

asymptotic analysis of the bootstrap methods 20030721

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## Asymptotic Analysis of the Bootstrap Methods

This documentation consists of three parts, namely "Exponential Family of Distributions", "Tube-Coordinates and  $z_c$ -formula", and "Bootstrap Methods". Each part is an independent *Mathematica* session, and should be run separately.

The calculation is third-order accurate, correct up to  $O(n^{-1})$  terms ignoring the error of  $O(n^{-3/2})$ . We use "o" to indicate  $O(n^{-1/2})$  quantities. So,  $o^2$  indicates  $O(n^{-1})$  and  $o^3$  indicates  $O(n^{-3/2})$ , etc. We repeatedly use a simplification function to keep only up to  $o^2$  terms.

In the first two parts, the tensor notation is heavily used. The add-on package "MathTensor" is required to run the *Mathematica* session by yourself.

### *Exponential Family of Distributions*

In this part, we will provide a canonical form the density function of the exponential family of distributions. First, some basic results for normal density is obtained. Then, the distribution function of the exponential family of distributions specified in the natural parameter will be transformed to an expression using the expectation parameter and the derivatives of the potential function.

#### ■ Startup

This section initializes the *Mathematica* session.

#### ■ packages

```
<< Statistics`ContinuousDistributions`
```

```
<< MathTens.m (Windows)
```

```
Loading MathTensor for DOS/Windows . . .
```

```
=====
MathTensor (TM) 2.2.1 (Windows) (September 17, 2000)
by Leonard Parker and Steven M. Christensen
Copyright (c) 1991-2000 MathTensor, Inc.
Runs with Mathematica (R) Versions 2.2, 3.0, 4.0
=====
No unit system is chosen. If you want one,
you must edit the file called Conventions.m,
or enter a command to interactively set units.
Units: {}
Sign conventions: Rmsign = 1 Rcsign = 1
MetricgSign = 1 DetgSign = -1
TensorForm turned on,
ShowTime turned off,
MetricgFlag = True.
=====
Null Windows
```

### ■ error messages

```
Off[General::spell1]
```

```
Off[General::spell]
```

### ■ distribution functions

```
gammadist[x_, m_, α_] := PDF[GammaDistribution[m, α], x]
Gammadist[x_, m_, α_] := CDF[GammaDistribution[m, α], x]
f[x_] := PDF[NormalDistribution[0, 1], x]
F[x_] := CDF[NormalDistribution[0, 1], x]
Q[x_] := Quantile[NormalDistribution[0, 1], x]
Chidist[x_, {di_, nc_}] := CDF[NoncentralChiSquareDistribution[di, nc], x]
```

### ■ Normal distribution

This section first calculates the moments of the normal variables, which will be used to calculate the expected value of the exponential of normal variables.

## ■ the moments of the multivariate normal distribution

We consider the multivariate normal random vector  $x = (x_1, \dots, x_{\text{dim}})$  of dim-dimensions with mean  $b = (b_1, \dots, b_{\text{dim}})$ , and the identity covariance matrix. The density function is  $f(x) = f[x_1 - b_1] f[x_2 - b_2] \dots f[x_{\text{dim}} - b_{\text{dim}}]$ . In this subsection, we define "ruleintx" to calculate the central moments of  $x$ , such as  $E(x_a x_b)$ ,  $E(x_a x_b x_c x_d)$ , and  $E(x_a x_b x_c x_d x_e x_f)$  for  $b = 0$ .

## ■ the central moments of the standard normal variable in one dimension

The following `intx2f[n]` =  $E(x^{2n}) = \int_{-\infty}^{\infty} x^{2n} f[x] dx$  gives  $\frac{(2n)!}{2^n n!}$ .

```
intx2f[n_] = FullSimplify[ $\int_{-\infty}^{\infty} x^{2n} f[x] dx$ ,  $n \geq 0 \wedge n \in \text{Integers}$ ]
```

$$\frac{2^n \text{Gamma}[\frac{1}{2} + n]}{\sqrt{\pi}}$$

```
Table[intx2f[n], {n, 10}]
```

```
{1, 3, 15, 105, 945, 10395, 135135, 2027025, 34459425, 654729075}
```

## ■ define tensors

This  $x_a$  or  $x^a$  denotes a component of the random vector  $x$ .

```
DefineTensor[tx, "x", {{1}, 1}]
```

```
PermWeight::def : Object x defined
```

```
PermWeight::def: Object x defined
```

This  $b_a$  or  $b^a$  denotes a component of the mean vector  $b$ .

```
DefineTensor[sb, "b", {{1}, 1}]
```

```
PermWeight::def : Object b defined
```

The following  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$ ,  $a_4$ ,  $a_5$ , and  $a_6$  are used for coefficients in a series expansion with respect to  $x$ .

```
DefineTensor[ta0, "a0", {{}, 1}]
```

```
PermWeight::def : Object a0 defined
```

```
PermWeight::def: Object a0 defined
```

```
DefineTensor[ta1, "a1", {{1}, 1}]
```

```
PermWeight::def : Object a1 defined
```

```
PermWeight::def: Object a1 defined
```

```

DefineTensor[ta2, "a2", {{2, 1}, 1}]
PermWeight::sym : Symmetries of a2 assigned
PermWeight::def : Object a2 defined
PermWeight::sym: Symmetries of a2 assigned
PermWeight::def: Object a2 defined

DefineTensor[ta3, "a3", {{1, 2, 3}, 1}]
PermWeight::def : Object a3 defined
PermWeight::def: Object a3 defined

SetSymmetric[ta3[la, lb, lc]]
PermWeight::sym : Symmetries of a3 assigned
PermWeight::sym: Symmetries of a3 assigned

DefineTensor[ta4, "a4", {{1, 2, 3, 4}, 1}]
PermWeight::def : Object a4 defined
PermWeight::def: Object a4 defined

SetSymmetric[ta4[la, lb, lc, ld]]
PermWeight::sym : Symmetries of a4 assigned
PermWeight::sym: Symmetries of a4 assigned

DefineTensor[ta6, "a6", {{1, 2, 3, 4, 5, 6}, 1}]
PermWeight::def : Object a6 defined

SetSymmetric[ta6[la, lb, lc, ld, le, lf]]
PermWeight::sym : Symmetries of a6 assigned

```

### ■ the central moments for the multivariate case

Here we assume  $b = 0$ , and define the second central moment  $\alpha_{ab} = E(x_a x_b)$ , the fourth central moment  $\alpha_{abcd} = E(x_a x_b x_c x_d)$ , etc. The central moments of odd degrees are zero. Considering the symmetry of the normal distribution, these central moments of even degrees are expressed by the following partition indicators.

```

kd2[la_, lb_] = Kdelta[la, lb];
kd4[la_, lb_, lc_, ld_] = 3 Symmetrize[Kdelta[la, lb] Kdelta[lc, ld], {la, lb, lc, ld}];
kd6[la_, lb_, lc_, ld_, le_, lf_] =
  15 Symmetrize[Kdelta[la, lb] Kdelta[lc, ld] Kdelta[le, lf], {la, lb, lc, ld, le, lf}];

```

Then,  $\alpha_{ab} = \text{kd2}[a, b]$ ,  $\alpha_{abcd} = \text{kd4}[a, b, c, d]$ ,  $\alpha_{abcdef} = \text{kd6}[a, b, c, d, e, f]$ , etc.

```

RuleUnique[ruleintx1, tx[ui_], 0]
RuleUnique[ruleintx2, tx[ui_] tx[uj_], kd2[ui, uj]]
RuleUnique[ruleintx3, tx[ui_] tx[uj_] tx[uk_], 0]

```

```

RuleUnique[ruleintx4, tx[ui_] tx[uj_] tx[uk_] tx[ul_], kd4[ui, uj, uk, ul]]
RuleUnique[ruleintx5, tx[ui_] tx[uj_] tx[uk_] tx[ul_] tx[um_], 0]
RuleUnique[ruleintx6,
  tx[ui_] tx[uj_] tx[uk_] tx[ul_] tx[um_] tx[un_], kd6[ui, uj, uk, ul, um, un]]
ruleintx = {ruleintx6, ruleintx5, ruleintx4, ruleintx3, ruleintx2, ruleintx1};

```

Check if this rule works for one-dimension case;  $\alpha_{11}$ ,  $\alpha_{1111}$ ,  $\alpha_{111111}$  are given by

```

{kd2[1, 1], kd4[1, 1, 1, 1], kd6[1, 1, 1, 1, 1, 1]}
{1, 3, 15}

```

They should be equal to  $E(x^2)$ ,  $E(x^4)$ ,  $E(x^6)$ .

```

{intx2f[1], intx2f[2], intx2f[3]}
{1, 3, 15}

```

$$\alpha_{1122} = E(x_1^2) E(x_2^2) = E(x^2)^2$$

```

{kd4[1, 1, 2, 2], intx2f[1]^2}
{1, 1}

```

$$\alpha_{112233} = E(x_1^2) E(x_2^2) E(x_3^2) = E(x^2)^3$$

```

{kd6[1, 1, 2, 2, 3, 3], intx2f[1]^3}
{1, 1}

```

$$\alpha_{112222} = E(x_1^2) E(x_2^4) = E(x^2) E(x^4)$$

```

{kd6[1, 1, 2, 2, 2, 2], intx2f[1] intx2f[2]}
{3, 3}

```

In the below, we rather use superscript to indicate the components of  $x$ . For example, we use  $x = (x^a)$ , instead of  $x=(x_a)$ .  $a_{2ij} x^i x^j$  denotes a quadratic form with symmetric matrix  $a_{2ij}$ .

```

ta2[1i, 1j] tx[ui] tx[uj]
(a2ij) (xi) (xj)

```

The expectation  $E(a_{2ij} x^i x^j)$  is

```

ApplyRules[%, ruleintx]
(Kdeltapq) (a2pq)
AbsorbKdelta[%]
a2qq
Tsimpify[%]
a2qq

```

Similarly, for the symmetric 4-form  $a_{ijkl} x^i x^j x^k x^l$

```

ta4[1i, 1j, 1k, 1l] tx[ui] tx[uj] tx[uk] tx[ul]
(a4ijkl) (xi) (xj) (xk) (xl)

ApplyRules[% , ruleintx]
3 (Kdeltapq) (Kdeltars) (a4pqrs)

AbsorbKdelta[%]
3 (a4qsqs)

```

Similarly, for the symmetric 6-form  $a_{ijklmn} x^i x^j x^k x^l x^m x^n$

```

ta6[1i, 1j, 1k, 1l, 1m, 1n] tx[ui] tx[uj] tx[uk] tx[ul] tx[um] tx[un]
(a6ijklmn) (xi) (xj) (xk) (xl) (xm) (xn)

ApplyRules[% , ruleintx]
15 (Kdeltapq) (Kdeltars) (Kdeltatu) (a6pqrstu)

AbsorbKdelta[%]
15 (a6qsuqsu)

```

### ■ the expectation of the exponential of polynomial functions

Here we would like to calculate the log of the expectation of the exponential of  $\text{poly}(x) = a_0 + a_1 x^i + a_2 x^i x^j + a_3 x^i x^j x^k + a_4 x^i x^j x^k x^l$ , where  $a_1, a_2$ , and  $a_3$  are of order  $O(n^{-1/2})$ , and  $a_4$  is  $O(n^{-1})$ . Note that  $x^i$  here indicates the  $i$ -th element of  $x = (x^1, \dots, x^{\text{dim}})$  instead of the  $i$ -th power of  $x$ .  $\text{logexpmpoly} = \log E \{ \exp(\text{poly}(x)) \}$  is first obtained for  $b = 0$ , and next for general  $b \neq 0$  up to  $O(n^{-1})$  terms.

### ■ central case (b=0)

First  $\text{poly}(x)-a_0$  is set in `foo1`. The constant term  $a_0$  can be removed from `poly` in the following argument, but only be added in `logexpmpoly` later.

```

foo1 =
o ta1[1i] tx[ui] + o ta2[1i, 1j] tx[ui] tx[uj] + o ta3[1i, 1j, 1k] tx[ui] tx[uj] tx[uk] +
o2 ta4[1i, 1j, 1k, 1l] tx[ui] tx[uj] tx[uk] tx[ul]
o (a1i) (xi) + o (a2ij) (xi) (xj) + o (a3ijk) (xi) (xj) (xk) + o2 (a4ijkl) (xi) (xj) (xk) (xl)

```

Make rule "rulepoly" to substitute "poly" for `foo1`.

```

RuleUnique[rulepoly, poly, foo1]

```

Considering

```
Series[Exp[x], {x, 0, 2}]
```

$$1 + x + \frac{x^2}{2} + O[x]^3$$

we can calculate  $\exp(\text{poly}(x))$  as follows, and stored in foo4 up to  $O(n^{-1})$  terms.

```
foo3 = ApplyRules[1 + poly + 1/2 poly^2, rulepoly];
```

```
foo4 = Sum[Tsimplify[Coefficient[foo3, o, i]] o^i, {i, 0, 2}]
```

$$1 + o \left( (a_{1p}) (x^p) + (a_{2pq}) (x^p) (x^q) + (a_{3pqr}) (x^p) (x^q) (x^r) \right) + o^2 \left( \frac{1}{2} (a_{1p}) (a_{1q}) (x^p) (x^q) + (a_{1p}) (a_{2qr}) (x^p) (x^q) (x^r) + \frac{1}{2} (a_{2pq}) (a_{2rs}) (x^p) (x^q) (x^r) (x^s) + (a_{1p}) (a_{3qrs}) (x^p) (x^q) (x^r) (x^s) + (a_{4pqrst}) (x^p) (x^q) (x^r) (x^s) + (a_{2pq}) (a_{3rst}) (x^p) (x^q) (x^r) (x^s) (x^t) + \frac{1}{2} (a_{3pqr}) (a_{3stu}) (x^p) (x^q) (x^r) (x^s) (x^t) (x^u) \right)$$

Then, we take the expectation of foo4, calculating  $E\{\exp(\text{poly}(x))\}$ , and stored in foo5 below.

```
ApplyRules[foo4, ruleintx]
```

$$1 + \frac{1}{2} o^2 (Kdelta^{pq}) (a_{1p}) (a_{1q}) + o (Kdelta^{pq}) (a_{2pq}) + o^2 (Kdelta^{pq}) (Kdelta^{rs}) (a_{2pr}) (a_{2qs}) + \frac{1}{2} o^2 (Kdelta^{pq}) (Kdelta^{rs}) (a_{2pq}) (a_{2rs}) + 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (a_{1p}) (a_{3qrs}) + 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (Kdelta^{tu}) (a_{3prt}) (a_{3qsu}) + \frac{3}{2} o^2 (Kdelta^{pq}) (Kdelta^{rs}) (Kdelta^{tu}) (a_{3prs}) (a_{3qtu}) + 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (Kdelta^{tu}) (a_{3pqr}) (a_{3stu}) + 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (a_{4pqrst})$$

```
AbsorbKdelta[%]
```

$$1 + \frac{1}{2} o^2 (a_{1q}) (a_{1q}) + o (a_{2q^q}) + \frac{1}{2} o^2 (a_{2q^q}) (a_{2s^s}) + o^2 (a_{2qs}) (a_{2qs}) + 3 o^2 (a_{1q}) (a_{3qs^s}) + 3 o^2 (a_{3q^qs}) (a_{3su^u}) + \frac{3}{2} o^2 (a_{3qu^u}) (a_{3s^qs}) + 3 o^2 (a_{3qsu}) (a_{3qs^su}) + 3 o^2 (a_{4qs^qs})$$

```
foo5 = Tsimplify[%]
```

$$1 + \frac{1}{2} o^2 (a_{1q}) (a_{1q}) + o (a_{2q^q}) + \frac{1}{2} o^2 (a_{2q^q}) (a_{2s^s}) + o^2 (a_{2qs}) (a_{2qs}) + 3 o^2 (a_{1q}) (a_{3qs^s}) + 3 o^2 (a_{3q^qs}) (a_{3su^u}) + \frac{3}{2} o^2 (a_{3qu^u}) (a_{3s^qs}) + 3 o^2 (a_{3qsu}) (a_{3qs^su}) + 3 o^2 (a_{4qs^qs})$$

Considering

```
Series[Log[1 + x], {x, 0, 2}]
```

$$x - \frac{x^2}{2} + O[x]^3$$

we take the log of foo5, and stored in foo8 up to  $O(n^{-1})$  terms below.

```
RuleUnique[foo6rule, foo6, foo5 - 1]
```

```
foo7 = ApplyRules[foo6 - foo6^2 / 2, foo6rule];
```

`foo8 = Sum[CanAll[Tsimplify[Coefficient[foo7, o, i]]] oi, {i, 0, 2}]`

$$o(a_{2p}^p) + o^2 \left( \frac{1}{2} (a_{1p}) (a_{1p}) + (a_{2pq}) (a_{2pq}) + 3 (a_{1p}) (a_{3q}^{pq}) + \frac{9}{2} (a_{3pq}^p) (a_{3r}^{qr}) + 3 (a_{3pqr}) (a_{3pq}^{qr}) + 3 (a_{4pq}^{pq}) \right)$$

This is logexppoly for b=0.

`logexppolyb0 = ta0 + foo8`

$$a_0 + o(a_{2p}^p) + o^2 \left( \frac{1}{2} (a_{1p}) (a_{1p}) + (a_{2pq}) (a_{2pq}) + 3 (a_{1p}) (a_{3q}^{pq}) + \frac{9}{2} (a_{3pq}^p) (a_{3r}^{qr}) + 3 (a_{3pqr}) (a_{3pq}^{qr}) + 3 (a_{4pq}^{pq}) \right)$$

The following expression may be easier to read for us, but violating the summation convention rule of subscripts.

`logexppolyb0 /. {u1 -> l1, u2 -> l2, u3 -> l3}`

$$a_0 + o(a_{2pp}) + o^2 \left( \frac{1}{2} (a_{1p})^2 + (a_{2pq})^2 + 3 (a_{1p}) (a_{3pq}) + 3 (a_{3pqr})^2 + \frac{9}{2} (a_{3ppq}) (a_{3qrr}) + 3 (a_{4ppqq}) \right)$$

### ■ noncentral case (b≠0)

We assume the mean of  $x$  is zero, but replacing  $x_i$  with  $x^i + b^i$  to calculate the case for  $b \neq 0$ . foo11 is the same as poly(x)-a0, but with this substitution.

`foo11 = foo1 /. {tx[ui_] -> tx[ui] + sb[ui]}`

$$o(a_{1i}) (b^i + x^i) + o(a_{2ij}) (b^i + x^i) (b^j + x^j) + o(a_{3ijk}) (b^i + x^i) (b^j + x^j) (b^k + x^k) + o^2(a_{4ijkl}) (b^i + x^i) (b^j + x^j) (b^k + x^k) (b^l + x^l)$$

Obtain the canonical expression of the tensor usage, and redefine "rulepoly".

`foo12 = CanAll[Expand[foo11]]`

$$o(b_p) (a_{1p}) + o(b_p) (b_q) (a_{2pq}) + o(b_p) (b_q) (b_r) (a_{3pqr}) + o^2(b_p) (b_q) (b_r) (b_s) (a_{4pqrs}) + o(a_{1p}) (x^p) + 2 o(b_p) (a_{2q}^p) (x^q) + o(a_{2pq}) (x^p) (x^q) + 3 o(b_p) (b_q) (a_{3r}^{pq}) (x^r) + 3 o(b_p) (a_{3qr}^p) (x^q) (x^r) + o(a_{3pqr}) (x^p) (x^q) (x^r) + 4 o^2(b_p) (b_q) (b_r) (a_{4s}^{pqr}) (x^s) + 6 o^2(b_p) (b_q) (a_{4rs}^{pq}) (x^r) (x^s) + 4 o^2(b_p) (a_{4qrs}^p) (x^q) (x^r) (x^s) + o^2(a_{4pqrs}) (x^p) (x^q) (x^r) (x^s)$$

`RuleUnique[rulepoly, poly, foo12]`

we can calculate exp(poly(x)) as follows, and stored in foo14 up to  $O(n^{-1})$  terms.

$$foo13 = ApplyRules[1 + poly + \frac{1}{2} poly^2, rulepoly];$$



**foo14 = Sum[Tsimplify[Coefficient[foo13, o, i]] o<sup>i</sup>, {i, 0, 2}]**

$$\begin{aligned}
 & 1 + o \left( (b_p) (a1^p) + (b_p) (b_q) (a2^{pq}) + \right. \\
 & \quad (b_p) (b_q) (b_r) (a3^{pqr}) + (a1_p) (x^p) + 2 (b_p) (a2_{q^p}) (x^q) + (a2_{pq}) (x^p) (x^q) + \\
 & \quad \left. 3 (b_p) (b_q) (a3_{r^{pq}}) (x^r) + 3 (b_p) (a3_{qr^p}) (x^q) (x^r) + (a3_{pqr}) (x^p) (x^q) (x^r) \right) + \\
 & o^2 \left( \frac{1}{2} (b_p) (b_q) (a1^p) (a1^q) + (b_p) (b_q) (b_r) (a1^r) (a2^{pq}) + \right. \\
 & \quad \frac{1}{2} (b_p) (b_q) (b_r) (b_s) (a2^{pq}) (a2^{rs}) + (b_p) (b_q) (b_r) (b_s) (a1^s) (a3^{pqr}) + \\
 & \quad (b_p) (b_q) (b_r) (b_s) (b_t) (a2^{st}) (a3^{pqr}) + \frac{1}{2} (b_p) (b_q) (b_r) (b_s) (b_t) (b_u) (a3^{pqr}) (a3^{stu}) + \\
 & \quad (b_p) (b_q) (b_r) (b_s) (a4^{pqr^s}) + (b_p) (a1_q) (a1^p) (x^q) + \frac{1}{2} (a1_p) (a1_q) (x^p) (x^q) + \\
 & \quad 2 (b_p) (b_q) (a1^q) (a2_{r^p}) (x^r) + (b_p) (b_q) (a1_r) (a2^{pq}) (x^r) + \\
 & \quad (b_p) (a1^p) (a2_{qr}) (x^q) (x^r) + 2 (b_p) (a1_q) (a2_{r^p}) (x^q) (x^r) + (a1_p) (a2_{qr}) (x^p) (x^q) (x^r) + \\
 & \quad 2 (b_p) (b_q) (b_r) (a2_{s^r}) (a2^{pq}) (x^s) + 3 (b_p) (b_q) (b_r) (a1^r) (a3_{s^{pq}}) (x^s) + \\
 & \quad (b_p) (b_q) (b_r) (a1_s) (a3^{pqr}) (x^s) + 4 (b_p) (b_q) (b_r) (a4_{s^{pqr}}) (x^s) + \\
 & \quad 2 (b_p) (b_q) (a2_{r^p}) (a2_{s^q}) (x^r) (x^s) + (b_p) (b_q) (a2_{rs}) (a2^{pq}) (x^r) (x^s) + \\
 & \quad 3 (b_p) (b_q) (a1^q) (a3_{rs^p}) (x^r) (x^s) + 3 (b_p) (b_q) (a1_r) (a3_{s^{pq}}) (x^r) (x^s) + \\
 & \quad 6 (b_p) (b_q) (a4_{rs^{pq}}) (x^r) (x^s) + 2 (b_p) (a2_{q^p}) (a2_{rs}) (x^q) (x^r) (x^s) + \\
 & \quad (b_p) (a1^p) (a3_{qrs}) (x^q) (x^r) (x^s) + 3 (b_p) (a1_q) (a3_{rs^p}) (x^q) (x^r) (x^s) + \\
 & \quad 4 (b_p) (a4_{qrs^p}) (x^q) (x^r) (x^s) + \frac{1}{2} (a2_{pq}) (a2_{rs}) (x^p) (x^q) (x^r) (x^s) + \\
 & \quad (a1_p) (a3_{qrs}) (x^p) (x^q) (x^r) (x^s) + (a4_{pqr^s}) (x^p) (x^q) (x^r) (x^s) + \\
 & \quad 3 (b_p) (b_q) (b_r) (b_s) (a2^{rs}) (a3_{t^{pq}}) (x^t) + 2 (b_p) (b_q) (b_r) (b_s) (a2_{t^s}) (a3^{pqr}) (x^t) + \\
 & \quad 3 (b_p) (b_q) (b_r) (a2^{qr}) (a3_{st^p}) (x^s) (x^t) + 6 (b_p) (b_q) (b_r) (a2_{s^r}) (a3_{t^{pq}}) (x^s) (x^t) + \\
 & \quad (b_p) (b_q) (b_r) (a2_{st}) (a3^{pqr}) (x^s) (x^t) + (b_p) (b_q) (a2^{pq}) (a3_{rst}) (x^r) (x^s) (x^t) + \\
 & \quad 6 (b_p) (b_q) (a2_{r^q}) (a3_{st^p}) (x^r) (x^s) (x^t) + 3 (b_p) (b_q) (a2_{rs}) (a3_{t^{pq}}) (x^r) (x^s) (x^t) + \\
 & \quad 2 (b_p) (a2_{q^p}) (a3_{rst}) (x^q) (x^r) (x^s) (x^t) + 3 (b_p) (a2_{qr}) (a3_{st^p}) (x^q) (x^r) (x^s) (x^t) + \\
 & \quad (a2_{pq}) (a3_{rst}) (x^p) (x^q) (x^r) (x^s) (x^t) + 3 (b_p) (b_q) (b_r) (b_s) (b_t) (a3_{u^{st}}) (a3^{pqr}) (x^u) + \\
 & \quad \frac{9}{2} (b_p) (b_q) (b_r) (b_s) (a3_{t^{pq}}) (a3_{u^{rs}}) (x^t) (x^u) + \\
 & \quad 3 (b_p) (b_q) (b_r) (b_s) (a3_{tu^s}) (a3^{pqr}) (x^t) (x^u) + \\
 & \quad 9 (b_p) (b_q) (b_r) (a3_{s^{pq}}) (a3_{tu^r}) (x^s) (x^t) (x^u) + (b_p) (b_q) (b_r) (a3_{st^u}) \\
 & \quad (a3^{pqr}) (x^s) (x^t) (x^u) + 3 (b_p) (b_q) (a3_{r^{pq}}) (a3_{st^u}) (x^r) (x^s) (x^t) (x^u) + \\
 & \quad \frac{9}{2} (b_p) (b_q) (a3_{rs^p}) (a3_{tu^q}) (x^r) (x^s) (x^t) (x^u) + 3 (b_p) (a3_{qr^p}) (a3_{st^u}) (x^q) \\
 & \quad \left. (x^r) (x^s) (x^t) (x^u) + \frac{1}{2} (a3_{pqr}) (a3_{st^u}) (x^p) (x^q) (x^r) (x^s) (x^t) (x^u) \right)
 \end{aligned}$$

Then, we take the expectation of foo14, calculating  $E \{ \exp(\text{poly}(x)) \}$ , and stored in foo15 below.

**ApplyRules[fool4, ruleintx]**

$$\begin{aligned}
 & 1 + \frac{1}{2} o^2 (Kdelta^{pq}) (a1_p) (a1_q) + o (b_p) (a1^p) + \\
 & \frac{1}{2} o^2 (b_p) (b_q) (a1^p) (a1^q) + o (Kdelta^{pq}) (a2_{pq}) + o^2 (Kdelta^{pq}) (b_r) (a1^r) (a2_{pq}) + \\
 & o^2 (Kdelta^{pq}) (Kdelta^{rs}) (a2_{pr}) (a2_{qs}) + 2 o^2 (Kdelta^{pq}) (b_r) (a1_p) (a2_q^r) + \\
 & 2 o^2 (Kdelta^{pq}) (b_r) (b_s) (a2_p^r) (a2_q^s) + \frac{1}{2} o^2 (Kdelta^{pq}) (Kdelta^{rs}) (a2_{pq}) (a2_{rs}) + \\
 & o (b_p) (b_q) (a2^{pq}) + o^2 (b_p) (b_q) (b_r) (a1^r) (a2^{pq}) + o^2 (Kdelta^{pq}) (b_r) (b_s) (a2_{pq}) (a2^{rs}) + \\
 & \frac{1}{2} o^2 (b_p) (b_q) (b_r) (b_s) (a2^{pq}) (a2^{rs}) + 3 o (Kdelta^{pq}) (b_r) (a3_{pq}^r) + \\
 & 3 o^2 (Kdelta^{pq}) (b_r) (b_s) (a1^s) (a3_{pq}^r) + 3 o^2 (Kdelta^{pq}) (b_r) (b_s) (b_t) (a2^{st}) (a3_{pq}^r) + \\
 & 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (a1_p) (a3_{qrs}) + 6 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (b_t) (a2_p^t) (a3_{qrs}) + \\
 & 9 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (b_t) (b_u) (a3_p^{tu}) (a3_{qrs}) + \\
 & 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (Kdelta^{tu}) (a3_{prt}) (a3_{qsu}) + \\
 & 6 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (b_t) (a2_{pr}) (a3_{qs}^t) + \\
 & 9 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (b_t) (b_u) (a3_{pr}^t) (a3_{qs}^u) + \\
 & \frac{3}{2} o^2 (Kdelta^{pq}) (Kdelta^{rs}) (Kdelta^{tu}) (a3_{prs}) (a3_{qtu}) + \\
 & 3 o^2 (Kdelta^{pq}) (b_r) (b_s) (a1_p) (a3_q^{rs}) + 6 o^2 (Kdelta^{pq}) (b_r) (b_s) (b_t) (a2_p^t) (a3_q^{rs}) + \\
 & \frac{9}{2} o^2 (Kdelta^{pq}) (b_r) (b_s) (b_t) (b_u) (a3_p^{rs}) (a3_q^{tu}) + \\
 & 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (b_t) (a2_{pq}) (a3_{rs}^t) + \\
 & \frac{9}{2} o^2 (Kdelta^{pq}) (Kdelta^{rs}) (b_t) (b_u) (a3_{pq}^t) (a3_{rs}^u) + \\
 & 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (Kdelta^{tu}) (a3_{pqr}) (a3_{stu}) + \\
 & o (b_p) (b_q) (b_r) (a3^{pqr}) + o^2 (b_p) (b_q) (b_r) (b_s) (a1^s) (a3^{pqr}) + \\
 & o^2 (b_p) (b_q) (b_r) (b_s) (b_t) (a2^{st}) (a3^{pqr}) + o^2 (Kdelta^{pq}) (b_r) (b_s) (b_t) (a2_{pq}) (a3^{rst}) + \\
 & 3 o^2 (Kdelta^{pq}) (b_r) (b_s) (b_t) (b_u) (a3_{pq}^u) (a3^{rst}) + \\
 & \frac{1}{2} o^2 (b_p) (b_q) (b_r) (b_s) (b_t) (b_u) (a3^{pqr}) (a3^{stu}) + 3 o^2 (Kdelta^{pq}) (Kdelta^{rs}) (a4_{pqrs}) + \\
 & 6 o^2 (Kdelta^{pq}) (b_r) (b_s) (a4_{pq}^{rs}) + o^2 (b_p) (b_q) (b_r) (b_s) (a4^{pqrs})
 \end{aligned}$$

**AbsorbKdelta[%]**

$$\begin{aligned}
 & 1 + o (b_p) (a1^p) + \frac{1}{2} o^2 (a1_q) (a1^q) + \frac{1}{2} o^2 (b_p) (b_q) (a1^p) (a1^q) + \\
 & o (a2_q^q) + o^2 (b_r) (a1^r) (a2_q^q) + 2 o^2 (b_r) (a1^q) (a2_q^r) + \frac{1}{2} o^2 (a2_q^q) (a2_s^s) + \\
 & o (b_p) (b_q) (a2^{pq}) + o^2 (b_p) (b_q) (b_r) (a1^r) (a2^{pq}) + 2 o^2 (b_r) (b_s) (a2_q^s) (a2^{qr}) + \\
 & o^2 (a2_{qs}) (a2^{qs}) + o^2 (b_r) (b_s) (a2_q^q) (a2^{rs}) + \frac{1}{2} o^2 (b_p) (b_q) (b_r) (b_s) (a2^{pq}) (a2^{rs}) + \\
 & 3 o^2 (a1^q) (a3_{qs}^s) + 6 o^2 (b_t) (a2^{qt}) (a3_{qs}^s) + 6 o^2 (b_t) (a2^{qs}) (a3_{qs}^t) + 3 o (b_r) (a3_q^{qr}) + \\
 & 3 o^2 (b_r) (b_s) (a1^s) (a3_q^{qr}) + 3 o^2 (b_r) (b_s) (b_t) (a2^{st}) (a3_q^{qr}) + 3 o^2 (b_r) (b_s) (a1^q) (a3_q^{rs}) + \\
 & 6 o^2 (b_r) (b_s) (b_t) (a2^{qt}) (a3_q^{rs}) + 3 o^2 (a3_q^{qs}) (a3_{su}^u) + \frac{3}{2} o^2 (a3_{qu}^u) (a3_s^{qs}) + \\
 & 3 o^2 (b_t) (a2_q^q) (a3_s^{st}) + \frac{9}{2} o^2 (b_t) (b_u) (a3_q^{qt}) (a3_s^{su}) + o (b_p) (b_q) (b_r) (a3^{pqr}) + \\
 & o^2 (b_p) (b_q) (b_r) (b_s) (a1^s) (a3^{pqr}) + o^2 (b_p) (b_q) (b_r) (b_s) (b_t) (a2^{st}) (a3^{pqr}) + \\
 & \frac{9}{2} o^2 (b_r) (b_s) (b_t) (b_u) (a3_q^{tu}) (a3^{qrs}) + 9 o^2 (b_t) (b_u) (a3_{qs}^u) (a3^{qst}) + \\
 & 3 o^2 (a3_{qsu}) (a3^{qsu}) + 9 o^2 (b_t) (b_u) (a3_{qs}^s) (a3^{qtu}) + o^2 (b_r) (b_s) (b_t) (a2_q^q) (a3^{rst}) + \\
 & 3 o^2 (b_r) (b_s) (b_t) (b_u) (a3_q^{qu}) (a3^{rst}) + \frac{1}{2} o^2 (b_p) (b_q) (b_r) (b_s) (b_t) (b_u) (a3^{pqr}) (a3^{stu}) + \\
 & 3 o^2 (a4_{qs}^{qs}) + 6 o^2 (b_r) (b_s) (a4_q^{qrs}) + o^2 (b_p) (b_q) (b_r) (b_s) (a4^{pqrs})
 \end{aligned}$$

**foo15 = Tsimplify[%]**

$$\begin{aligned}
 & 1 + o(b_p)(a_1^p) + \frac{1}{2} o^2(a_1^q)(a_1^q) + \frac{1}{2} o^2(b_p)(b_q)(a_1^p)(a_1^q) + \\
 & o(a_2^q) + o^2(b_r)(a_1^r)(a_2^q) + 2 o^2(b_r)(a_1^q)(a_2^r) + \frac{1}{2} o^2(a_2^q)(a_2^s) + \\
 & o(b_p)(b_q)(a_2^{pq}) + o^2(b_p)(b_q)(b_r)(a_1^r)(a_2^{pq}) + 2 o^2(b_r)(b_s)(a_2^q)(a_2^{qr}) + \\
 & o^2(a_2^{qs})(a_2^{qs}) + o^2(b_r)(b_s)(a_2^q)(a_2^{rs}) + \frac{1}{2} o^2(b_p)(b_q)(b_r)(b_s)(a_2^{pq})(a_2^{rs}) + \\
 & 3 o^2(a_1^q)(a_3^{qs}) + 6 o^2(b_t)(a_2^{qt})(a_3^{qs}) + 6 o^2(b_t)(a_2^{qs})(a_3^{qt}) + 3 o(b_r)(a_3^{qr}) + \\
 & 3 o^2(b_r)(b_s)(a_1^s)(a_3^{qr}) + 3 o^2(b_r)(b_s)(b_t)(a_2^{st})(a_3^{qr}) + 3 o^2(b_r)(b_s)(a_1^q)(a_3^{rs}) + \\
 & 6 o^2(b_r)(b_s)(b_t)(a_2^{qt})(a_3^{rs}) + 3 o^2(a_3^{qs})(a_3^{su}) + \frac{3}{2} o^2(a_3^{qu})(a_3^{qs}) + \\
 & 3 o^2(b_t)(a_2^q)(a_3^{st}) + \frac{9}{2} o^2(b_t)(b_u)(a_3^{qt})(a_3^{su}) + o(b_p)(b_q)(b_r)(a_3^{pqr}) + \\
 & o^2(b_p)(b_q)(b_r)(b_s)(a_1^s)(a_3^{pqr}) + o^2(b_p)(b_q)(b_r)(b_s)(b_t)(a_2^{st})(a_3^{pqr}) + \\
 & \frac{9}{2} o^2(b_r)(b_s)(b_t)(b_u)(a_3^{tu})(a_3^{rs}) + 9 o^2(b_t)(b_u)(a_3^{su})(a_3^{st}) + \\
 & 3 o^2(a_3^{su})(a_3^{su}) + 9 o^2(b_t)(b_u)(a_3^{su})(a_3^{tu}) + o^2(b_r)(b_s)(b_t)(a_2^q)(a_3^{rst}) + \\
 & 3 o^2(b_r)(b_s)(b_t)(b_u)(a_3^{qu})(a_3^{rst}) + \frac{1}{2} o^2(b_p)(b_q)(b_r)(b_s)(b_t)(b_u)(a_3^{pqr})(a_3^{stu}) + \\
 & 3 o^2(a_4^{qs}) + 6 o^2(b_r)(b_s)(a_4^{rs}) + o^2(b_p)(b_q)(b_r)(b_s)(a_4^{pqr})
 \end{aligned}$$

we take the log of foo15, and stored in foo18 up to  $O(n^{-1})$  terms below.

**RuleUnique[foo16rule, foo16, foo15 - 1]**

**foo17 = ApplyRules[foo16 - foo16<sup>2</sup> / 2, foo16rule];**

**foo18 = Sum[CanAll[Tsimplify[Coefficient[foo17, o, i]]] o<sup>i</sup>, {i, 0, 2}]**

$$\begin{aligned}
 & o((b_p)(a_1^p) + a_2^p + (b_p)(b_q)(a_2^{pq}) + 3(b_p)(a_3^{pq}) + (b_p)(b_q)(b_r)(a_3^{pqr})) + \\
 & o^2\left(\frac{1}{2}(a_1^p)(a_1^p) + 2(b_p)(a_1^q)(a_2^{pq}) + (a_2^{pq})(a_2^{pq}) + \right. \\
 & \quad 2(b_p)(b_q)(a_2^r)(a_2^{qr}) + 3(a_1^p)(a_3^{pq}) + 6(b_p)(a_2^p)(a_3^{qr}) + \\
 & \quad \frac{9}{2}(a_3^{pq})(a_3^{qr}) + 3(b_p)(b_q)(a_1^r)(a_3^{pqr}) + 6(b_p)(a_2^{qr})(a_3^{pqr}) + \\
 & \quad 3(a_3^{pqr})(a_3^{pqr}) + 9(b_p)(b_q)(a_3^{rs})(a_3^{pq}) + 6(b_p)(b_q)(b_r)(a_2^p)(a_3^{rs}) + \\
 & \quad 9(b_p)(b_q)(a_3^{rs})(a_3^{rs}) + \frac{9}{2}(b_p)(b_q)(b_r)(b_s)(a_3^{tr})(a_3^{st}) + \\
 & \quad \left. 3(a_4^{pq}) + 6(b_p)(b_q)(a_4^{qr}) + (b_p)(b_q)(b_r)(b_s)(a_4^{pqr})\right)
 \end{aligned}$$

This is logexpoly for  $b \neq 0$ .

**logexpoly = ta0 + foo18**

$$\begin{aligned}
 & a_0 + o((b_p)(a_1^p) + a_2^p + (b_p)(b_q)(a_2^{pq}) + 3(b_p)(a_3^{pq}) + (b_p)(b_q)(b_r)(a_3^{pqr})) + \\
 & o^2\left(\frac{1}{2}(a_1^p)(a_1^p) + 2(b_p)(a_1^q)(a_2^{pq}) + (a_2^{pq})(a_2^{pq}) + \right. \\
 & \quad 2(b_p)(b_q)(a_2^r)(a_2^{qr}) + 3(a_1^p)(a_3^{pq}) + 6(b_p)(a_2^p)(a_3^{qr}) + \\
 & \quad \frac{9}{2}(a_3^{pq})(a_3^{qr}) + 3(b_p)(b_q)(a_1^r)(a_3^{pqr}) + 6(b_p)(a_2^{qr})(a_3^{pqr}) + \\
 & \quad 3(a_3^{pqr})(a_3^{pqr}) + 9(b_p)(b_q)(a_3^{rs})(a_3^{pq}) + 6(b_p)(b_q)(b_r)(a_2^p)(a_3^{rs}) + \\
 & \quad 9(b_p)(b_q)(a_3^{rs})(a_3^{rs}) + \frac{9}{2}(b_p)(b_q)(b_r)(b_s)(a_3^{tr})(a_3^{st}) + \\
 & \quad \left. 3(a_4^{pq}) + 6(b_p)(b_q)(a_4^{qr}) + (b_p)(b_q)(b_r)(b_s)(a_4^{pqr})\right)
 \end{aligned}$$

**InputForm[logeexpoly]**

```

ta0 + o*(sb[l1]*ta1[u1] + ta2[l1, u1] +
  sb[l1]*sb[l2]*ta2[u1, u2] + 3*sb[l1]*ta3[l2, u1, u2] +
  sb[l1]*sb[l2]*sb[l3]*ta3[u1, u2, u3]) +
o^2*((ta1[l1]*ta1[u1])/2 + 2*sb[l1]*ta1[l2]*ta2[u1, u2] +
  ta2[l1, l2]*ta2[u1, u2] + 2*sb[l1]*sb[l2]*ta2[l3, u1]*
  ta2[u2, u3] + 3*ta1[l1]*ta3[l2, u1, u2] +
  6*sb[l1]*ta2[l2, u1]*ta3[l3, u2, u3] +
  (9*ta3[l1, l2, u1]*ta3[l3, u2, u3])/2 +
  3*sb[l1]*sb[l2]*ta1[l3]*ta3[u1, u2, u3] +
  6*sb[l1]*ta2[l2, l3]*ta3[u1, u2, u3] +
  3*ta3[l1, l2, l3]*ta3[u1, u2, u3] +
  9*sb[l1]*sb[l2]*ta3[l3, l4, u3]*ta3[u1, u2, u4] +
  6*sb[l1]*sb[l2]*sb[l3]*ta2[l4, u1]*ta3[u2, u3, u4] +
  9*sb[l1]*sb[l2]*ta3[l3, l4, u1]*ta3[u2, u3, u4] +
  (9*sb[l1]*sb[l2]*sb[l3]*sb[l4]*ta3[l5, u1, u3]*
  ta3[u2, u4, u5])/2 + 3*ta4[l1, l2, u1, u2] +
  6*sb[l1]*sb[l2]*ta4[l3, u1, u2, u3] +
  sb[l1]*sb[l2]*sb[l3]*sb[l4]*ta4[u1, u2, u3, u4])

```

The following expression may be easier to read for us, but violating the summation convention rule of subscripts.

**Collect[logeexpoly,**

**{o, sb[l1] sb[l2] sb[l3] sb[l4], sb[l1] sb[l2] sb[l3], sb[l1] sb[l2], sb[l1]}**]

```

a0 + o (a2pp + (bp) (bq) (a2pq) + (bp) (a1p + 3 (a3qpq)) + (bp) (bq) (br) (a3pqr)) +
o2 (  $\frac{1}{2}$  (a1p) (a1p) + (a2pq) (a2pq) + 3 (a1p) (a3qpq) +  $\frac{9}{2}$  (a3pqp) (a3rqr) +
  3 (a3pqr) (a3pqr) + (bp) (2 (a1q) (a2pq) + 6 (a2qp) (a3rqr) + 6 (a2qr) (a3pqr)) +
  6 (bp) (bq) (br) (a2sp) (a3qrs) + 3 (a4pqpq) + (bp) (bq)
  (2 (a2rp) (a2qr) + 3 (a1r) (a3pqr) + 9 (a3rsr) (a3pqs) + 9 (a3rsp) (a3qrs) + 6 (a4rpqr)) +
  (bp) (bq) (br) (bs) (  $\frac{9}{2}$  (a3tprt) (a3qst) + a4pqrst ) )

```

**% /. {u1 -> l1, u2 -> l2, u3 -> l3, u4 -> l4, u5 -> l5}**

```

a0 + o (a2pp + (bp) (bq) (a2pq) + (bp) (a1p + 3 (a3pqq)) + (bp) (bq) (br) (a3pqr)) +
o2 (  $\frac{1}{2}$  (a1p)2 + (a2pq)2 + 3 (a1p) (a3pqq) + 3 (a3pqr)2 +
   $\frac{9}{2}$  (a3ppq) (a3qrr) + (bp) (2 (a1q) (a2pq) + 6 (a2qr) (a3pqr) + 6 (a2pq) (a3qrr)) +
  6 (bp) (bq) (br) (a2ps) (a3qrs) + 3 (a4ppqq) + (bp) (bq)
  (2 (a2pr) (a2qr) + 3 (a1r) (a3pqr) + 9 (a3prs) (a3qrs) + 9 (a3pqs) (a3rrs) + 6 (a4pqrr)) +
  (bp) (bq) (br) (bs) (  $\frac{9}{2}$  (a3prt) (a3qst) + a4pqrst ) )

```

## ■ Exponential family

The density function of the exponential family is first specified by using the natural parameter vector. This standard form is transformed into our canonical expression of the density with respect to the expectation parameter vector. Since the exponential family is not uniquely expressed up to the affine transformation, we assume without loss of generality that origin of the expectation parameter coincides with that of the natural parameter, and the covariance matrix of the random variable is identity at the origin. We consider only the continuous random variable throughout. The canonical form will be stored in "logdensity".

## ■ the standard form

Let  $f(y; \theta) = \exp(\theta^a y_a - h(y) - \psi(\theta))$  denote the density function of random variable  $y = (y_1, \dots, y_{\dim})$  with the natural parameter vector  $\theta = (\theta^1, \dots, \theta^{\dim})$ . The log of the density function is specified by `logdensity=log f(y;θ)` using the cumulant function  $\psi(\theta)$  and the measure function  $h(y)$ .

## ■ simplification functions

Some simplification functions are defined here for later use

```
tsimp[exp_] := CanAll[AbsorbKdelta[CanAll[exp]]]
geto2[exp_] := Sum[Simplify[Coefficient[exp, o, i]] oi, {i, -1, 2}]
tgeto2[exp_] := Sum[tsimp[Coefficient[exp, o, i]] oi, {i, -1, 2}]
```

Define differential operator (for type-a index)

```
difa[exp_, ru_, ala_] := (exp - (exp /. {ru[al_] → 0})) /.
{ru[al1_] ru[al2_] ru[al3_] ru[al4_] → ru[al1] ru[al2] ru[al3] Kdelta[al4, ala] +
ru[al1] ru[al2] ru[al4] Kdelta[al3, ala] + ru[al1] ru[al4] ru[al3]
Kdelta[al2, ala] + ru[al4] ru[al2] ru[al3] Kdelta[al1, ala],
ru[al1_] ru[al2_] ru[al3_] → ru[al1] ru[al2] Kdelta[al3, ala] +
ru[al1] ru[al3] Kdelta[al2, ala] + ru[al2] ru[al3] Kdelta[al1, ala],
ru[al1_] ru[al2_] → ru[al1] Kdelta[al2, ala] + ru[al2] Kdelta[al1, ala],
ru[al1_] → Kdelta[al1, ala]}
```

## ■ define tensors

$\theta = (\theta^1, \dots, \theta^{\dim})$  is the natural parameter vector

```
DefineTensor[st, "θ", {{1}, 1}]
PermWeight::def : Object θ defined
```

$\eta = (\eta_1, \dots, \eta_{\dim})$  is the expectation parameter vector

```
DefineTensor[se, "η", {{1}, 1}]
PermWeight::def : Object η defined
```

$\phi_3^{abc} = \frac{\partial^3 \phi}{\partial \eta_a \partial \eta_b \partial \eta_c} \Big|_0$  is the third derivative of the potential function  $\phi(\eta)$  at the origin  $\eta=0$ .

```
DefineTensor[tp3, "φ3", {{1, 2, 3}, 1}]
PermWeight::def : Object φ3 defined
```

```
SetSymmetric[tp3[la, lb, lc]]
PermWeight::sym : Symmetries of φ3 assigned
```

$\phi_4^{abcd} = \frac{\partial^4 \phi}{\partial \eta_a \partial \eta_b \partial \eta_c \partial \eta_d} \Big|_0$  is the fourth derivative of the potential function  $\phi(\eta)$  at the origin  $\eta=0$ .

**DefineTensor[tp4, "φ4", {{1, 2, 3, 4}, 1}]**

PermWeight::def : Object φ4 defined

**SetSymmetric[tp4[la, lb, lc, ld]]**

PermWeight::sym : Symmetries of φ4 assigned

$\psi_{3\text{abc}} = \frac{\partial^3 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c} \Big|_0$  is the third derivative of the cumulant function  $\psi(\theta)$  at the origin  $\theta=0$ .

**DefineTensor[tq3, "ψ3", {{1, 2, 3}, 1}]**

PermWeight::def : Object ψ3 defined

**SetSymmetric[tq3[la, lb, lc]]**

PermWeight::sym : Symmetries of ψ3 assigned

$\psi_{4\text{abcd}} = \frac{\partial^4 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c \partial \theta^d} \Big|_0$  is the fourth derivative of the cumulant function  $\psi(\theta)$  at the origin  $\theta=0$ .

**DefineTensor[tq4, "ψ4", {{1, 2, 3, 4}, 1}]**

PermWeight::def : Object ψ4 defined

**SetSymmetric[tq4[la, lb, lc, ld]]**

PermWeight::sym : Symmetries of ψ4 assigned

$y = (y_1, \dots, y_{\text{dim}})$  is the random variable

**DefineTensor[ry, "y", {{1}, 1}]**

PermWeight::def : Object y defined

$h1^a = \frac{\partial h}{\partial y_a} \Big|_0$  is the first derivative of  $h(y)$  at the origin  $y = 0$ .

**DefineTensor[th1, "h1", {{1}, 1}]**

PermWeight::def : Object h1 defined

$h2^{ab} = \frac{\partial^2 h}{\partial y_a \partial y_b} \Big|_0$  is the second derivative of  $h(y)$  at the origin  $y = 0$ .

**DefineTensor[th2, "h2", {{2, 1}, 1}]**

PermWeight::sym : Symmetries of h2 assigned

PermWeight::def : Object h2 defined

$ih2_{ab} = (h2^{ab})^{-1}$  is the inverse matrix of  $h2^{ab}$ .

**DefineTensor[tih2, "ih2", {{2, 1}, 1}]**

PermWeight::sym : Symmetries of ih2 assigned

PermWeight::def : Object ih2 defined

$h3^{abc} = \frac{\partial^3 h}{\partial y_a \partial y_b \partial y_c} \Big|_0$  is the third derivative of  $h(y)$  at the origin  $y = 0$ .

**DefineTensor[th3, "h3", {{1, 2, 3}, 1}]**

PermWeight::def : Object h3 defined

```
SetSymmetric[th3[la, lb, lc]]
```

```
PermWeight::sym : Symmetries of h3 assigned
```

$h4^{abcd} = \frac{\partial^4 h}{\partial y_a \partial y_b \partial y_c \partial y_d} \Big|_0$  is the fourth derivative of  $h(y)$  at the origin  $y = 0$ .

```
DefineTensor[th4, "h4", {{1, 2, 3, 4}, 1}]
```

```
PermWeight::def : Object h4 defined
```

```
SetSymmetric[th4[la, lb, lc, ld]]
```

```
PermWeight::sym : Symmetries of h4 assigned
```

### ■ the log of the density function

$\text{logdensity} = \log f(y; \theta)$  is specified here.

```
logdensity = st[ua] ry[la] - psi[theta] - h[y]
```

```
-h[y] - psi[theta] + (y_a) (\theta^a)
```

Since  $\int f(y; \theta) dy = 1$ , the cumulant function is defined formally by  $\psi(\theta) = \log \int \exp(\theta^a y_a - h(y)) dy$ . The expectation parameter vector is defined by  $\eta = E(y; \theta) = \int y f(y; \theta) dy$ . The potential function  $\phi(\eta)$  is defined by  $\phi(\eta) = \max_{\theta} \{\theta^a \eta_a - \psi(\theta)\}$ . The two parametrizations are related to each other by  $\eta_a = \frac{\partial \psi}{\partial \theta^a}$  and  $\theta^a = \frac{\partial \phi}{\partial \eta_a}$ .

Without losing generality, we assume  $\frac{\partial \phi}{\partial \eta_a} \Big|_0 = 0$  and  $\frac{\partial^2 \phi}{\partial \eta_a \partial \eta_b} \Big|_0 = \delta^{ab}$ .

### ■ the expression of $\psi(\theta)$ in terms of $\eta$

In this subsection, we derive the expression of  $\psi(\theta)$  using  $\eta$  and the  $\phi$  derivatives. The result will be stored in "psieta".

#### ■ derivation

Define "ruleeta1" for the Taylor series of  $\eta_a$  is  $\eta_a = \frac{\partial \psi}{\partial \theta^a} = \frac{\partial \psi}{\partial \theta^a} \Big|_0 + \frac{\partial^2 \psi}{\partial \theta^a \partial \theta^b} \Big|_0 \theta^b + \frac{1}{2} \frac{\partial^3 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c} \Big|_0 \theta^b \theta^c + \frac{1}{6} \frac{\partial^4 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c \partial \theta^d} \Big|_0 \theta^b \theta^c \theta^d$ , where  $\psi_{3abc} = O(n^{-1/2})$  and  $\psi_{4abcd} = O(n^{-1})$ .

```
RuleUnique[ruleeta1, se[la_], Kdelta[la, lb] st[ub] +
```

```
1/2 o tq3[la, lb, lc] st[ub] st[uc] + 1/6 o^2 tq4[la, lb, lc, ld] st[ub] st[uc] st[ud]]
```

```
ApplyRules[se[la], ruleeta1]
```

```
(Kdelta_{pa}) (\theta^p) + 1/2 o (\theta^p) (\theta^q) (\psi_{3pqa}) + 1/6 o^2 (\theta^p) (\theta^q) (\theta^r) (\psi_{4pqr a})
```

Define "ruletheta1" for the Taylor series of  $\theta^a = \frac{\partial \phi}{\partial \eta_a} = \frac{\partial \phi}{\partial \eta_a} \Big|_0 + \frac{\partial^2 \phi}{\partial \eta_a \partial \eta_b} \Big|_0 \eta_b + \frac{1}{2} \frac{\partial^3 \phi}{\partial \eta_a \partial \eta_b \partial \eta_c} \Big|_0 \eta_b \eta_c + \frac{1}{6} \frac{\partial^4 \phi}{\partial \eta_a \partial \eta_b \partial \eta_c \partial \eta_d} \Big|_0 \eta_b \eta_c \eta_d$ , where  $\phi_{3abc} = O(n^{-1/2})$  and  $\phi_{4abcd} = O(n^{-1})$ .

```

RuleUnique[ruletheta1, st[ua_],
  Kdelta[ua, ub] se[lb] +  $\frac{1}{2}$  o tp3[ua, ub, uc] se[lb] se[lc] +
   $\frac{1}{6}$  o2 tp4[ua, ub, uc, ud] se[lb] se[lc] se[ld]]
foo21 = ApplyRules[st[ua], ruletheta1]
(Kdeltapa) (ηp) +  $\frac{1}{2}$  o (ηp) (ηq) (φ3pqa) +  $\frac{1}{6}$  o2 (ηp) (ηq) (ηr) (φ4pqra)

```

Calculate  $\frac{\partial^2 \phi}{\partial \eta_a \partial \eta_b} = \frac{\partial \theta^a}{\partial \eta_b} = \delta^{ab} + \frac{\partial^3 \phi}{\partial \eta_a \partial \eta_b \partial \eta_c} \Big|_0 \eta_c + \frac{1}{2} \frac{\partial^4 \phi}{\partial \eta_a \partial \eta_b \partial \eta_c \partial \eta_d} \Big|_0 \eta_c \eta_d$  by taking the partial differentiation of  $\theta^a$  with respect to  $\eta_b$ . Define "rulephi2" for  $\frac{\partial^2 \phi}{\partial \eta_a \partial \eta_b}$ .

```

foo22 = tsimp[difa[foo21, se, ub]]
Kdeltaab + o (ηp) (φ3pab) +  $\frac{1}{2}$  o2 (ηp) (ηq) (φ4pqab)
DefineTensor[dp2, {{2, 1}, 1}]
PermWeight::sym : Symmetries of dp2 assigned
PermWeight::def : Object dp2 defined
RuleUnique[rulephi2, dp2[ua_, ub_], foo22]

```

Apply  $(I + A)^{-1} = I - A + A^2 + O(n^{-3/2})$  for  $A = O(n^{-1/2})$  to  $\frac{\partial^2 \phi}{\partial \eta_a \partial \eta_b}$

```

foo23 = tgeto2[ApplyRules[Kdelta[ua, ub] - (dp2[ua, ub] - Kdelta[ua, ub]) +
  (dp2[ua, uc] - Kdelta[ua, uc]) (dp2[lc, ub] - Kdelta[lc, ub]), rulephi2]]
Kdeltaab - o (ηp) (φ3pab) + o2 ((ηp) (ηq) (φ3rpb) (φ3qra) -  $\frac{1}{2}$  (ηp) (ηq) (φ4pqab))

```

Substitute ruleeta1 for  $\eta_a$  to get  $\frac{\partial^2 \psi}{\partial \theta^a \partial \theta^b} = \left( \frac{\partial^2 \phi}{\partial \eta_a \partial \eta_b} \right)^{-1}$  using  $\phi$  derivatives as well as  $\psi$  derivatives.

```

foo24 = tgeto2[ApplyRules[foo23, ruleeta1]]
Kdeltaab - o (θp) (φ3pab) +
  o2 ((θp) (θq) (φ3rpb) (φ3qra) -  $\frac{1}{2}$  (θp) (θq) (φ4pqab) -  $\frac{1}{2}$  (θp) (θq) (φ3rab) (ψ3pqr))

```

The above expression is compared with  $\frac{\partial^2 \psi}{\partial \theta^a \partial \theta^b} = \delta_{ab} + \frac{\partial^3 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c} \Big|_0 \theta^c + \frac{\partial^4 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c \partial \theta^d} \Big|_0 \theta^c \theta^d$ , and the coefficients are obtained below.

```

foo25 = Collect[CoefficientList[foo24 /. {st[l1_] -> x}, x], o, tsimp[
  CanAll[# /. {u1 -> uc, u2 -> ud, u3 -> ue, u4 -> uf, l1 -> lc, l2 -> ld, l3 -> le, l4 -> lf}]] &]
{Kdeltaab, -o (φ3abc), o2 ((φ3pad) (φ3pbc) -  $\frac{1}{2}$  (φ4abcd) -  $\frac{1}{2}$  (φ3pab) (ψ3pcd))}
foo26 = Simplify[{foo25[[2]] / o, foo25[[3]] (2 / o2)}]
{- (φ3abc), 2 (φ3pad) (φ3pbc) - φ4abcd - (φ3pab) (ψ3pcd)}
RuleUnique[ruletq3, tq3[ua_, ub_, uc_], foo26[[1]]]
RuleUnique[ruletq4, tq4[ua_, ub_, uc_, ud_], ApplyRules[foo26[[2]], ruletq3]]

```



We have obtained  $\frac{\partial^3 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c} \Big|_0$ , and  $\frac{\partial^4 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c \partial \theta^d} \Big|_0$  as follows.

```
ApplyRules[tq3[ua, ub, uc], ruletq3]
```

```
-(phi3abc)
```

```
ApplyRules[tq4[ua, ub, uc, ud], ruletq4]
```

```
2 (phi3ad) (phi3bc) + (phi3ab) (phi3cd) - phi4abcd
```

Let us write down the Taylor series

$$\psi(\theta) = \psi(0) + \frac{\partial \psi}{\partial \theta^a} \Big|_0 \theta^a + \frac{1}{2} \frac{\partial^2 \psi}{\partial \theta^a \partial \theta^b} \Big|_0 \theta^a \theta^b + \frac{1}{6} \frac{\partial^3 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c} \Big|_0 \theta^a \theta^b \theta^c + \frac{1}{24} \frac{\partial^4 \psi}{\partial \theta^a \partial \theta^b \partial \theta^c \partial \theta^d} \Big|_0 \theta^a \theta^b \theta^c \theta^d$$

```
psitheta =
```

```
psi[0] + 1/2 Kdelta[la, lb] st[ua] st[ub] + 1/6 o tq3[la, lb, lc] st[ua] st[ub] st[uc] +
```

```
1/24 o^2 tq4[la, lb, lc, ld] st[ua] st[ub] st[uc] st[ud]
```

```
psi[0] + 1/2 (Kdeltaab) (thetaa) (thetab) +
```

```
1/6 o (thetaa) (thetab) (thetac) (psiabc) + 1/24 o^2 (thetaa) (thetab) (thetac) (thetad) (psiabcd)
```

### ■ result

Now express  $\psi(\theta)$  in terms of  $\eta$  and  $\phi$  derivatives. This gives eq.(3.8) of SH02.

```
psieta = CanAll[
```

```
ApplyRules[CanAll[tgeto2[ApplyRules[psitheta, ruletheta1]]], {ruletq3, ruletq4}]]
```

```
psi[0] + 1/2 (etap) (etap) + 1/3 o (etap) (etaq) (etar) (phi3pqr) + 1/8 o^2 (etap) (etaq) (etar) (etas) (phi4pqrs)
```

```
psieta // InputForm
```

```
psi[0] + (se[l1]*se[u1])/2 +
(o*se[l1]*se[l2]*se[l3]*tp3[u1, u2, u3])/3 +
(o^2*se[l1]*se[l2]*se[l3]*se[l4]*tp4[u1, u2, u3, u4])/8
```

### ■ the expression of h(y) in terms of $\phi$ derivatives

In this subsection, we derive the expression of h(y) using  $\phi$  derivatives. The result will be stored in "hinyphi".

### ■ derivation

Consider Taylor series  $h(y) = h(0) + h1^a y_a + \frac{1}{2} h2^{ab} y_a y_b + \frac{1}{6} h3^{abc} y_a y_b y_c + \frac{1}{24} h4^{abcd} y_a y_b y_c y_d$ , where  $h1^a = O(n^{1/2})$ ,  $h2^{ab} = O(1)$ ,  $h3^{abc} = O(n^{-1/2})$ ,  $h4^{abcd} = O(n^{-1})$ .

$$\begin{aligned} \text{hiny} &= \mathbf{h}[0] + \mathbf{o}^{-1} \text{th1}[\mathbf{ua}] \text{ry}[\mathbf{la}] + \\ &\quad \frac{1}{2} \text{th2}[\mathbf{ua}, \mathbf{ub}] \text{ry}[\mathbf{la}] \text{ry}[\mathbf{lb}] + \frac{1}{6} \mathbf{o} \text{th3}[\mathbf{ua}, \mathbf{ub}, \mathbf{uc}] \text{ry}[\mathbf{la}] \text{ry}[\mathbf{lb}] \text{ry}[\mathbf{lc}] + \\ &\quad \frac{1}{24} \mathbf{o}^2 \text{th4}[\mathbf{ua}, \mathbf{ub}, \mathbf{uc}, \mathbf{ud}] \text{ry}[\mathbf{la}] \text{ry}[\mathbf{lb}] \text{ry}[\mathbf{lc}] \text{ry}[\mathbf{ld}] \\ \text{h}[0] &+ \frac{(\mathbf{Y}_a) (\mathbf{h1}^a)}{\mathbf{o}} + \frac{1}{2} (\mathbf{Y}_a) (\mathbf{Y}_b) (\mathbf{h2}^{ab}) + \\ &\quad \frac{1}{6} \mathbf{o} (\mathbf{Y}_a) (\mathbf{Y}_b) (\mathbf{Y}_c) (\mathbf{h3}^{abc}) + \frac{1}{24} \mathbf{o}^2 (\mathbf{Y}_a) (\mathbf{Y}_b) (\mathbf{Y}_c) (\mathbf{Y}_d) (\mathbf{h4}^{abcd}) \end{aligned}$$

Define foo31 and foo32 below, which will satisfy  $\text{foo31} + \text{foo32} = \theta^a y_a - h(y) + O(n^{-1/2})$  as shown later.

$$\begin{aligned} \text{foo31} &= \frac{-1}{2} \text{th2}[\mathbf{ua}, \mathbf{ub}] (\text{ry}[\mathbf{la}] - \text{tih2}[\mathbf{la}, \mathbf{lc}] (\text{st}[\mathbf{uc}] - \mathbf{o}^{-1} \text{th1}[\mathbf{uc}])) \\ &\quad (\text{ry}[\mathbf{lb}] - \text{tih2}[\mathbf{lb}, \mathbf{ld}] (\text{st}[\mathbf{ud}] - \mathbf{o}^{-1} \text{th1}[\mathbf{ud}])) \\ &\quad - \frac{1}{2} (\mathbf{h2}^{ab}) \left( \mathbf{Y}_a - \left( \theta^c - \frac{\mathbf{h1}^c}{\mathbf{o}} \right) (\text{ih2}_{ac}) \right) \left( \mathbf{Y}_b - \left( \theta^d - \frac{\mathbf{h1}^d}{\mathbf{o}} \right) (\text{ih2}_{bd}) \right) \\ \text{foo32} &= -\mathbf{h}[0] + \frac{1}{2} \text{tih2}[\mathbf{la}, \mathbf{lb}] (\text{st}[\mathbf{ua}] - \mathbf{o}^{-1} \text{th1}[\mathbf{ua}]) (\text{st}[\mathbf{ub}] - \mathbf{o}^{-1} \text{th1}[\mathbf{ub}]) \\ &\quad -\mathbf{h}[0] + \frac{1}{2} \left( \theta^a - \frac{\mathbf{h1}^a}{\mathbf{o}} \right) \left( \theta^b - \frac{\mathbf{h1}^b}{\mathbf{o}} \right) (\text{ih2}_{ab}) \end{aligned}$$

Define a rule to make  $\mathbf{h2}_a^b \text{ih2}^{ac} = \delta^{bc}$ , thus ih2 is the inverse matrix of h2.

$$\text{RuleUnique}[\text{absorbth2}, \text{th2}[\mathbf{la}_-, \mathbf{ub}_-] \text{tih2}[\mathbf{uc}_-, \mathbf{ua}_-], \text{Kdelta}[\mathbf{ub}, \mathbf{uc}]]$$

Apply this rule to foo31+foo32 to get foo33.

$$\begin{aligned} \text{foo33} &= \text{CanAll}[\text{AbsorbKdelta}[\text{ApplyRules}[\text{CanAll}[\text{foo31} + \text{foo32}], \text{absorbth2}]]] \\ &\quad -\mathbf{h}[0] + (\mathbf{Y}_p) (\theta^p) - \frac{(\mathbf{Y}_p) (\mathbf{h1}^p)}{\mathbf{o}} - \frac{1}{2} (\mathbf{Y}_p) (\mathbf{Y}_q) (\mathbf{h2}^{pq}) \end{aligned}$$

Confirming  $\text{foo33} = \text{foo31} + \text{foo32} = \theta^a y_a - h(y) + O(n^{-1/2})$ .

$$\begin{aligned} &\text{CanAll}[\text{foo33} - (\text{ry}[\mathbf{la}] \text{st}[\mathbf{ua}] - \text{hiny})] \\ &\quad \frac{1}{6} \mathbf{o} (\mathbf{Y}_p) (\mathbf{Y}_q) (\mathbf{Y}_r) (\mathbf{h3}^{pqr}) + \frac{1}{24} \mathbf{o}^2 (\mathbf{Y}_p) (\mathbf{Y}_q) (\mathbf{Y}_r) (\mathbf{Y}_s) (\mathbf{h4}^{pqrs}) \end{aligned}$$

Since  $(2\pi)^{-\frac{\dim}{2}} \det(\mathbf{h2}^{ab})^{\frac{1}{2}} \exp(\text{foo31})$  is the multivariate normal density function with mean specified above and  $\text{ih2}_{ab}$  covariance,  $\int \exp(\theta^a y_a - h(y) - \text{foo32} + O(n^{-1/2})) d\mathbf{y} = \int \exp(\text{foo31}) d\mathbf{y} = (2\pi)^{\frac{\dim}{2}} \det(\mathbf{h2}^{ab})^{-\frac{1}{2}}$ . Then,  $\psi(\theta) = \log \int \exp(\theta^a y_a - h(y)) d\mathbf{y} = \frac{\dim}{2} \log(2\pi) - \frac{1}{2} \log \det(\mathbf{h2}^{ab}) + \text{foo32} + O(n^{-1/2})$ .

$$\begin{aligned} \text{foo34} &= \frac{\dim}{2} \text{Log}[2\pi] - \frac{1}{2} \text{deth2} + \text{CanAll}[\text{Expand}[\text{foo32}]] \\ &\quad - \frac{\text{deth2}}{2} - \mathbf{h}[0] + \frac{1}{2} \dim \text{Log}[2\pi] + \\ &\quad \frac{1}{2} (\theta_p) (\theta_q) (\text{ih2}^{pq}) - \frac{(\theta_p) (\mathbf{h1}_q)}{\mathbf{o}} (\text{ih2}^{pq}) + \frac{(\mathbf{h1}_p) (\mathbf{h1}_q) (\text{ih2}^{pq})}{2 \mathbf{o}^2} \end{aligned}$$

Considering  $\frac{\partial \psi}{\partial \theta^a} \Big|_0 = 0$ ,  $\frac{\partial^2 \psi}{\partial \theta^a \partial \theta^b} \Big|_0 = \delta_{ab}$ , we find that  $\text{ih2}^{ab} = \delta^{ab} + O(n^{-1/2})$  and  $\mathbf{h1}_a = O(n^{-1/2})$  from the above expression of  $\psi(\theta) = \text{foo34} + O(n^{-1/2})$ . Let us write  $\mathbf{h2}^{ab} = \delta^{ab} + \mathbf{ah2}^{ab}$  with  $\mathbf{ah2}^{ab} = O(n^{-1/2})$ .

```

DefineTensor[tah2, "ah2", {{2, 1}, 1}]
PermWeight::sym : Symmetries of ah2 assigned
PermWeight::def : Object ah2 defined

ruleth2ah2 = th2[ua_, ub_] -> Kdelta[ua, ub] + o tah2[ua, ub];

```

Rewrite the Taylor series of  $h(y)$  by noting the first derivative  $h_1$  is in fact  $O(n^{-1/2})$ .

```

hiny = h[0] + o th1[ua] ry[la] +
      1/2 th2[ua, ub] ry[la] ry[lb] + 1/6 o th3[ua, ub, uc] ry[la] ry[lb] ry[lc] +
      1/24 o^2 th4[ua, ub, uc, ud] ry[la] ry[lb] ry[lc] ry[ld] /. ruleth2ah2

h[0] + 1/2 (Ya) (Yb) (Kdelta^ab + o (ah2^ab)) + o (Ya) (h1^a) +
      1/6 o (Ya) (Yb) (Yc) (h3^abc) + 1/24 o^2 (Ya) (Yb) (Yc) (Yd) (h4^abcd)

```

In the following,  $\exp(\theta^a y_a - h(y)) = \exp(\text{foo35}) = \exp(\text{foo36}) \exp(\text{foo37} + O(n^{-3/2}))$ , where  $\int \exp(\text{foo31}) dy = 1$ .

```

foo35 = ry[la] st[ua] - hiny

-h[0] + (Ya) (theta^a) - 1/2 (Ya) (Yb) (Kdelta^ab + o (ah2^ab)) -
      o (Ya) (h1^a) - 1/6 o (Ya) (Yb) (Yc) (h3^abc) - 1/24 o^2 (Ya) (Yb) (Yc) (Yd) (h4^abcd)

foo36 = -dim/2 Log[2 Pi] + -1/2 (ry[la] - st[la]) (ry[ua] - st[ua])

-1/2 dim Log[2 pi] - 1/2 (Ya - theta_a) (Y^a - theta^a)

foo37 = CanAll[AbsorbKdelta[CanAll[foo35 - foo36]]]

-h[0] + 1/2 dim Log[2 pi] + 1/2 (theta_p) (theta^p) - 1/2 o (Yp) (Yq) (ah2^pq) -
      o (Yp) (h1^p) - 1/6 o (Yp) (Yq) (Yr) (h3^pqr) - 1/24 o^2 (Yp) (Yq) (Yr) (Ys) (h4^pqrs)

```

Noting  $\psi(\theta) = \log \int \exp(\text{foo35}) dy = \log E(\exp(\text{foo37} + O(n^{-3/2})))$ , where the expectation is taken for the multivariate normal with mean  $(\theta^1, \dots, \theta^{\dim})$  and covariance identity. We apply "logeexpoly" to foo37. First, we get  $\text{foo38}=\{a_0, a_1, a_2, a_3, a_4\}$  for the coefficients of  $a_0 + a_1^i x_i + a_2^{ij} x_i x_j + a_3^{ijk} x_i x_j x_k + a_4^{ijkl} x_i x_j x_k x_l$ , and  $\psi(\theta) = \text{foo39}$  below.

```

foo38 = CoefficientList[foo37 /. ry[la_] -> x, x] / {1, o, o, o, o^2}

{-h[0] + 1/2 dim Log[2 pi] + 1/2 (theta_p) (theta^p), - (h1^p), -1/2 (ah2^pq), -1/6 (h3^pqr), -1/24 (h4^pqrs)}

```

```
foo39 = CanAll[logeexpoly / .
  {sb → st, ta0 → foo38[[1]], ta1[u1_] → foo38[[2]], ta2[u1_, u2_] → foo38[[3]],
  ta3[u1_, u2_, u3_] → foo38[[4]], ta4[u1_, u2_, u3_, u4_] → foo38[[5]]}]
-h[0] + 1/2 dim Log[2 π] + 1/2 (θp) (θp) - 1/2 o (ah2pp) - 1/2 o (θp) (θq) (ah2pq) +
  1/4 o2 (ah2pq) (ah2pq) + 1/2 o2 (θp) (θq) (ah2rp) (ah2qr) - o (θp) (h1p) +
  1/2 o2 (h1p) (h1p) + o2 (θp) (ah2qp) (h1q) - 1/2 o (θp) (h3qpq) + 1/2 o2 (h1p) (h3qpq) +
  1/2 o2 (θp) (ah2qp) (h3rqr) + 1/8 o2 (h3pqp) (h3rqr) - 1/6 o (θp) (θq) (θr) (h3pqr) +
  1/2 o2 (θp) (ah2qr) (h3pqr) + 1/2 o2 (θp) (θq) (h1r) (h3pqr) + 1/12 o2 (h3pqr) (h3pqr) +
  1/4 o2 (θp) (θq) (h3rsr) (h3qs) + 1/2 o2 (θp) (θq) (θr) (ah2sp) (h3qrs) +
  1/4 o2 (θp) (θq) (h3rsp) (h3qrs) + 1/8 o2 (θp) (θq) (θr) (θs) (h3tpq) (h3rst) -
  1/8 o2 (h4pqpq) - 1/4 o2 (θp) (θq) (h4rpqr) - 1/24 o2 (θp) (θq) (θr) (θs) (h4pqrs)
```

Now substitute  $\theta^a = \frac{\partial \phi}{\partial \eta_a} = \delta^{ab} \eta_b + \frac{1}{2} \phi^{abc} \eta_b \eta_c + \frac{1}{6} \phi^{abcd} \eta_b \eta_c \eta_d$  for  $\theta^a$  in foo39 to get  $\psi(\theta)=\text{foo40}$  in terms of  $\eta$  below. The coefficients for the polynomial of  $\eta$  is stored in foo41.

```
foo40 = CanAll[tgeto2[ApplyRules[foo39, ruletheta1]]];
foo41 = Collect[CoefficientList[foo40 /. {se[l1_] → x}, x], o,
  tsimp[# /. {u1 → ua, u2 → ub, u3 → uc, u4 → ud, l1 → la, l2 → lb, l3 → lc, l4 → ld}] &]
{-h[0] + 1/2 dim Log[2 π] - 1/2 o (ah2pp) +
  o2 (1/4 (ah2pq) (ah2pq) + 1/2 (h1p) (h1p) + 1/2 (h1p) (h3qpq) +
  1/8 (h3pqp) (h3rqr) + 1/12 (h3pqr) (h3pqr) - 1/8 (h4pqpq)) ,
  o (- (h1a) - 1/2 (h3ppa)) + o2 ((ah2pa) (h1p) + 1/2 (ah2pa) (h3qpq) + 1/2 (ah2pq) (h3pqa)) ,
  1/2 - 1/2 o (ah2ab) + o2 (1/2 (ah2pa) (ah2pb) + 1/4 (h3pqa) (h3pqb) + 1/2 (h1p) (h3pab) +
  1/4 (h3pqp) (h3qab) - 1/4 (h4ppab) - 1/2 (h1p) (φ3pab) - 1/4 (h3pqp) (φ3qab)) ,
  o2 (1/2 (ah2pa) (h3pbc) - 1/2 (ah2pa) (φ3pbc)) + o (- 1/6 (h3abc) + 1/2 (φ3abc)) ,
  o2 (1/8 (h3pab) (h3pcd) - 1/24 (h4abcd) - 1/4 (h3pab) (φ3pcd) + 1/8 (φ3pab) (φ3pcd) + 1/6 (φ4abcd)) }
```

Since foo40= $\psi(\theta)=\text{psieta}$ , foo41 must be equal to foo42 below.

```
foo42 = CoefficientList[psieta /. se[la_] → x, x] /. {u1 → ua, u2 → ub, u3 → uc, u4 → ud}
{psi[0], 0, 1/2, 1/3 o (φ3abc), 1/8 o2 (φ4abcd)}
```

At first, we compare the coefficient for  $\eta^a \eta^b$ .

```
foo41[[3]]
1/2 - 1/2 o (ah2ab) +
  o2 (1/2 (ah2pa) (ah2pb) + 1/4 (h3pqa) (h3pqb) + 1/2 (h1p) (h3pab) + 1/4 (h3pqp) (h3qab) -
  1/4 (h4ppab) - 1/2 (h1p) (φ3pab) - 1/4 (h3pqp) (φ3qab))
```

foo42[[3]]

$$\frac{1}{2}$$

Thus, ah2 is in fact  $O(n^{-1})$  instead of  $O(n^{-1/2})$ .

hiny = hiny /. { tah2[ua\_, ub\_] -> o tah2[ua, ub]}

$$h[0] + \frac{1}{2} (Y_a) (Y_b) (Kdelta^{ab} + o^2 (ah2^{ab})) + o (Y_a) (h1^a) + \frac{1}{6} o (Y_a) (Y_b) (Y_c) (h3^{abc}) + \frac{1}{24} o^2 (Y_a) (Y_b) (Y_c) (Y_d) (h4^{abcd})$$

We rewrite foo43=foo42-foo41.

foo43 = Map[tgeto2, (foo42 - foo41) /. { tah2[u1\_, u2\_] -> o tah2[u1, u2]}]

$$\left\{ h[0] - \frac{1}{2} \dim \text{Log}[2 \pi] + \text{psi}[0] + o^2 \left( \frac{1}{2} (ah2_p^p) - \frac{1}{2} (h1_p) (h1^p) - \frac{1}{2} (h1_p) (h3_q^{pq}) - \frac{1}{8} (h3_{pq}^p) (h3_r^{qr}) - \frac{1}{12} (h3_{pqr}) (h3^{pqr}) + \frac{1}{8} (h4_{pq}^{pq}) \right), o \left( h1^a + \frac{1}{2} (h3_p^{pa}) \right), o^2 \left( \frac{1}{2} (ah2^{ab}) - \frac{1}{4} (h3_{pq}^a) (h3^{pqb}) - \frac{1}{2} (h1_p) (h3^{pab}) - \frac{1}{4} (h3_{pq}^p) (h3^{qab}) + \frac{1}{4} (h4_p^{pab}) + \frac{1}{2} (h1_p) (\phi3^{pab}) + \frac{1}{4} (h3_{pq}^p) (\phi3^{qab}) \right), o \left( \frac{1}{6} (h3^{abc}) - \frac{1}{6} (\phi3^{abc}) \right), o^2 \left( -\frac{1}{8} (h3_p^{ab}) (h3^{pcd}) + \frac{1}{24} (h4^{abcd}) + \frac{1}{4} (h3_p^{ab}) (\phi3^{pcd}) - \frac{1}{8} (\phi3_p^{ab}) (\phi3^{pcd}) - \frac{1}{24} (\phi4^{abcd}) \right) \right\}$$

We solve these five equations == 0. At first, foo43[[4]]==0 gives  $h3^{abc} = \phi3^{abc}$ .

foo44 = Solve[foo43[[4]] == 0, th3[ua, ub, uc]]

$$\{ \{ h3^{abc} \rightarrow \phi3^{abc} \} \}$$

RuleUnique[rule44, th3[ua\_, ub\_, uc\_], foo44[[1, 1, 2]]]

foo45 = Solve[ApplyRules[foo43[[2]], rule44] == 0, th1[ua]]

$$\{ \{ h1^a \rightarrow -\frac{1}{2} (\phi3_p^{pa}) \} \}$$

RuleUnique[rule45, th1[ua\_], foo45[[1, 1, 2]]]

foo46 = Solve[ApplyRules[foo43[[5]], {rule44, rule45}] == 0, th4[ua, ub, uc, ud]]

$$\{ \{ h4^{abcd} \rightarrow \phi4^{abcd} \} \}$$

RuleUnique[rule46, th4[ua\_, ub\_, uc\_, ud\_], foo46[[1, 1, 2]]]

foo47 =

Simplify[Solve[ApplyRules[foo43[[3]], {rule44, rule45, rule46}] == 0, tah2[ua, ub]]]

$$\{ \{ ah2^{ab} \rightarrow \frac{1}{2} ((\phi3_{pq}^a) (\phi3^{pqb}) - \phi4_p^{pab}) \} \}$$

RuleUnique[rule47, tah2[ua\_, ub\_], foo47[[1, 1, 2]]]

```
foo48 =
Simplify[Solve[ApplyRules[foo43[[1]], {rule44, rule45, rule46, rule47}] == 0, h[0]]]
{{h[0] -> 1/24 (12 dim Log[2 Pi] - 24 psi[0] - 3 o^2 (phi3_pq^q) (phi3_r^p) +
3 o^2 (phi3_pq^p) (phi3_r^q) - 4 o^2 (phi3_pqr) (phi3_pqr) + 3 o^2 (phi4_pq^pq))}}
RuleUnique[rule48, h[0], foo48[[1, 1, 2]]]
```

■ result

Now, it is time to express  $h(y)$  in terms of the  $\phi$  derivatives.

```
hinyphi =
CanAll[AbsorbKdelta[ApplyRules[hiny, {rule44, rule45, rule46, rule47, rule48}]]]
```

$$\frac{1}{2} \dim \text{Log}[2 \pi] - \text{psi}[0] + \frac{1}{2} (Y_p) (Y^p) - \frac{1}{2} o (Y_p) (\phi_{3_q}^{pq}) +$$

$$\frac{1}{6} o (Y_p) (Y_q) (Y_r) (\phi_{3_pqr}^{pqr}) - \frac{1}{6} o^2 (\phi_{3_pqr}) (\phi_{3_pqr}^{pqr}) + \frac{1}{4} o^2 (Y_p) (Y_q) (\phi_{3_{rs}^p}) (\phi_{3_{rs}^q}) +$$

$$\frac{1}{8} o^2 (\phi_{4_{pq}^{pq}}) - \frac{1}{4} o^2 (Y_p) (Y_q) (\phi_{4_{rs}^{pqr}}) + \frac{1}{24} o^2 (Y_p) (Y_q) (Y_r) (Y_s) (\phi_{4_{pqrs}^{pqrs}})$$

```
hinyphi // InputForm
```

```
(dim*Log[2*Pi])/2 - psi[0] + (ry[l1]*ry[u1])/2 -
(o*ry[l1]*tp3[l2, u1, u2])/2 +
(o*ry[l1]*ry[l2]*ry[l3]*tp3[u1, u2, u3])/6 -
(o^2*tp3[l1, l2, l3]*tp3[u1, u2, u3])/6 +
(o^2*ry[l1]*ry[l2]*tp3[l3, l4, u1]*tp3[u2, u3, u4])/4 +
(o^2*tp4[l1, l2, u1, u2])/8 -
(o^2*ry[l1]*ry[l2]*tp4[l3, u1, u2, u3])/4 +
(o^2*ry[l1]*ry[l2]*ry[l3]*ry[l4]*tp4[u1, u2, u3, u4])/24
```

The coefficients of  $h(y)$  as a polynomial of  $y$  are as follows.

```
foo49 = Collect[CoefficientList[hinyphi /. ry[l1_] -> x, x] /.
{u1 -> ua, u2 -> ub, u3 -> uc, u4 -> ud, l1 -> la, l2 -> lb, l3 -> lc, l4 -> ld}, o, tsimp[#] &]
```

$$\left\{ \frac{1}{2} \dim \text{Log}[2 \pi] - \text{psi}[0] + o^2 \left( -\frac{1}{6} (\phi_{3_pqr}) (\phi_{3_pqr}^{pqr}) + \frac{1}{8} (\phi_{4_{pq}^{pq}}) \right), -\frac{1}{2} o (\phi_{3_p}^{pa}), \right.$$

$$\left. \frac{1}{2} + o^2 \left( \frac{1}{4} (\phi_{3_{pq}^a}) (\phi_{3_{pq}^{pb}}) - \frac{1}{4} (\phi_{4_p}^{pab}) \right), \frac{1}{6} o (\phi_{3^{abc}}), \frac{1}{24} o^2 (\phi_{4^{abcd}}) \right\}$$

■ the canonical form

Now we get the canonical form of  $\log f(y; \eta)$  in "logdensityy".

■ the summary of the previous sections

The standard form of the density function is specified by  $\text{logdensity} = \log f(y; \theta)$ .

```
logdensity
```

$$-h[y] - \text{psi}[\text{theta}] + (y_a) (\theta^a)$$

By applying "ruletheta1" to logdensity,  $\theta$  can be expressed in terms of  $\eta$  and  $\phi$  derivatives.

**foo51 = ApplyRules[logdensity, ruletheta1]**

$$-h[y] - \text{psi}[\text{theta}] + (\text{Kdelta}^{\text{pq}}) (Y_p) (\eta_q) + \frac{1}{2} \circ (Y_p) (\eta_q) (\eta_r) (\phi_3^{\text{pqr}}) + \frac{1}{6} \circ^2 (Y_p) (\eta_q) (\eta_r) (\eta_s) (\phi_4^{\text{pqrs}})$$

The cumulant function  $\psi(\theta)$  can be expressed in terms of  $\eta$  and  $\phi$  derivatives as shown in psieta.

**psieta**

$$\text{psi}[0] + \frac{1}{2} (\eta_p) (\eta^p) + \frac{1}{3} \circ (\eta_p) (\eta_q) (\eta_r) (\phi_3^{\text{pqr}}) + \frac{1}{8} \circ^2 (\eta_p) (\eta_q) (\eta_r) (\eta_s) (\phi_4^{\text{pqrs}})$$

The measure function  $h(y)$  can be expressed in terms of  $y$  and  $\phi$  derivatives as shown in hinyphi.

**hinyphi**

$$\begin{aligned} & \frac{1}{2} \dim \text{Log}[2 \pi] - \text{psi}[0] + \frac{1}{2} (Y_p) (Y^p) - \frac{1}{2} \circ (Y_p) (\phi_3^{\text{pq}}) + \\ & \frac{1}{6} \circ (Y_p) (Y_q) (Y_r) (\phi_3^{\text{pqr}}) - \frac{1}{6} \circ^2 (\phi_3^{\text{pqr}}) (\phi_3^{\text{pqr}}) + \frac{1}{4} \circ^2 (Y_p) (Y_q) (\phi_3^{\text{rs}^p}) (\phi_3^{\text{qrs}}) + \\ & \frac{1}{8} \circ^2 (\phi_4^{\text{pq}^{\text{pq}}}) - \frac{1}{4} \circ^2 (Y_p) (Y_q) (\phi_4^{\text{r}^{\text{pqr}}}) + \frac{1}{24} \circ^2 (Y_p) (Y_q) (Y_r) (Y_s) (\phi_4^{\text{pqrs}}) \end{aligned}$$

## ■ result

By substituting psieta and hinyphi for psi[theta] and h[y] respectively in foo51=log f(y;θ), we obtain the canonical form of log f(y;η) as follows.

**foo52 = Collect[foo51 /. {psi[theta] → psieta, h[y] → hinyphi}, o, tsimp]**

$$\begin{aligned} & -\frac{1}{2} \dim \text{Log}[2 \pi] - \frac{1}{2} (Y_p) (Y^p) + (Y_p) (\eta^p) - \\ & \frac{1}{2} (\eta_p) (\eta^p) + \circ \left( \frac{1}{2} (Y_p) (\phi_3^{\text{pq}}) - \frac{1}{6} (Y_p) (Y_q) (Y_r) (\phi_3^{\text{pqr}}) + \right. \\ & \quad \left. \frac{1}{2} (Y_p) (\eta_q) (\eta_r) (\phi_3^{\text{pqr}}) - \frac{1}{3} (\eta_p) (\eta_q) (\eta_r) (\phi_3^{\text{pqr}}) \right) + \\ & \circ^2 \left( \frac{1}{6} (\phi_3^{\text{pqr}}) (\phi_3^{\text{pqr}}) - \frac{1}{4} (Y_p) (Y_q) (\phi_3^{\text{rs}^p}) (\phi_3^{\text{qrs}}) - \frac{1}{8} (\phi_4^{\text{pq}^{\text{pq}}}) + \right. \\ & \quad \left. \frac{1}{4} (Y_p) (Y_q) (\phi_4^{\text{r}^{\text{pqr}}}) - \frac{1}{24} (Y_p) (Y_q) (Y_r) (Y_s) (\phi_4^{\text{pqrs}}) + \right. \\ & \quad \left. \frac{1}{6} (Y_p) (\eta_q) (\eta_r) (\eta_s) (\phi_4^{\text{pqrs}}) - \frac{1}{8} (\eta_p) (\eta_q) (\eta_r) (\eta_s) (\phi_4^{\text{pqrs}}) \right) \end{aligned}$$

This is the canonical form of log f(y;η).

**logdensity = Expand[foo52];**

**logdensity // InputForm**

$$\begin{aligned} & -(\dim * \text{Log}[2 * \text{Pi}])/2 - (\text{ry}[11] * \text{ry}[u1])/2 + \text{ry}[11] * \text{se}[u1] - \\ & (\text{se}[11] * \text{se}[u1])/2 + (\circ * \text{ry}[11] * \text{tp3}[12, u1, u2])/2 - \\ & (\circ * \text{ry}[11] * \text{ry}[12] * \text{ry}[13] * \text{tp3}[u1, u2, u3])/6 + \\ & (\circ * \text{ry}[11] * \text{se}[12] * \text{se}[13] * \text{tp3}[u1, u2, u3])/2 - \\ & (\circ * \text{se}[11] * \text{se}[12] * \text{se}[13] * \text{tp3}[u1, u2, u3])/3 + \\ & (\circ^2 * \text{tp3}[11, 12, 13] * \text{tp3}[u1, u2, u3])/6 - \\ & (\circ^2 * \text{ry}[11] * \text{ry}[12] * \text{tp3}[13, 14, u1] * \text{tp3}[u2, u3, u4])/4 - \\ & (\circ^2 * \text{tp4}[11, 12, u1, u2])/8 + \\ & (\circ^2 * \text{ry}[11] * \text{ry}[12] * \text{tp4}[13, u1, u2, u3])/4 - \\ & (\circ^2 * \text{ry}[11] * \text{ry}[12] * \text{ry}[13] * \text{ry}[14] * \text{tp4}[u1, u2, u3, u4])/24 + \\ & (\circ^2 * \text{ry}[11] * \text{se}[12] * \text{se}[13] * \text{se}[14] * \text{tp4}[u1, u2, u3, u4])/6 - \\ & (\circ^2 * \text{se}[11] * \text{se}[12] * \text{se}[13] * \text{se}[14] * \text{tp4}[u1, u2, u3, u4])/8 \end{aligned}$$

We also show the metric  $\frac{\partial^2 \phi}{\partial \eta_a \partial \eta_b}$  by using rulephi2, and name it "phi2eta" for later use.

```
phi2eta = ApplyRules[dp2[ua, ub], rulephi2]

Kdeltaab + o(ηp) (φ3pab) +  $\frac{1}{2}$  o2(ηp) (ηq) (φ4pqab)

InputForm[phi2eta]

Kdelta[ua, ub] + o*se[l1]*tp3[u1, ua, ub] +
(o2*se[l1]*se[l2]*tp4[u1, u2, ua, ub])/2
```

## Tube-Coordinates and $z_c$ -formula

In this part, we first give an expression of the smooth surface in  $R^{\dim}$  which specifies the boundary of the region of interest in the  $\eta$ -space. The tube-coordinate system is then defined as a pair of the coordinate system on the surface and the coordinate along the normal direction. The signed distance from the boundary is slightly modified for generalization, and named as a modified signed distance characterized by a coefficient vector  $c$ . The  $z_c$ -formula is derived as an expression of the distribution function of the modified signed distance, which is obtained up to  $O(n^{-1})$  terms ignoring the error of  $O(n^{-3/2})$ .

### ■ Startup

This section initializes the *Mathematica* session.

#### ■ packages

```
<< Statistics`ContinuousDistributions`
```



**<< MathTens.m (Windows)**

Loading MathTensor for DOS/Windows . . .

```

=====
MathTensor (TM) 2.2.1 (Windows) (September 17, 2000)
by Leonard Parker and Steven M. Christensen
Copyright (c) 1991-2000 MathTensor, Inc.
Runs with Mathematica (R) Versions 2.2, 3.0, 4.0
=====
No unit system is chosen. If you want one,
you must edit the file called Conventions.m,
or enter a command to interactively set units.
Units: {}
Sign conventions: Rmsign = 1 Rcsign = 1
MetricgSign = 1 DetgSign = -1
TensorForm turned on,
ShowTime turned off,
MetricgFlag = True.
=====
Null Windows

```

**■ error messages**

```
Off[General::spell1]
```

```
Off[General::spell]
```

**■ distribution functions**

```

gammadist[x_, m_,  $\alpha$ _] := PDF[GammaDistribution[m,  $\alpha$ ], x]
Gammadist[x_, m_,  $\alpha$ _] := CDF[GammaDistribution[m,  $\alpha$ ], x]
f[x_] := PDF[NormalDistribution[0, 1], x]
F[x_] := CDF[NormalDistribution[0, 1], x]
Q[x_] := Quantile[NormalDistribution[0, 1], x]
Chidist[x_, {di_, nc_}] := CDF[NoncentralChiSquareDistribution[di, nc], x]

```

**■ Exponential family**

This section summarizes the results for the exponential family derived in the previous part.

## ■ the expectation of the exponential of a polynomial function of the normal vector

Here we give the log of the expectation of the exponential of  $\text{poly}(x) = a_0 + a_1 x^i + a_{2ij} x^i x^j + a_{3ijk} x^i x^j x^k + a_{4ijkl} x^i x^j x^k x^l$ , where  $a_1$ ,  $a_2$ , and  $a_3$  are of order  $O(n^{-1/2})$ , and  $a_4$  is  $O(n^{-1})$ .  $x$  is a multivariate normal random vector  $x = (x^1, \dots, x^{\dim})$  of  $\dim$ -dimensions with mean  $b = (b^1, \dots, b^{\dim})$ , and the identity covariance matrix.  $\text{logeexpoly} = \log E \{\exp(\text{poly}(x))\}$  is obtained up to  $O(n^{-1})$  terms.

## ■ define tensors

This  $b_a$  or  $b^a$  denotes a component of the mean vector  $b$ .

```
DefineTensor[sb, "b", {{1}, 1}]
PermWeight::def : Object b defined
```

The following  $a_0$ ,  $a_1$ ,  $a_2$ ,  $a_3$ ,  $a_4$ ,  $a_5$ , and  $a_6$  are used for coefficients in a series expansion with respect to  $x$ .

```
DefineTensor[ta0, "a0", {{}, 1}]
PermWeight::def : Object a0 defined
PermWeight::def: Object a0 defined
```

```
DefineTensor[ta1, "a1", {{1}, 1}]
PermWeight::def : Object a1 defined
PermWeight::def: Object a1 defined
```

```
DefineTensor[ta2, "a2", {{2, 1}, 1}]
PermWeight::sym : Symmetries of a2 assigned
PermWeight::def : Object a2 defined
PermWeight::sym: Symmetries of a2 assigned
PermWeight::def: Object a2 defined
```

```
DefineTensor[ta3, "a3", {{1, 2, 3}, 1}]
PermWeight::def : Object a3 defined
PermWeight::def: Object a3 defined
```

```
SetSymmetric[ta3[la, lb, lc]]
PermWeight::sym : Symmetries of a3 assigned
PermWeight::sym: Symmetries of a3 assigned
```

```
DefineTensor[ta4, "a4", {{1, 2, 3, 4}, 1}]
PermWeight::def : Object a4 defined
PermWeight::def: Object a4 defined
```

```
SetSymmetric[ta4[la, lb, lc, ld]]
```

```
PermWeight::sym : Symmetries of a4 assigned
```

```
PermWeight::sym: Symmetries of a4 assigned
```

```
DefineTensor[ta6, "a6", {{1, 2, 3, 4, 5, 6}, 1}]
```

```
PermWeight::def : Object a6 defined
```

```
SetSymmetric[ta6[la, lb, lc, ld, le, lf]]
```

```
PermWeight::sym : Symmetries of a6 assigned
```

## ■ "logeexpoly"

```
logeexpoly = ta0 + o * (sb[11] * ta1[u1] + ta2[11, u1] + sb[11] * sb[12] * ta2[u1, u2] +
  3 * sb[11] * ta3[12, u1, u2] + sb[11] * sb[12] * sb[13] * ta3[u1, u2, u3]) + o^2 *
  ((ta1[11] * ta1[u1]) / 2 + 2 * sb[11] * ta1[12] * ta2[u1, u2] + ta2[11, 12] * ta2[u1, u2] +
  2 * sb[11] * sb[12] * ta2[13, u1] * ta2[u2, u3] + 3 * ta1[11] * ta3[12, u1, u2] +
  6 * sb[11] * ta2[12, u1] * ta3[13, u2, u3] + (9 * ta3[11, 12, u1] * ta3[13, u2, u3]) / 2 +
  3 * sb[11] * sb[12] * ta1[13] * ta3[u1, u2, u3] +
  6 * sb[11] * ta2[12, 13] * ta3[u1, u2, u3] + 3 * ta3[11, 12, 13] * ta3[u1, u2, u3] +
  9 * sb[11] * sb[12] * ta3[13, 14, u3] * ta3[u1, u2, u4] +
  6 * sb[11] * sb[12] * sb[13] * ta2[14, u1] * ta3[u2, u3, u4] +
  9 * sb[11] * sb[12] * ta3[13, 14, u1] * ta3[u2, u3, u4] +
  (9 * sb[11] * sb[12] * sb[13] * sb[14] * ta3[15, u1, u3] * ta3[u2, u4, u5]) / 2 +
  3 * ta4[11, 12, u1, u2] + 6 * sb[11] * sb[12] * ta4[13, u1, u2, u3] +
  sb[11] * sb[12] * sb[13] * sb[14] * ta4[u1, u2, u3, u4])
```

```
a0 + o ((b_p) (a1^p) + a2_p^p + (b_p) (b_q) (a2^p q) + 3 (b_p) (a3_q^p q) + (b_p) (b_q) (b_r) (a3^p q r)) +
  o^2 ( (1/2) (a1_p) (a1^p) + 2 (b_p) (a1_q) (a2^p q) + (a2_p q) (a2^p q) +
  2 (b_p) (b_q) (a2_r^p) (a2^q r) + 3 (a1_p) (a3_q^p q) + 6 (b_p) (a2_q^p) (a3_r^q r) +
  9/2 (a3_p q^p) (a3_r^q r) + 3 (b_p) (b_q) (a1_r) (a3^p q r) + 6 (b_p) (a2_q r) (a3^p q r) +
  3 (a3_p q r) (a3^p q r) + 9 (b_p) (b_q) (a3_r s^r) (a3^p q s) + 6 (b_p) (b_q) (b_r) (a2_s^p) (a3^q r s) +
  9 (b_p) (b_q) (a3_r s^p) (a3^q r s) + 9/2 (b_p) (b_q) (b_r) (b_s) (a3_t^p r) (a3^q s t) +
  3 (a4_p q^p q) + 6 (b_p) (b_q) (a4_r^p q r) + (b_p) (b_q) (b_r) (b_s) (a4^p q r s) )
```

## ■ the canonical form of the density function

Here we give the canonical form of  $\log f(y;\eta)$  for the exponential family of distributions, and store it in logdensity.

The metric  $\text{phi2eta} = \frac{\partial^2 \phi(\eta)}{\partial \eta_a \partial \eta_b}$  is also given here.

## ■ define tensors

$\theta = (\theta^1, \dots, \theta^{\text{dim}})$  is the natural parameter vector

```
DefineTensor[st, "theta", {{1}, 1}]
```

```
PermWeight::def : Object theta defined
```

$\eta = (\eta_1, \dots, \eta_{\text{dim}})$  is the expectation parameter vector

```
DefineTensor[se, "η", {{1}, 1}]
```

```
PermWeight::def : Object η defined
```

$y = (y_1, \dots, y_{\dim})$  is the random variable

```
DefineTensor[ry, "y", {{1}, 1}]
```

```
PermWeight::def : Object y defined
```

$\phi_3^{abc} = \frac{\partial^3 \phi}{\partial \eta_a \partial \eta_b \partial \eta_c} \Big|_0$  is the third derivative of the potential function  $\phi(\eta)$  at the origin  $\eta=0$ .

```
DefineTensor[tp3, "φ3", {{1, 2, 3}, 1}]
```

```
PermWeight::def : Object φ3 defined
```

```
SetSymmetric[tp3[la, lb, lc]]
```

```
PermWeight::sym : Symmetries of φ3 assigned
```

$\phi_4^{abcd} = \frac{\partial^4 \phi}{\partial \eta_a \partial \eta_b \partial \eta_c \partial \eta_d} \Big|_0$  is the fourth derivative of the potential function  $\phi(\eta)$  at the origin  $\eta=0$ .

```
DefineTensor[tp4, "φ4", {{1, 2, 3, 4}, 1}]
```

```
PermWeight::def : Object φ4 defined
```

```
SetSymmetric[tp4[la, lb, lc, ld]]
```

```
PermWeight::sym : Symmetries of φ4 assigned
```

## ■ "logdensityy"

```
logdensityy =
```

$$\begin{aligned}
& - (\dim * \text{Log}[2 * \text{Pi}]) / 2 - (\text{ry}[11] * \text{ry}[u1]) / 2 + \text{ry}[11] * \text{se}[u1] - (\text{se}[11] * \text{se}[u1]) / 2 + \\
& (\text{o} * \text{ry}[11] * \text{tp3}[12, u1, u2]) / 2 - (\text{o} * \text{ry}[11] * \text{ry}[12] * \text{ry}[13] * \text{tp3}[u1, u2, u3]) / 6 + \\
& (\text{o} * \text{ry}[11] * \text{se}[12] * \text{se}[13] * \text{tp3}[u1, u2, u3]) / 2 - \\
& (\text{o} * \text{se}[11] * \text{se}[12] * \text{se}[13] * \text{tp3}[u1, u2, u3]) / 3 + \\
& (\text{o}^2 * \text{tp3}[11, 12, 13] * \text{tp3}[u1, u2, u3]) / 6 - \\
& (\text{o}^2 * \text{ry}[11] * \text{ry}[12] * \text{tp3}[13, 14, u1] * \text{tp3}[u2, u3, u4]) / 4 - \\
& (\text{o}^2 * \text{tp4}[11, 12, u1, u2]) / 8 + (\text{o}^2 * \text{ry}[11] * \text{ry}[12] * \text{tp4}[13, u1, u2, u3]) / 4 - \\
& (\text{o}^2 * \text{ry}[11] * \text{ry}[12] * \text{ry}[13] * \text{ry}[14] * \text{tp4}[u1, u2, u3, u4]) / 24 + \\
& (\text{o}^2 * \text{ry}[11] * \text{se}[12] * \text{se}[13] * \text{se}[14] * \text{tp4}[u1, u2, u3, u4]) / 6 - \\
& (\text{o}^2 * \text{se}[11] * \text{se}[12] * \text{se}[13] * \text{se}[14] * \text{tp4}[u1, u2, u3, u4]) / 8 \\
& - \frac{1}{2} \dim \text{Log}[2 \pi] - \frac{1}{2} (Y_p) (Y^p) + (Y_p) (\eta^p) - \frac{1}{2} (\eta_p) (\eta^p) + \\
& \frac{1}{2} \circ (Y_p) (\phi_{3_q}^{pq}) - \frac{1}{6} \circ (Y_p) (Y_q) (Y_r) (\phi_{3^{pqr}}) + \frac{1}{2} \circ (Y_p) (\eta_q) (\eta_r) (\phi_{3^{pqr}}) - \\
& \frac{1}{3} \circ (\eta_p) (\eta_q) (\eta_r) (\phi_{3^{pqr}}) + \frac{1}{6} \circ^2 (\phi_{3_{pq}}) (\phi_{3^{pqr}}) - \frac{1}{4} \circ^2 (Y_p) (Y_q) (\phi_{3_{rs}^p}) (\phi_{3^{qrs}}) - \\
& \frac{1}{8} \circ^2 (\phi_{4_{pq}}^{pq}) + \frac{1}{4} \circ^2 (Y_p) (Y_q) (\phi_{4_r}^{pqr}) - \frac{1}{24} \circ^2 (Y_p) (Y_q) (Y_r) (Y_s) (\phi_{4^{pqrs}}) + \\
& \frac{1}{6} \circ^2 (Y_p) (\eta_q) (\eta_r) (\eta_s) (\phi_{4^{pqrs}}) - \frac{1}{8} \circ^2 (\eta_p) (\eta_q) (\eta_r) (\eta_s) (\phi_{4^{pqrs}})
\end{aligned}$$

## ■ "phi2eta"

$$\text{phi2eta} = \text{Kdelta}[\text{ua}, \text{ub}] + \text{o} * \text{se}[11] * \text{tp3}[\text{u1}, \text{ua}, \text{ub}] + (\text{o}^2 * \text{se}[11] * \text{se}[12] * \text{tp4}[\text{u1}, \text{u2}, \text{ua}, \text{ub}]) / 2$$

$$\text{Kdelta}^{\text{ab}} + \text{o}(\eta_p)(\phi_3^{\text{pab}}) + \frac{1}{2} \text{o}^2(\eta_p)(\eta_q)(\phi_4^{\text{pqab}})$$

## ■ Tube-coordinates

First, the expression of the surface is specified in the Taylor series. Then, the tangent vectors and the normal vector are obtained. The tube-coordinates (u,v) are defined and used instead of the  $\eta$ -parametrization. Here u is dim-1 dimensional vector specifying a point on the surface, and v is the signed distance. The density function  $f(u, v | v_0)$  is obtained from  $f(y | \eta)$ , where the parameter value is specified as  $\eta = (0, \dots, 0, v_0)$  without losing the generality.

### ■ preliminary

Some functions and tensors are defined here.

### ■ indices

Here the dimension of the space is denoted by "9" for the index, whereas it is denoted by "dim" for the regular number. type-a index may run from 1 to 8, although it is not used explicitly, but only assumes type-a index cannot be 9.

```
AddIndexTypes
```

### ■ simplification functions

type-a index cannot be "9".

```
RuleUnique[rulekdelta1, Kdelta[a_, 9], 0, IndexaQ[a]]
```

```
RuleUnique[rulekdelta2, Kdelta[a_, -9], 0, IndexaQ[a]]
```

using the above fact.

```
tsimp[exp_] :=
  CanAll[AbsorbKdelta[CanAll[ApplyRules[exp, {rulekdelta1, rulekdelta2}]]]]];
```

raising -9 to 9 for a unique expression.

```
ruletps9 =
  {tp3[-9, 11_, 12_] → tp3[9, 11, 12], tp4[-9, 11_, 12_, 13_] → tp4[9, 11, 12, 13]};
```

further simplification

```
tsimpp[exp_] := Tsimplify[
  CanAll[AbsorbKdelta[CanAll[ApplyRules[exp /. ruletps9 /. ruletps9 /. ruletps9 /.
    ruletps9, {rulekdelta1, rulekdelta2}]]]]];
```

Ignore  $O(n^{-3/2})$  terms for scalar

```
geto2[exp_] := Sum[Simplify[Coefficient[exp, o, i]] oi, {i, -1, 2}]
```

Ignore  $O(n^{-3/2})$  terms for tensor.

```
tgeto2[exp_] := Sum[tsimp[Coefficient[exp, o, i]] oi, {i, -1, 2}]
```

Series expansion for scalar ignoring  $O(n^{-3/2})$  terms.

```
gets2[exp_] := geto2[Series[exp, {o, 0, 2}]]
```

Series expansion for tensor ignoring  $O(n^{-3/2})$  terms.

```
tgetrule[tx_] := Module[{coefs, coef0, coef1, coef2, rule0, rule1, rule2},
  coefs = CoefficientList[tx, o]; RuleUnique[rule0, coef0, coefs[[1]]];
  RuleUnique[rule1, coef1, coefs[[2]]]; RuleUnique[rule2, coef2, coefs[[3]]];
  {{coef0, coef1, coef2}, {rule0, rule1, rule2}}]

tgets2[exp_, x_, tx_] := Module[{xcoef, xrule}, {xcoef, xrule} = tgetrule[tx];
  ApplyRules[gets2[exp /. {x → Sum[xcoef[[i]] oi-1, {i, 3}}], xrule]]

tgets2[exp_, x_, tx_, y_, ty_] := Module[{xcoef, xrule, ycoef, yrule},
  {xcoef, xrule} = tgetrule[tx]; {ycoef, yrule} = tgetrule[ty]; ApplyRules[
  gets2[exp /. {x → Sum[xcoef[[i]] oi-1, {i, 3}], y → Sum[ycoef[[i]] oi-1, {i, 3}}],
  Join[xrule, yrule]]]
```

Define an operator to separate the regular index into the type-a index and dim.

```
sepa[foo_, l_] := Module[{aup, alo},
  UpLoa[{aup}, {alo}]; MakeSumRange[foo, {l, alo, -9}]];
```

Define differential operator (for type-a index)

```
difa[exp_, ru_, ala_] := (exp - (exp /. {ru[al_] → 0})) /.
  {ru[al1_] ru[al2_] ru[al3_] ru[al4_] → ru[al1] ru[al2] ru[al3] Kdelta[al4, ala] +
  ru[al1] ru[al2] ru[al4] Kdelta[al3, ala] + ru[al1] ru[al4] ru[al3]
  Kdelta[al2, ala] + ru[al4] ru[al2] ru[al3] Kdelta[al1, ala],
  ru[al1_] ru[al2_] ru[al3_] → ru[al1] ru[al2] Kdelta[al3, ala] +
  ru[al1] ru[al3] Kdelta[al2, ala] + ru[al2] ru[al3] Kdelta[al1, ala],
  ru[al1_] ru[al2_] → ru[al1] Kdelta[al2, ala] + ru[al2] Kdelta[al1, ala],
  ru[al1_] → Kdelta[al1, ala]}
```

## ■ define tensors

$u = (u_1, \dots, u_{\dim-1})$  is the parametrization of the surface. Type-a index indicate the suffix such as  $u = (u_{b'})$ , where  $b' = 1, \dots, \dim - 1$ .

```
DefineTensor[ru, "u", {{1}, 1}]
PermWeight::def : Object u defined
```

$d^{a'b'} = O(n^{-1/2})$  is the curvature matrix (second derivative) of the surface at the origin.

```
DefineTensor[td, "d", {{2, 1}, 1}]
PermWeight::sym : Symmetries of d assigned
PermWeight::def : Object d defined
```

$e^{a'b'c'} = O(n^{-1})$  is the third derivative at the origin.

```
DefineTensor[te, "e", {{1, 2, 3}, 1}]
PermWeight::def : Object e defined
SetSymmetric[te[la, lb, lc]]
PermWeight::sym : Symmetries of e assigned
```

$B_b^{a'} = \frac{\partial \eta_b}{\partial u_{a'}}$ ,  $b=1, \dots, \text{dim}$  is the tangent vector for  $a'=1, \dots, \text{dim}-1$ . Here the regular type index runs  $1, \dots, \text{dim}$ , whereas the type-a index runs  $1, \dots, \text{dim}-1$ .

```
DefineTensor[tB, "B", {{1, 2}, 1}]
PermWeight::def : Object B defined
tB[lb, aua]
B_b^{a'}
```

$\phi^{a'b'}(u) = \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta(u)} B_p^{a'}(u) B_q^{b'}(u)$  is the metric in the tangent space.

```
DefineTensor[tpa, "phi", {{2, 1}, 1}]
PermWeight::sym : Symmetries of phi assigned
PermWeight::def : Object phi defined
```

## ■ the coordinates around the smooth surface

The surface is specified by  $\eta_{b'}(u) = u_{b'}$ ,  $b' = 1, \dots, \text{dim} - 1$  and  $\eta_{\text{dim}}(u) = -d^{a'b'} u_{a'} u_{b'} - e^{a'b'c'} u_{a'} u_{b'} u_{c'}$ . They are stored in "foo1" and "foo2" or corresponding "rule1" and "rule2". The region of interest is specified by  $\eta_{\text{dim}} \leq \eta_{\text{dim}}(u)$ . The tangent vectors are given by  $\text{foo3} = B_{b'}^{a'} = \frac{\partial \eta_{b'}}{\partial u_{a'}}$  and  $\text{foo4} = B_{\text{dim}}^{a'} = \frac{\partial \eta_{\text{dim}}}{\partial u_{a'}}$ , or corresponding "rule3" and "rule4". We also obtain  $\text{phi2bu} = \phi^{a'b'}(u) = \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta(u)} B_p^{a'}(u) B_q^{b'}(u)$ , which is the metric in the tangent space. The elements of the normal vector are denoted as  $B_a^{\text{dim}}$ ,  $a=1, \dots, \text{dim}$ , which are given in  $\text{foo15} = B_a^{\text{dim}}(u)$  and  $\text{foo16} = B_{\text{dim}}^{\text{dim}}(u)$ , or in the corresponding "rule15" and "rule16". The reparametrization between  $\eta$ -coordinates and  $(u,v)$ -coordinates are specified by  $\eta_a(u, v) = \eta_a(u) + B_a^{\text{dim}}(u) v$ , and given in  $\text{foo21} = \eta_a(u, v)$  and  $\text{foo22} = \eta_{\text{dim}}(u, v)$ , or in "rule21", "rule22", and "rule22b".

## ■ smooth surface

Define rules for the surface.

```
RuleUnique[rule1, se[ala_], Kdelta[ala, aub] ru[alb], IndexaQ[ala]]
RuleUnique[rule2, se[-9],
-o td[aua, aub] ru[ala] ru[alb] - o^2 te[aua, aub, auc] ru[ala] ru[alb] ru[alc]]
```

$$\eta_{b'}(u) = u_{b'}, b' = 1, \dots, \text{dim} - 1$$

```
foo1 = ApplyRules[se[alb], {rule1, rule2}]
(Kdelta_{b',p'}) (u_{p'})
```

$$\eta_{\text{dim}}(u) = -d^{a'b'} u_a' u_{b'} - e^{a'b'c'} u_a' u_{b'} u_{c'}$$

```
foo2 = ApplyRules[se[-9], {rule1, rule2}]
-o (u_{p'}) (u_{q'}) (d^{p'q'}) - o^2 (u_{p'}) (u_{q'}) (u_{r'}) (e^{p'q'r'})
```

### ■ tangent vectors

$$B_{b'}^{a'} = \frac{\partial \eta_{b'}}{\partial u_a'}$$

```
foo3 = tsimp[difa[foo1, ru, aua]]
Kdelta_{b',a'}
```

$$B_{\text{dim}}^{a'} = \frac{\partial \eta_{\text{dim}}}{\partial u_a'}$$

```
foo4 = tsimp[difa[foo2, ru, aua]]
-2 o (u_{p'}) (d^{p'a'}) - 3 o^2 (u_{p'}) (u_{q'}) (e^{p'q'a'})
```

Define rules for the tangent vectors.

```
RuleUnique[rule3, tB[alb_, aua_], foo3, IndexaQ[alb] ^ IndexaQ[aua]]
RuleUnique[rule4, tB[-9, aua_], foo4, IndexaQ[aua]]
```

check if they work

```
ApplyRules[tB[alb, aua], {rule3, rule4}]
Kdelta_{b',a'}
ApplyRules[tB[-9, aua], {rule3, rule4}]
-2 o (u_{p'}) (d^{p'a'}) - 3 o^2 (u_{p'}) (u_{q'}) (e^{p'q'a'})
```

Next, we will calculate  $\phi^{a'b'}(u) = \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta(u)} B_p^{a'}(u) B_q^{b'}(u)$  below.

Apply the separate operator to  $\text{phi2eta} = \frac{\partial^2 \phi(\eta)}{\partial \eta_a \partial \eta_b}$ , and evaluate it on the surface to get  $\text{phi2u} = \frac{\partial^2 \phi(\eta)}{\partial \eta_a \partial \eta_b} \Big|_{\eta(u)}$ .

**phi2eta**

$$Kdelta^{ab} + o(\eta_p) (\phi_3^{pab}) + \frac{1}{2} o^2(\eta_p) (\eta_q) (\phi_4^{pqab})$$

```
tsimp[sepa[sepa[phi2eta, 11], 12]]
```

$$Kdelta^{ab} + o(\eta_9) (\phi_3^{9ab}) + o(\eta_{p'}) (\phi_3^{p'ab}) + \frac{1}{2} o^2(\eta_9)^2 (\phi_4^{99ab}) + o^2(\eta_9) (\eta_{p'}) (\phi_4^{9p'ab}) + \frac{1}{2} o^2(\eta_{p'}) (\eta_{q'}) (\phi_4^{p'q'ab})$$



**phi2u = tgeto2[ApplyRules[%, {rule1, rule2}]]**

$$Kdelta^{ab} + o(u_{p'}) (\phi 3^{p'ab}) + o^2 \left( - (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{9ab}) + \frac{1}{2} (u_{p'}) (u_{q'}) (\phi 4^{p'q'ab}) \right)$$

Using phi2u above, we write phi2bu =  $\phi^{a'b'}(u) = \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta(u)} B_p^a(u) B_q^{b'}(u)$  as follows. First, the summation range of phi2bu is separated into type-a and dim. Then,  $B_p^a(u)$  are substituted by their expressions.

**phi2u tB[1a, aua] tB[1b, aub]**

$$(B_a^{a'}) (B_b^{b'}) \left( Kdelta^{ab} + o(u_{p'}) (\phi 3^{p'ab}) + o^2 \left( - (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{9ab}) + \frac{1}{2} (u_{p'}) (u_{q'}) (\phi 4^{p'q'ab}) \right) \right)$$

**CanAll[sepa[sepa[%, 1a], 1b]]**

$$\begin{aligned} & (B_9^{a'}) (B_9^{b'}) + (Kdelta^{9p'}) (B_9^{b'}) (B_{p'}^{a'}) + (Kdelta^{9p'}) (B_9^{a'}) (B_{p'}^{b'}) + \\ & (Kdelta^{p'q'}) (B_{p'}^{a'}) (B_{q'}^{b'}) - o^2 (u_{p'}) (u_{q'}) (B_9^{a'}) (B_9^{b'}) (d^{p'q'}) (\phi 3^{999}) + \\ & o(u_{p'}) (B_9^{a'}) (B_9^{b'}) (\phi 3^{99p'}) - o^2 (u_{p'}) (u_{q'}) (B_9^{b'}) (B_{r'}^{a'}) (d^{p'q'}) (\phi 3^{99r'}) - \\ & o^2 (u_{p'}) (u_{q'}) (B_9^{a'}) (B_{r'}^{b'}) (d^{p'q'}) (\phi 3^{99r'}) + o(u_{p'}) (B_9^{b'}) (B_{q'}^{a'}) (\phi 3^{9p'q'}) + \\ & o(u_{p'}) (B_9^{a'}) (B_{q'}^{b'}) (\phi 3^{9p'q'}) - o^2 (u_{p'}) (u_{q'}) (B_{r'}^{a'}) (B_s^{b'}) (d^{p'q'}) (\phi 3^{9r's'}) + \\ & o(u_{p'}) (B_{q'}^{a'}) (B_{r'}^{b'}) (\phi 3^{p'q'r'}) + \frac{1}{2} o^2 (u_{p'}) (u_{q'}) (B_9^{a'}) (B_9^{b'}) (\phi 4^{99p'q'}) + \\ & \frac{1}{2} o^2 (u_{p'}) (u_{q'}) (B_9^{b'}) (B_{r'}^{a'}) (\phi 4^{9p'q'r'}) + \\ & \frac{1}{2} o^2 (u_{p'}) (u_{q'}) (B_9^{a'}) (B_{r'}^{b'}) (\phi 4^{9p'q'r'}) + \frac{1}{2} o^2 (u_{p'}) (u_{q'}) (B_{r'}^{a'}) (B_s^{b'}) (\phi 4^{p'q'r's'}) \end{aligned}$$

**phi2bu = tgeto2[ApplyRules[%, {rule3, rule4}]]**

$$\begin{aligned} & Kdelta^{a'b'} + o(u_{p'}) (\phi 3^{p'a'b'}) + o^2 \\ & \left( 4 (u_{p'}) (u_{q'}) (d^{p'a'}) (d^{q'b'}) - 2 (u_{p'}) (u_{q'}) (d^{q'b'}) (\phi 3^{9p'a'}) - 2 (u_{p'}) (u_{q'}) (d^{q'a'}) (\phi 3^{9p'b'}) - \right. \\ & \left. (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{9a'b'}) + \frac{1}{2} (u_{p'}) (u_{q'}) (\phi 4^{p'q'a'b'}) \right) \end{aligned}$$

We may symmetrize the coefficients of phi2bu.

**phi2bucoef = Simplify[CoefficientList[phi2bu /. {ru[all\_] -> x}, x] / {1, o, o^2}] / .  
{au1 -> auc, au2 -> aud}**

$$\left\{ Kdelta^{a'b'}, \phi 3^{a'b'c'}, \frac{1}{2} (8 (d^{a'c'}) (d^{b'd'}) - 2 (d^{c'd'}) (\phi 3^{9a'b'}) - 4 (d^{b'd'}) (\phi 3^{9a'c'}) - 4 (d^{a'd'}) (\phi 3^{9b'c'}) + \phi 4^{a'b'c'd'}) \right\}$$

**phi2bucoef[[3]] =**

**tsimp[Symmetrize[Symmetrize[phi2bucoef[[3]], {aua, aub}], {auc, aud}]]**

$$\begin{aligned} & 2 (d^{a'd'}) (d^{b'c'}) + 2 (d^{a'c'}) (d^{b'd'}) - (d^{c'd'}) (\phi 3^{9a'b'}) - (d^{b'd'}) (\phi 3^{9a'c'}) - \\ & (d^{b'c'}) (\phi 3^{9a'd'}) - (d^{a'd'}) (\phi 3^{9b'c'}) - (d^{a'c'}) (\phi 3^{9b'd'}) + \frac{1}{2} (\phi 4^{a'b'c'd'}) \end{aligned}$$

**phi2bu =**

**phi2bucoef[[1]] + o phi2bucoef[[2]] ru[alc] + o^2 phi2bucoef[[3]] ru[alc] ru[ald]**

$$\begin{aligned} & Kdelta^{a'b'} + o(u_{c'}) (\phi 3^{a'b'c'}) + \\ & o^2 (u_{c'}) (u_{d'}) \left( 2 (d^{a'd'}) (d^{b'c'}) + 2 (d^{a'c'}) (d^{b'd'}) - (d^{c'd'}) (\phi 3^{9a'b'}) - (d^{b'd'}) (\phi 3^{9a'c'}) - \right. \\ & \left. (d^{b'c'}) (\phi 3^{9a'd'}) - (d^{a'd'}) (\phi 3^{9b'c'}) - (d^{a'c'}) (\phi 3^{9b'd'}) + \frac{1}{2} (\phi 4^{a'b'c'd'}) \right) \end{aligned}$$

Further simplification is possible. Here the phi2bu is essentially the same as above although the warning messages appear.

```
tsimpp[phi2bu]
```

```
The assigned symmetries may be inconsistent.
```

```
The assigned symmetries may be inconsistent.
```

```
The assigned symmetries may be inconsistent.
```

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The assigned symmetries may be inconsistent.
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The assigned symmetries may be inconsistent.
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The assigned symmetries may be inconsistent.
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The assigned symmetries may be inconsistent.
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The assigned symmetries may be inconsistent.
```

```
The assigned symmetries may be inconsistent.
```

$$K\delta a^{a'b'} + 4 o^2 (u_{p'}) (u_{q'}) (d^{p'b'}) (d^{q'a'}) - 2 o^2 (u_{p'}) (u_{q'}) (d^{q'b'}) (\phi 3^{9p'a'}) - 2 o^2 (u_{p'}) (u_{q'}) (d^{q'a'}) (\phi 3^{9p'b'}) - o^2 (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{9a'b'}) + o (u_{p'}) (\phi 3^{p'a'b'}) + \frac{1}{2} o^2 (u_{p'}) (u_{q'}) (\phi 4^{p'q'a'b'})$$

```
phi2bu = %;
```

■ the normal vector

The elements of the normal vector are denoted as  $B_a^{\dim}$ ,  $a=1,\dots,\dim$ . But for the moment, we use "norma" for  $B_a^{\dim}$ , and "normb" for  $B_{\dim}^{\dim}$ . First of all, we assume the following expressions of these values using unknown na2, na3, nb2, nb3.

```
DefineTensor[tna2, "na2", {{1, 2}, 1}]
```

```
PermWeight::def : Object na2 defined
```

```
DefineTensor[tna3, "na3", {{1, 3, 2}, 1}]
```

```
PermWeight::sym : Symmetries of na3 assigned
```

```
PermWeight::def : Object na3 defined
```

```
norma = o tna2[ala, aub] ru[alb] + o^2 tna3[ala, aub, auc] ru[alb] ru[alc]
```

```
o (u_{b'}) (na2_{a'}^{b'}) + o^2 (u_{b'}) (u_{c'}) (na3_{a'}^{b'c'})
```

```
RuleUnique[rule5, tB[ala_, 9], norma, IndexaQ[ala]]
```

**DefineTensor[tnb1, "nb1", {{1}, 1}]**

PermWeight::def : Object nb1 defined

**DefineTensor[tnb2, "nb2", {{2}, 1, 1}]**

PermWeight::sym : Symmetries of nb2 assigned

PermWeight::def : Object nb2 defined

**normb = 1 + o tnb1[aub] ru[alb] + o<sup>2</sup> tnb2[aub, auc] ru[alb] ru[alc]**

$1 + o(u_{b'}) (nb1^{b'}) + o^2(u_{b'}) (u_{c'}) (nb2^{b'c'})$

**RuleUnique[rule6, tB[-9, 9], normb]**

The inner product of the normal vector  $B_a^{\dim}$  and a tangent vector  $B_a^{a'}$  is  $foo7 = \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta(u)} B_p^{a'}(u) B_q^{\dim}(u)$ .

**phi2u tB[1a, aua] tB[1b, 9]**

$(B_a^{a'}) (B_b^9)$   
 $\left( Kdelta^{ab} + o(u_{p'}) (\phi3^{p'ab}) + o^2 \left( - (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi3^{9ab}) + \frac{1}{2} (u_{p'}) (u_{q'}) (\phi4^{p'q'ab}) \right) \right)$

**CanAll[sepa[sepa[%, 1a], 1b]]**

$(B_9^9) (B_9^{a'}) + (Kdelta^{9p'}) (B_9^{a'}) (B_p^9) + (Kdelta^{9p'}) (B_9^9) (B_p^{a'}) +$   
 $(Kdelta^{p'q'}) (B_p^{a'}) (B_q^9) - o^2(u_{p'}) (u_{q'}) (B_9^9) (B_9^{a'}) (d^{p'q'}) (\phi3^{999}) +$   
 $o(u_{p'}) (B_9^9) (B_9^{a'}) (\phi3^{99p'}) - o^2(u_{p'}) (u_{q'}) (B_9^{a'}) (B_r^9) (d^{p'q'}) (\phi3^{99r'}) -$   
 $o^2(u_{p'}) (u_{q'}) (B_9^9) (B_r^{a'}) (d^{p'q'}) (\phi3^{99r'}) + o(u_{p'}) (B_9^{a'}) (B_q^9) (\phi3^{9p'q'}) +$   
 $o(u_{p'}) (B_9^9) (B_q^{a'}) (\phi3^{9p'q'}) - o^2(u_{p'}) (u_{q'}) (B_r^{a'}) (B_s^9) (d^{p'q'}) (\phi3^{9r's'}) +$   
 $o(u_{p'}) (B_q^{a'}) (B_r^9) (\phi3^{p'q'r'}) + \frac{1}{2} o^2(u_{p'}) (u_{q'}) (B_9^9) (B_9^{a'}) (\phi4^{99p'q'}) +$   
 $\frac{1}{2} o^2(u_{p'}) (u_{q'}) (B_9^{a'}) (B_r^9) (\phi4^{9p'q'r'}) +$   
 $\frac{1}{2} o^2(u_{p'}) (u_{q'}) (B_9^9) (B_r^{a'}) (\phi4^{9p'q'r'}) + \frac{1}{2} o^2(u_{p'}) (u_{q'}) (B_r^{a'}) (B_s^9) (\phi4^{p'q'r's'})$

**foo7 = tgeto2[ApplyRules[%, {rule3, rule4, rule5, rule6}]]**

$o(-2(u_{p'}) (d^{p'a'}) + (u_{p'}) (na2^{a'p'}) + (u_{p'}) (\phi3^{9p'a'})) +$   
 $o^2 \left( -3(u_{p'}) (u_{q'}) (e^{p'q'a'}) + (u_{p'}) (u_{q'}) (na3^{a'p'q'}) - 2(u_{p'}) (u_{q'}) (d^{q'a'}) (nb1^{p'}) - \right.$   
 $2(u_{p'}) (u_{q'}) (d^{q'a'}) (\phi3^{99p'}) - (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi3^{99a'}) +$   
 $\left. (u_{p'}) (u_{q'}) (nb1^{q'}) (\phi3^{9p'a'}) + (u_{p'}) (u_{q'}) (na2_{r,q'}) (\phi3^{p'r'a'}) + \frac{1}{2} (u_{p'}) (u_{q'}) (\phi4^{9p'q'a'}) \right)$

The squared norm of the normal vector  $B_a^{\dim}$  is  $foo8 = \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta(u)} B_p^{\dim}(u) B_q^{\dim}(u)$ .

**phi2u tB[1a, 9] tB[1b, 9]**

$(B_a^9) (B_b^9)$   
 $\left( Kdelta^{ab} + o(u_{p'}) (\phi3^{p'ab}) + o^2 \left( - (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi3^{9ab}) + \frac{1}{2} (u_{p'}) (u_{q'}) (\phi4^{p'q'ab}) \right) \right)$

**CanAll[sepa[sepa[%, la], lb]]**

$$\begin{aligned} & (B_9^9)^2 + 2 (Kdelta^{9p'}) (B_9^9) (B_p^9) + \\ & (Kdelta^{p'q'}) (B_p^9) (B_q^9) - o^2 (u_p') (u_q') (B_9^9)^2 (d^{p'q'}) (\phi_3^{999}) + \\ & o (u_p') (B_9^9)^2 (\phi_3^{99p'}) - 2 o^2 (u_p') (u_q') (B_9^9) (B_r^9) (d^{p'q'}) (\phi_3^{99r'}) + \\ & 2 o (u_p') (B_9^9) (B_q^9) (\phi_3^{9p'q'}) - o^2 (u_p') (u_q') (B_r^9) (B_s^9) (d^{p'q'}) (\phi_3^{9r's'}) + \\ & o (u_p') (B_q^9) (B_r^9) (\phi_3^{p'q'r'}) + \frac{1}{2} o^2 (u_p') (u_q') (B_9^9)^2 (\phi_4^{99p'q'}) + \\ & o^2 (u_p') (u_q') (B_9^9) (B_r^9) (\phi_4^{9p'q'r'}) + \frac{1}{2} o^2 (u_p') (u_q') (B_r^9) (B_s^9) (\phi_4^{p'q'r's'}) \end{aligned}$$

**foo8 = tgeto2[ApplyRules[%, {rule3, rule4, rule5, rule6}]]**

$$\begin{aligned} & 1 + o (2 (u_p') (nb1^{p'}) + (u_p') (\phi_3^{99p'})) + \\ & o^2 \left( (u_p') (u_q') (na2_{r,q'}) (na2^{r'p'}) + (u_p') (u_q') (nb1^{p'}) (nb1^{q'}) + \right. \\ & \quad 2 (u_p') (u_q') (nb2^{p'q'}) - (u_p') (u_q') (d^{p'q'}) (\phi_3^{999}) + 2 (u_p') (u_q') (nb1^{q'}) (\phi_3^{99p'}) + \\ & \quad \left. 2 (u_p') (u_q') (na2_{r,q'}) (\phi_3^{9p'r'}) + \frac{1}{2} (u_p') (u_q') (\phi_4^{99p'q'}) \right) \end{aligned}$$

Now, we will solve na2, na3, nb2, nb3 from the equations foo7==0, foo8==1. First we get the coefficients in foo7 and foo8, and relabel nonfree indexes.

**foo9 =**

$$\begin{aligned} & \text{Simplify[CoefficientList[foo7 /. {ru[al_] \to x}, x] / {1, o, o^2}] /. {au1 \to aub, au2 \to auc}] \\ & \{0, -2 (d^{a'b'}) + na2^{a'b'} + \phi_3^{9a'b'}, -3 (e^{a'b'c'}) + na3^{a'b'c'} - 2 (d^{a'c'}) (nb1^{b'}) - (d^{b'c'}) (\phi_3^{99a'}) - \\ & \quad 2 (d^{a'c'}) (\phi_3^{99b'}) + (nb1^{c'}) (\phi_3^{9a'b'}) + (na2_{r,c'}) (\phi_3^{r'a'b'}) + \frac{1}{2} (\phi_4^{9a'b'c'}) \} \end{aligned}$$

**foo10 = Simplify[CoefficientList[foo8 - 1 /. {ru[al\_] \to x}, x] / {1, o, o^2}] /. {au1 \to aub, au2 \to auc}**

$$\begin{aligned} & \{0, 2 (nb1^{b'}) + \phi_3^{99b'}, (nb1^{b'}) (nb1^{c'}) + 2 (nb2^{b'c'}) - (d^{b'c'}) (\phi_3^{999}) + \\ & \quad 2 (nb1^{c'}) (\phi_3^{99b'}) + (na2_{r,c'}) (na2^{r'b'}) + 2 (\phi_3^{9r'b'}) + \frac{1}{2} (\phi_4^{99b'c'}) \} \end{aligned}$$

**ao0 = Solve[foo9[[2]] == 0, tna2[aua, aub]]**

$$\{\{na2^{a'b'} \to 2 (d^{a'b'}) - \phi_3^{9a'b'}\}\}$$

**RuleUnique[rule11, tna2[aua\_, aub\_], ao0[[1, 1, 2]], IndexaQ[aua] \wedge IndexaQ[aub]]**

**ao0 = Solve[foo10[[2]] == 0, tnb1[aub]]**

$$\{\{nb1^{b'} \to -\frac{1}{2} (\phi_3^{99b'})\}\}$$

**RuleUnique[rule12, tnb1[aub\_], ao0[[1, 1, 2]], IndexaQ[aub]]**

**ao0 = Solve[ApplyRules[foo9[[3]], {rule11, rule12}] == 0, tna3[aua, aub, auc]]**

$$\begin{aligned} & \{\{na3^{a'b'c'} \to 3 (e^{a'b'c'}) + (d^{b'c'}) (\phi_3^{99a'}) + (d^{a'c'}) (\phi_3^{99b'}) + \\ & \quad \frac{1}{2} (\phi_3^{99c'}) (\phi_3^{9a'b'}) - 2 (d_{p,c'}) (\phi_3^{p'a'b'}) + (\phi_3^{9p,c'}) (\phi_3^{p'a'b'}) - \frac{1}{2} (\phi_4^{9a'b'c'})\}\}\} \end{aligned}$$

```

ao2 = tsimp[Symmetrize[ao[[1, 1, 2]], {aub, auc}]]
3 (ea'b'c') + (db'c') (φ399a') +  $\frac{1}{2}$  (da'c') (φ399b') +  $\frac{1}{2}$  (da'b') (φ399c') +
 $\frac{1}{4}$  (φ399c') (φ399a'b') +  $\frac{1}{4}$  (φ399b') (φ399a'c') - (dp,c') (φ3p'a'b') +
 $\frac{1}{2}$  (φ39p,c') (φ3p'a'b') - (dp,b') (φ3p'a'c') +  $\frac{1}{2}$  (φ39p,b') (φ3p'a'c') -  $\frac{1}{2}$  (φ499a'b'c')

RuleUnique[rule13, tna3[aua_, aub_, auc_],
ao2, IndexaQ[aua] ^ IndexaQ[aub] ^ IndexaQ[auc]]

ao = Solve[ApplyRules[foo10[[3]], {rule11, rule12, rule13}] = 0, tnb2[aub, auc]]
{ {nb2b'c' →  $\frac{1}{2}$  ( -4 (dp,c') (dp'b') + (db'c') (φ3999) +  $\frac{3}{4}$  (φ399b') (φ399c') +
2 (dp'b') (φ39p,c') - 2 (dp,c') (φ39p'b') + (φ39p,c') (φ39p'b') -  $\frac{1}{2}$  (φ499b'c')) } }

ao2 = tsimp[Symmetrize[ao[[1, 1, 2]], {aub, auc}]]
- (dp,c') (dp'b') - (dp,b') (dp'c') +  $\frac{1}{2}$  (db'c') (φ3999) +  $\frac{3}{8}$  (φ399b') (φ399c') +
 $\frac{1}{2}$  (dp'c') (φ39p,b') +  $\frac{1}{2}$  (dp'b') (φ39p,c') -  $\frac{1}{2}$  (dp,c') (φ39p'b') +
 $\frac{1}{4}$  (φ39p,c') (φ39p'b') -  $\frac{1}{2}$  (dp,b') (φ39p'c') +  $\frac{1}{4}$  (φ39p,b') (φ39p'c') -  $\frac{1}{4}$  (φ499b'c')

ao2 = tsimpp[%]
-2 (dp,c') (dp'b') +  $\frac{1}{2}$  (db'c') (φ3999) +
 $\frac{3}{8}$  (φ399b') (φ399c') +  $\frac{1}{2}$  (φ39p,c') (φ39p'b') -  $\frac{1}{4}$  (φ499b'c')

RuleUnique[rule14, tnb2[aub_, auc_], ao2, IndexaQ[aub] ^ IndexaQ[auc]]

ApplyRules[tnb2[aua, aub], rule14]
-2 (dp,b') (dp'a') +  $\frac{1}{2}$  (da'b') (φ3999) +
 $\frac{3}{8}$  (φ399a') (φ399b') +  $\frac{1}{2}$  (φ39p,b') (φ39p'a') -  $\frac{1}{4}$  (φ499a'b')
    
```

We get  $foo15 = B_{a'}^{\dim}(u)$  and  $foo16 = B_{\dim}^{\dim}(u)$  below.

**norma**

$$o(u_{b'}) (na2_{a',b'}) + o^2(u_{b'}) (u_{c'}) (na3_{a',b'c'})$$

**foo15 = tgeto2[ApplyRules[norma, {rule11, rule12, rule13, rule14}]]**

$$\begin{aligned}
 & o(2(u_{p'}) (d_{a,p'}) - (u_{p'}) (φ^{3^{99a,p'}})) + \\
 & o^2 \left( 3(u_{p'}) (u_{q'}) (e_{a,p'q'}) + (u_{p'}) (u_{q'}) (d^{p'q'}) (φ^{3^{99a'}}) + \frac{1}{2} (u_{p'}) (u_{q'}) (d_{a,q'}) (φ^{3^{99p'}}) + \right. \\
 & \quad \frac{1}{2} (u_{p'}) (u_{q'}) (d_{a,p'}) (φ^{3^{99q'}}) + \frac{1}{4} (u_{p'}) (u_{q'}) (φ^{3^{99q'}}) (φ^{3^{99a,p'}}) + \\
 & \quad \frac{1}{4} (u_{p'}) (u_{q'}) (φ^{3^{99p'}}) (φ^{3^{99a,q'}}) - (u_{p'}) (u_{q'}) (d_{r,q'}) (φ^{3_{a,p'r'}}) + \\
 & \quad \frac{1}{2} (u_{p'}) (u_{q'}) (φ^{3_{r,q'}}) (φ^{3_{a,p'r'}}) - (u_{p'}) (u_{q'}) (d_{r,p'}) (φ^{3_{a,q'r'}}) + \\
 & \quad \left. \frac{1}{2} (u_{p'}) (u_{q'}) (φ^{3_{r,p'}}) (φ^{3_{a,q'r'}}) - \frac{1}{2} (u_{p'}) (u_{q'}) (φ^{4_{a,p'q'}}) \right)
 \end{aligned}$$

**foo15 = tsimpp[foo15]**

$$2 \circ (u_{p'}) (d_{a'}^{p'}) + 3 \circ^2 (u_{p'}) (u_{q'}) (e_{a'}^{p'q'}) + \circ^2 (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{99a'}) + \circ^2 (u_{p'}) (u_{q'}) (d_{a'}^{q'}) (\phi 3^{99p'}) - \circ (u_{p'}) (\phi 3^{9a'}^{p'}) + \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (\phi 3^{99q'}) (\phi 3^{9a'}^{p'}) - 2 \circ^2 (u_{p'}) (u_{q'}) (d_{r'}^{q'}) (\phi 3_{a'}^{p'r'}) + \circ^2 (u_{p'}) (u_{q'}) (\phi 3_{r'}^{9q'}) (\phi 3_{a'}^{p'r'}) - \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (\phi 4_{a'}^{9p'q'})$$

**RuleUnique[rule15, tB[ala\_, 9], foo15, IndexaQ[ala]]**

**ApplyRules[tB[ala, 9], rule15]**

$$2 \circ (u_{p'}) (d_{a'}^{p'}) + 3 \circ^2 (u_{p'}) (u_{q'}) (e_{a'}^{p'q'}) + \circ^2 (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{99a'}) + \circ^2 (u_{p'}) (u_{q'}) (d_{a'}^{q'}) (\phi 3^{99p'}) - \circ (u_{p'}) (\phi 3^{9a'}^{p'}) + \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (\phi 3^{99q'}) (\phi 3^{9a'}^{p'}) - 2 \circ^2 (u_{p'}) (u_{q'}) (d_{r'}^{q'}) (\phi 3_{a'}^{p'r'}) + \circ^2 (u_{p'}) (u_{q'}) (\phi 3_{r'}^{9q'}) (\phi 3_{a'}^{p'r'}) - \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (\phi 4_{a'}^{9p'q'})$$

**normb**

$$1 + \circ (u_{b'}) (nb1^{b'}) + \circ^2 (u_{b'}) (u_{c'}) (nb2^{b'c'})$$

**foo16 = tgeto2[ApplyRules[normb, {rule11, rule12, rule13, rule14}]]**

$$1 - \frac{1}{2} \circ (u_{p'}) (\phi 3^{99p'}) + \circ^2 \left( -2 (u_{p'}) (u_{q'}) (d_{r'}^{q'}) (d^{p'r'}) + \frac{1}{2} (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{999}) + \frac{3}{8} (u_{p'}) (u_{q'}) (\phi 3^{99p'}) (\phi 3^{99q'}) + \frac{1}{2} (u_{p'}) (u_{q'}) (\phi 3_{r'}^{9q'}) (\phi 3^{9p'r'}) - \frac{1}{4} (u_{p'}) (u_{q'}) (\phi 4^{99p'q'}) \right)$$

**RuleUnique[rule16, tB[-9, 9], foo16]**

**ApplyRules[tB[-9, 9], rule16]**

$$1 - 2 \circ^2 (u_{p'}) (u_{q'}) (d_{r'}^{q'}) (d^{p'r'}) + \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{999}) - \frac{1}{2} \circ (u_{p'}) (\phi 3^{99p'}) + \frac{3}{8} \circ^2 (u_{p'}) (u_{q'}) (\phi 3^{99p'}) (\phi 3^{99q'}) + \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (\phi 3_{r'}^{9q'}) (\phi 3^{9p'r'}) - \frac{1}{4} \circ^2 (u_{p'}) (u_{q'}) (\phi 4^{99p'q'})$$

In the below, we confirm if the normal vector is orthogonal to the tangent vectors and if the length of the normal vector is 1.

The inner product of the normal vector  $B_a^{\dim}$  and a tangent vector  $B_a^{a'}$  is  $foo17 = \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta(u)} B_p^{a'}(u) B_q^{\dim}(u)$ .

**phi2u tB[la, aua] tB[lb, 9]**

$$(B_a^{a'}) (B_b^9) \left( Kdelta^{ab} + \circ (u_{p'}) (\phi 3^{p'ab}) + \circ^2 \left( - (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi 3^{9ab}) + \frac{1}{2} (u_{p'}) (u_{q'}) (\phi 4^{p'q'ab}) \right) \right)$$

**CanAll[sepa[sepa[%, la], lb]];**

**foo17 = tgeto2[ApplyRules[%, {rule3, rule4, rule15, rule16}]]**

0

The squared norm of the normal vector  $B_a^{\dim}$  is  $foo18 = \frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta(u)} B_p^{\dim}(u) B_q^{\dim}(u)$ .

```

phi2u tB[1a, 9] tB[1b, 9]
(Ba^9) (Bb^9)
(Kdelta^ab + o(u_p') (phi3^p'ab) + o^2 (- (u_p') (u_q') (d^p'q') (phi3^9ab) + 1/2 (u_p') (u_q') (phi4^p'q'ab)))

CanAll[sepa[sepa[%, 1a], 1b]];

foo18 = tgeto2[ApplyRules[%, {rule3, rule4, rule15, rule16}]]
1 + o^2 (-2 (u_p') (u_q') (d^p'r') (phi3^9_r,q') + 2 (u_p') (u_q') (d_r,q') (phi3^9_p'r'))

tsimpp[foo18]
1

```

### ■ (u,v)-coordinate system

foo20 =  $\eta_a(u, v) = \eta_a(u) + B_a^{\dim}(u) v$ .

```

foo20 = se[1a] + tB[1a, 9] v
eta_a + v (Ba^9)

```

foo21 =  $\eta_{a'}(u, v)$ .

```

foo21 = ApplyRules[foo20 /. {1a -> a1a}, {rule1, rule2, rule15, rule16}]
(Kdelta_a,p') (u_p') + 2 o v (u_p') (d_a,p') + 3 o^2 v (u_p') (u_q') (e_a,p'q') +
o^2 v (u_p') (u_q') (d^p'q') (phi3^9_a') + o^2 v (u_p') (u_q') (d_a,q') (phi3^9_p') - o v (u_p') (phi3^9_a,p') +
1/2 o^2 v (u_p') (u_q') (phi3^9_q') (phi3^9_a,p') - 2 o^2 v (u_p') (u_q') (d_r,q') (phi3_a,p'r') +
o^2 v (u_p') (u_q') (phi3^9_r,q') (phi3_a,p'r') - 1/2 o^2 v (u_p') (u_q') (phi4^9_a,p'q')

RuleUnique[rule21, se[a1a_], foo21, IndexaQ[a1a]]

```

foo22 =  $\eta_{\dim}(u, v)$ .

```

foo22 = ApplyRules[foo20 /. {1a -> -9}, {rule1, rule2, rule15, rule16}]
v - o (u_p') (u_q') (d^p'q') - 2 o^2 v (u_p') (u_q') (d_r,q') (d^p'r') - o^2 (u_p') (u_q') (u_r') (e^p'q'r') +
1/2 o^2 v (u_p') (u_q') (d^p'q') (phi3^9_q) - 1/2 o v (u_p') (phi3^9_p') + 3/8 o^2 v (u_p') (u_q') (phi3^9_p') (phi3^9_q') +
1/2 o^2 v (u_p') (u_q') (phi3^9_r,q') (phi3^9_p'r') - 1/4 o^2 v (u_p') (u_q') (phi4^9_p'q')

RuleUnique[rule22, se[-9], foo22]
RuleUnique[rule22b, se[9], foo22]

```

### ■ change of variables

The Jacobian of the change of variables  $\eta \leftrightarrow (u, v)$  is  $J = \det\left(\frac{\partial \eta(u, v)}{\partial (u, v)}\right)$ . The asymptotic expression of  $\log \det J$  is obtained up to  $O(n^{-1})$  term in "logdetJ". The density function  $f(u, v | v_0)$  is obtained from  $f(y | \eta)$  as shown in "logdensityuv", where the parameter value is specified as  $\eta = (0, \dots, 0, v_0)$ .

## ■ Jacobian

Here we will calculate the log of the Jacobian  $J = \det\left(\frac{\partial \eta_a(u,v)}{\partial(u,v)}\right)$ .

First, we obtain the expression of  $\begin{pmatrix} \frac{\partial \eta_a(u,v)}{\partial u_B} & \frac{\partial \eta_a(u,v)}{\partial v} \\ \frac{\partial \eta_{\text{dim}}(u,v)}{\partial u_B} & \frac{\partial \eta_{\text{dim}}(u,v)}{\partial v} \end{pmatrix} = \begin{pmatrix} \text{foo23} & \text{foo25} \\ \text{foo24} & \text{foo26} \end{pmatrix}$ .

$$\text{foo23} = \frac{\partial \eta_a(u,v)}{\partial u_B}$$

**foo23 = tsimp[difa[foo21, ru, aub]]**

$$\begin{aligned} & \text{Kdelta}_{a,b'} + 2 \circ v (d_{a,b'}) + 6 \circ^2 v (u_{p'}) (e_{a,p'b'}) + \\ & 2 \circ^2 v (u_{p'}) (d^{p'b'}) (\phi_{3^{99a'}}) + \circ^2 v (u_{p'}) (d_{a,b'}) (\phi_{3^{99p'}}) + \circ^2 v (u_{p'}) (d_{a,p'}) (\phi_{3^{99b'}}) + \\ & \frac{1}{2} \circ^2 v (u_{p'}) (\phi_{3^{99b'}}) (\phi_{3^{9a,p'}}) - \circ v (\phi_{3^{9a,b'}}) + \frac{1}{2} \circ^2 v (u_{p'}) (\phi_{3^{99p'}}) (\phi_{3^{9a,b'}}) - \\ & 2 \circ^2 v (u_{p'}) (d_{q,b'}) (\phi_{3_{a,p'q'}}) + \circ^2 v (u_{p'}) (\phi_{3_{q,b'}}) (\phi_{3_{a,p'q'}}) - \\ & 2 \circ^2 v (u_{p'}) (d_{q,p'}) (\phi_{3_{a,q'b'}}) + \circ^2 v (u_{p'}) (\phi_{3_{q,p'}}) (\phi_{3_{a,q'b'}}) - \circ^2 v (u_{p'}) (\phi_{4_{a,p'b'}}) \end{aligned}$$

$$\text{foo24} = \frac{\partial \eta_{\text{dim}}(u,v)}{\partial u_B}$$

**foo24 = tsimp[difa[foo22, ru, aub]]**

$$\begin{aligned} & -2 \circ^2 v (u_{p'}) (d_{q,b'}) (d^{p'q'}) - 2 \circ (u_{p'}) (d^{p'b'}) - 2 \circ^2 v (u_{p'}) (d_{q,p'}) (d^{q'b'}) - \\ & 3 \circ^2 (u_{p'}) (u_{q'}) (e^{p'q'b'}) + \circ^2 v (u_{p'}) (d^{p'b'}) (\phi_{3^{999}}) - \frac{1}{2} \circ v (\phi_{3^{99b'}}) + \\ & \frac{3}{4} \circ^2 v (u_{p'}) (\phi_{3^{99p'}}) (\phi_{3^{99b'}}) + \frac{1}{2} \circ^2 v (u_{p'}) (\phi_{3_{q,b'}}) (\phi_{3^{99p'q'}}) + \\ & \frac{1}{2} \circ^2 v (u_{p'}) (\phi_{3_{q,p'}}) (\phi_{3^{9q'b'}}) - \frac{1}{2} \circ^2 v (u_{p'}) (\phi_{4^{99p'b'}}) \end{aligned}$$

$$\text{foo25} = \frac{\partial \eta_a(u,v)}{\partial v}$$

**foo25 = tsimp[D[foo21, v]]**

$$\begin{aligned} & 2 \circ (u_{p'}) (d_{a,p'}) + 3 \circ^2 (u_{p'}) (u_{q'}) (e_{a,p'q'}) + \\ & \circ^2 (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi_{3^{99a'}}) + \circ^2 (u_{p'}) (u_{q'}) (d_{a,q'}) (\phi_{3^{99p'}}) - \circ (u_{p'}) (\phi_{3^{9a,p'}}) + \\ & \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (\phi_{3^{99q'}}) (\phi_{3^{9a,p'}}) - 2 \circ^2 (u_{p'}) (u_{q'}) (d_{r,q'}) (\phi_{3_{a,p'r'}}) + \\ & \circ^2 (u_{p'}) (u_{q'}) (\phi_{3_{r,q'}}) (\phi_{3_{a,p'r'}}) - \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (\phi_{4_{a,p'q'}}) \end{aligned}$$

$$\text{foo26} = \frac{\partial \eta_{\text{dim}}(u,v)}{\partial v}$$

**foo26 = tsimp[D[foo22, v]]**

$$\begin{aligned} & 1 - 2 \circ^2 (u_{p'}) (u_{q'}) (d_{r,q'}) (d^{p'r'}) + \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (d^{p'q'}) (\phi_{3^{999}}) - \\ & \frac{1}{2} \circ (u_{p'}) (\phi_{3^{99p'}}) + \frac{3}{8} \circ^2 (u_{p'}) (u_{q'}) (\phi_{3^{99p'}}) (\phi_{3^{99q'}}) + \\ & \frac{1}{2} \circ^2 (u_{p'}) (u_{q'}) (\phi_{3_{r,q'}}) (\phi_{3^{9p'r'}}) - \frac{1}{4} \circ^2 (u_{p'}) (u_{q'}) (\phi_{4^{99p'q'}}) \end{aligned}$$

$$\text{foo27} = \frac{\text{foo25}}{\text{foo26}}$$



$$\text{foo27} = \text{tsimp}[tgets2[y/x, x, \text{foo26}, y, \text{foo25}]]$$

$$2 o(u_{p'}) (d_{a', p'}) + 3 o^2(u_{p'}) (u_{q'}) (e_{a', p'q'}) + o^2(u_{p'}) (u_{q'}) (d^{p'q'}) (\phi_{3^{99}a'}) + \\ 2 o^2(u_{p'}) (u_{q'}) (d_{a', q'}) (\phi_{3^{99}p'}) - o(u_{p'}) (\phi_{3^9a', p'}) - 2 o^2(u_{p'}) (u_{q'}) (d_{r', q'}) (\phi_{3a', p'r'}) + \\ o^2(u_{p'}) (u_{q'}) (\phi_{3^9r', q'}) (\phi_{3a', p'r'}) - \frac{1}{2} o^2(u_{p'}) (u_{q'}) (\phi_{4^9a', p'q'})$$

$$\text{foo28} = \text{foo27} \text{foo24} = \frac{\text{foo24} \text{foo25}}{\text{foo26}}$$

$$\text{foo28} = \text{tsimp}[tgets2[x y, x, \text{foo27}, y, \text{foo24}]]$$

$$-4 o^2(u_{p'}) (u_{q'}) (d_{a', p'}) (d^{q'b'}) - o^2 v(u_{p'}) (d_{a', p'}) (\phi_{3^{99}b'}) + \\ 2 o^2(u_{p'}) (u_{q'}) (d^{q'b'}) (\phi_{3^9a', p'}) + \frac{1}{2} o^2 v(u_{p'}) (\phi_{3^{99}b'}) (\phi_{3^9a', p'})$$

$$\text{foo29} = \text{foo23} - \text{foo28} - \delta_{a'}^{b'} = \text{foo23} - \frac{\text{foo24} \text{foo25}}{\text{foo26}} - \delta_{a'}^{b'}$$

$$\text{foo29} = \text{tsimp}[tgets2[x - y, x, \text{foo23}, y, \text{foo28}]] - \text{Kdelta}[ala, aub]$$

$$2 o v(d_{a', b'}) + 4 o^2(u_{p'}) (u_{q'}) (d_{a', p'}) (d^{q'b'}) + 6 o^2 v(u_{p'}) (e_{a', p'b'}) + \\ 2 o^2 v(u_{p'}) (d^{p'b'}) (\phi_{3^{99}a'}) + o^2 v(u_{p'}) (d_{a', b'}) (\phi_{3^{99}p'}) + 2 o^2 v(u_{p'}) (d_{a', p'}) (\phi_{3^{99}b'}) - \\ 2 o^2(u_{p'}) (u_{q'}) (d^{q'b'}) (\phi_{3^9a', p'}) - o v(\phi_{3^9a', b'}) + \frac{1}{2} o^2 v(u_{p'}) (\phi_{3^{99}p'}) (\phi_{3^9a', b'}) - \\ 2 o^2 v(u_{p'}) (d_{q', b'}) (\phi_{3a', p'q'}) + o^2 v(u_{p'}) (\phi_{3^9q', b'}) (\phi_{3a', p'q'}) - \\ 2 o^2 v(u_{p'}) (d_{q', p'}) (\phi_{3a', q'b'}) + o^2 v(u_{p'}) (\phi_{3^9q', p'}) (\phi_{3a', q'b'}) - o^2 v(u_{p'}) (\phi_{4^9a', p'b'})$$

Now,  $\begin{pmatrix} \text{foo23} & \text{foo25} \\ \text{foo24} & \text{foo26} \end{pmatrix}$  is transformed to  $\begin{pmatrix} I + \text{foo29} & 0 \\ \text{foo24} & \text{foo26} \end{pmatrix}$  by the simple conventions preserving the determinant.

Then,  $\log J = \log \det(I + \text{foo29}) + \log(1 + (\text{foo26} - 1)) = \text{trace}(\text{foo29}) - \frac{1}{2} \text{trace}(\text{foo29}^2) + \text{foo26} - 1 - \frac{1}{2} (\text{foo26} - 1)^2$ .

$$\text{foo30} = \text{trace}(\text{foo29})$$

$$\text{foo30} = \text{tsimp}[\text{Kdelta}[aua, alb] \text{foo29}]$$

$$2 o v(d_{p', p'}) + 4 o^2(u_{p'}) (u_{q'}) (d_{r', p'}) (d^{q'r'}) + 6 o^2 v(u_{p'}) (e_{q', p'q'}) + \\ 4 o^2 v(u_{p'}) (d^{p'q'}) (\phi_{3^{99}q'}) + o^2 v(u_{p'}) (d_{q', q'}) (\phi_{3^{99}p'}) - o v(\phi_{3^9p', p'}) + \\ \frac{1}{2} o^2 v(u_{p'}) (\phi_{3^{99}p'}) (\phi_{3^9q', q'}) - 2 o^2(u_{p'}) (u_{q'}) (d^{q'r'}) (\phi_{3^9r', p'}) - \\ 2 o^2 v(u_{p'}) (d_{q', r'}) (\phi_{3r', p'q'}) + o^2 v(u_{p'}) (\phi_{3^9q', r'}) (\phi_{3r', p'q'}) - \\ 2 o^2 v(u_{p'}) (d_{q', p'}) (\phi_{3r', q'r'}) + o^2 v(u_{p'}) (\phi_{3^9q', p'}) (\phi_{3r', q'r'}) - o^2 v(u_{p'}) (\phi_{4^9q', p'q'})$$

$$\text{foo31} = \text{trace}(\text{foo29}^2)$$

$$\text{foo31} = \text{tsimp}[tgets2[x y, x, \text{foo29}, y, \text{foo29} /. \{ala \to aua, aub \to alb\}]]$$

$$4 o^2 v^2(d_{p', q'}) (d_{q', p'}) - 4 o^2 v^2(d_{p', q'}) (\phi_{3^9q', p'}) + o^2 v^2(\phi_{3^9p', q'}) (\phi_{3^9q', p'})$$

$$\text{foo32} = (\text{foo26} - 1)^2$$

$$\text{foo32} = \text{tsimp}[tgets2[x^2, x, \text{foo26} - 1]]$$

$$\frac{1}{4} o^2(u_{p'}) (u_{q'}) (\phi_{3^{99}p'}) (\phi_{3^{99}q'})$$

Finally,  $\log \det J = \log \det J = \text{foo30} - \frac{1}{2} \text{foo31} + \text{foo26} - 1 - \frac{1}{2} \text{foo32}$ .

$$\begin{aligned} \text{logdetJ} = & \text{tgeto2}\left[\text{tsimp}\left[\text{foo30} - \frac{1}{2} \text{foo31} + \text{foo26} - 1 - \frac{1}{2} \text{foo32}\right]\right] \\ & \circ \left(2 \mathbf{v} \left(\mathbf{d}_{\mathbf{p}, \mathbf{p}'}\right) - \frac{1}{2} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\phi_{3^{99\mathbf{p}'}}\right) - \mathbf{v} \left(\phi_{3^9 \mathbf{p}, \mathbf{p}'}\right)\right) + \\ & \circ^2 \left(-2 \mathbf{v}^2 \left(\mathbf{d}_{\mathbf{p}, \mathbf{q}'}\right) \left(\mathbf{d}_{\mathbf{q}, \mathbf{p}'}\right) + 2 \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{u}_{\mathbf{q}, \mathbf{p}'}\right) \left(\mathbf{d}_{\mathbf{r}, \mathbf{q}'}\right) \left(\mathbf{d}^{\mathbf{p}' \mathbf{r}'}\right) + \right. \\ & 6 \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{e}_{\mathbf{q}, \mathbf{p}' \mathbf{q}'}\right) + \frac{1}{2} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{u}_{\mathbf{q}, \mathbf{p}'}\right) \left(\mathbf{d}^{\mathbf{p}' \mathbf{q}'}\right) \left(\phi_{3^{999}}\right) + 4 \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{d}^{\mathbf{p}' \mathbf{q}'}\right) \left(\phi_{3^{99} \mathbf{q}'}\right) + \\ & \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{d}_{\mathbf{q}, \mathbf{q}'}\right) \left(\phi_{3^{99\mathbf{p}'}}\right) + \frac{1}{4} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{u}_{\mathbf{q}, \mathbf{p}'}\right) \left(\phi_{3^{99\mathbf{p}'}}\right) \left(\phi_{3^{99\mathbf{q}'}}\right) + \\ & 2 \mathbf{v}^2 \left(\mathbf{d}_{\mathbf{p}, \mathbf{q}'}\right) \left(\phi_{3^9 \mathbf{q}, \mathbf{p}'}\right) - \frac{1}{2} \mathbf{v}^2 \left(\phi_{3^9 \mathbf{p}, \mathbf{q}'}\right) \left(\phi_{3^9 \mathbf{q}, \mathbf{p}'}\right) + \frac{1}{2} \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\phi_{3^{99\mathbf{p}'}}\right) \left(\phi_{3^9 \mathbf{q}, \mathbf{q}'}\right) - \\ & 2 \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{u}_{\mathbf{q}, \mathbf{p}'}\right) \left(\mathbf{d}^{\mathbf{q}' \mathbf{r}'}\right) \left(\phi_{3^9 \mathbf{r}, \mathbf{p}'}\right) + \frac{1}{2} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{u}_{\mathbf{q}, \mathbf{p}'}\right) \left(\phi_{3^9 \mathbf{r}, \mathbf{q}'}\right) \left(\phi_{3^9 \mathbf{p}' \mathbf{r}'}\right) - \\ & 2 \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{d}_{\mathbf{q}, \mathbf{r}'}\right) \left(\phi_{3_{\mathbf{r}, \mathbf{p}' \mathbf{q}'}}\right) + \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\phi_{3^9 \mathbf{q}, \mathbf{r}'}\right) \left(\phi_{3_{\mathbf{r}, \mathbf{p}' \mathbf{q}'}}\right) - 2 \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{d}_{\mathbf{q}, \mathbf{p}'}\right) \left(\phi_{3_{\mathbf{r}, \mathbf{q}' \mathbf{r}'}}\right) + \\ & \left. \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\phi_{3^9 \mathbf{q}, \mathbf{p}'}\right) \left(\phi_{3_{\mathbf{r}, \mathbf{q}' \mathbf{r}'}}\right) - \frac{1}{4} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\mathbf{u}_{\mathbf{q}, \mathbf{p}'}\right) \left(\phi_{4^{99\mathbf{p}' \mathbf{q}'}}\right) - \mathbf{v} \left(\mathbf{u}_{\mathbf{p}, \mathbf{p}'}\right) \left(\phi_{4^9 \mathbf{q}, \mathbf{p}' \mathbf{q}'}\right)\right) \end{aligned}$$

**Collect[logdetJ /. {ru[al\_] -> u}, {o, v, u}, Simplify]**

$$\begin{aligned} & \circ \left(-\frac{1}{2} \mathbf{u} \left(\phi_{3^{99\mathbf{p}'}}\right) + \mathbf{v} \left(2 \left(\mathbf{d}_{\mathbf{p}, \mathbf{p}'}\right) - \phi_{3^9 \mathbf{p}, \mathbf{p}'}\right)\right) + \\ & \circ^2 \left(\mathbf{v}^2 \left(-2 \left(\mathbf{d}_{\mathbf{p}, \mathbf{q}'}\right) \left(\mathbf{d}_{\mathbf{q}, \mathbf{p}'}\right) - \phi_{3^9 \mathbf{q}, \mathbf{p}'}\right) - \frac{1}{2} \left(\phi_{3^9 \mathbf{p}, \mathbf{q}'}\right) \left(\phi_{3^9 \mathbf{q}, \mathbf{p}'}\right)\right) + \\ & \frac{1}{4} \mathbf{u}^2 \left(8 \left(\mathbf{d}_{\mathbf{r}, \mathbf{q}'}\right) \left(\mathbf{d}^{\mathbf{p}' \mathbf{r}'}\right) + 2 \left(\mathbf{d}^{\mathbf{p}' \mathbf{q}'}\right) \left(\phi_{3^{999}}\right) + \left(\phi_{3^{99\mathbf{p}'}}\right) \left(\phi_{3^{99\mathbf{q}'}}\right) - \right. \\ & \left. 8 \left(\mathbf{d}^{\mathbf{q}' \mathbf{r}'}\right) \left(\phi_{3^9 \mathbf{r}, \mathbf{p}'}\right) + 2 \left(\phi_{3^9 \mathbf{r}, \mathbf{q}'}\right) \left(\phi_{3^9 \mathbf{p}' \mathbf{r}'}\right) - \phi_{4^{99\mathbf{p}' \mathbf{q}'}}\right) + \\ & \mathbf{u} \mathbf{v} \left(6 \left(\mathbf{e}_{\mathbf{q}, \mathbf{p}' \mathbf{q}'}\right) + 4 \left(\mathbf{d}^{\mathbf{p}' \mathbf{q}'}\right) \left(\phi_{3^9 \mathbf{q}, \mathbf{p}'}\right) + \left(\mathbf{d}_{\mathbf{q}, \mathbf{q}'}\right) \left(\phi_{3^{99\mathbf{p}'}}\right) + \frac{1}{2} \left(\phi_{3^{99\mathbf{p}'}}\right) \left(\phi_{3^9 \mathbf{q}, \mathbf{q}'}\right) - 2 \left(\mathbf{d}_{\mathbf{q}, \mathbf{r}'}\right) \right. \\ & \left. \left(\phi_{3_{\mathbf{r}, \mathbf{p}' \mathbf{q}'}}\right) + \left(\phi_{3^9 \mathbf{q}, \mathbf{r}'}\right) \left(\phi_{3_{\mathbf{r}, \mathbf{p}' \mathbf{q}'}}\right) - 2 \left(\mathbf{d}_{\mathbf{q}, \mathbf{p}'}\right) \left(\phi_{3_{\mathbf{r}, \mathbf{q}' \mathbf{r}'}}\right) + \left(\phi_{3^9 \mathbf{q}, \mathbf{p}'}\right) \left(\phi_{3_{\mathbf{r}, \mathbf{q}' \mathbf{r}'}}\right) - \phi_{4^9 \mathbf{q}, \mathbf{p}' \mathbf{q}'}\right) \end{aligned}$$

■ **density function f(u,v|v0)**

log f(y | η) is given as follows.

**tgeto2[logdensityy]**

$$\begin{aligned} & -\frac{1}{2} \text{dim} \text{Log}[2 \pi] - \frac{1}{2} \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\mathbf{Y}^{\mathbf{p}}\right) + \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\eta^{\mathbf{p}}\right) - \\ & \frac{1}{2} \left(\eta_{\mathbf{p}}\right) \left(\eta^{\mathbf{p}}\right) + \circ \left(\frac{1}{2} \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\phi_{3_{\mathbf{q}}^{\mathbf{p} \mathbf{q}}}\right) - \frac{1}{6} \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\mathbf{Y}_{\mathbf{q}}\right) \left(\mathbf{Y}_{\mathbf{r}}\right) \left(\phi_{3^{\mathbf{p} \mathbf{q} \mathbf{r}}}\right) + \right. \\ & \left. \frac{1}{2} \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\eta_{\mathbf{q}}\right) \left(\eta_{\mathbf{r}}\right) \left(\phi_{3^{\mathbf{p} \mathbf{q} \mathbf{r}}}\right) - \frac{1}{3} \left(\eta_{\mathbf{p}}\right) \left(\eta_{\mathbf{q}}\right) \left(\eta_{\mathbf{r}}\right) \left(\phi_{3^{\mathbf{p} \mathbf{q} \mathbf{r}}}\right)\right) + \\ & \circ^2 \left(\frac{1}{6} \left(\phi_{3_{\mathbf{p} \mathbf{q} \mathbf{r}}}\right) \left(\phi_{3^{\mathbf{p} \mathbf{q} \mathbf{r}}}\right) - \frac{1}{4} \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\mathbf{Y}_{\mathbf{q}}\right) \left(\phi_{3_{\mathbf{r} \mathbf{s}}^{\mathbf{p}}}\right) \left(\phi_{3^{\mathbf{q} \mathbf{r} \mathbf{s}}}\right) - \frac{1}{8} \left(\phi_{4_{\mathbf{p} \mathbf{q}}^{\mathbf{p} \mathbf{q}}}\right) + \right. \\ & \frac{1}{4} \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\mathbf{Y}_{\mathbf{q}}\right) \left(\phi_{4_{\mathbf{r}}^{\mathbf{p} \mathbf{q} \mathbf{r}}}\right) - \frac{1}{24} \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\mathbf{Y}_{\mathbf{q}}\right) \left(\mathbf{Y}_{\mathbf{r}}\right) \left(\mathbf{Y}_{\mathbf{s}}\right) \left(\phi_{4^{\mathbf{p} \mathbf{q} \mathbf{r} \mathbf{s}}}\right) + \\ & \left. \frac{1}{6} \left(\mathbf{Y}_{\mathbf{p}}\right) \left(\eta_{\mathbf{q}}\right) \left(\eta_{\mathbf{r}}\right) \left(\eta_{\mathbf{s}}\right) \left(\phi_{4^{\mathbf{p} \mathbf{q} \mathbf{r} \mathbf{s}}}\right) - \frac{1}{8} \left(\eta_{\mathbf{p}}\right) \left(\eta_{\mathbf{q}}\right) \left(\eta_{\mathbf{r}}\right) \left(\eta_{\mathbf{s}}\right) \left(\phi_{4^{\mathbf{p} \mathbf{q} \mathbf{r} \mathbf{s}}}\right)\right) \end{aligned}$$

First, we set η=(0,...,0,v0). In other words, η<sub>a'</sub> = 0, and η<sub>dim</sub> = v0. Here we use symbol v0 for λ.

**RuleUnique[rule35, se[la\_], v0 Kdelta[la, 9]]**

**foo35 = tsimp[ApplyRules[logdensityy, rule35]]**

$$\begin{aligned}
 & -\frac{v0^2}{2} - \frac{1}{2} \dim \text{Log}[2 \pi] + v0 (Y^9) - \frac{1}{2} (Y_p) (Y^p) - \frac{1}{3} \circ v0^3 (\phi3^{999}) + \frac{1}{2} \circ v0^2 (Y_p) (\phi3^{99p}) + \\
 & \frac{1}{2} \circ (Y_p) (\phi3_q^{pq}) - \frac{1}{6} \circ (Y_p) (Y_q) (Y_r) (\phi3^{pqr}) + \frac{1}{6} \circ^2 (\phi3_{pqr}) (\phi3^{pqr}) - \\
 & \frac{1}{4} \circ^2 (Y_p) (Y_q) (\phi3_{rs}^p) (\phi3^{qrs}) - \frac{1}{8} \circ^2 v0^4 (\phi4^{9999}) + \frac{1}{6} \circ^2 v0^3 (Y_p) (\phi4^{999p}) - \\
 & \frac{1}{8} \circ^2 (\phi4_{pq}^{pq}) + \frac{1}{4} \circ^2 (Y_p) (Y_q) (\phi4_r^{pqr}) - \frac{1}{24} \circ^2 (Y_p) (Y_q) (Y_r) (Y_s) (\phi4^{pqrs})
 \end{aligned}$$

Then, change of variables  $y=\eta(u,v)$ .

**foo36 = tsimp[**

**CanAll[sepa[CanAll[sepa[CanAll[sepa[CanAll[sepa[foo35, 11]], 11]], 11]], 11]], 11]]]**

$$\begin{aligned}
 & -\frac{v0^2}{2} - \frac{1}{2} \dim \text{Log}[2 \pi] + v0 (Y^9) - \frac{1}{2} (Y_9) (Y^9) - \frac{1}{2} (Y_{p'}) (Y^{p'}) - \frac{1}{3} \circ v0^3 (\phi3^{999}) + \\
 & \frac{1}{2} \circ (Y_9) (\phi3^{999}) + \frac{1}{2} \circ v0^2 (Y_9) (\phi3^{999}) - \frac{1}{6} \circ (Y_9)^3 (\phi3^{999}) + \frac{1}{6} \circ^2 (\phi3^{999})^2 - \\
 & \frac{1}{4} \circ^2 (Y_9)^2 (\phi3^{999})^2 + (Y_{p'}) \left( \frac{\circ}{2} + \frac{\circ v0^2}{2} - \frac{1}{2} \circ (Y_9)^2 - \frac{1}{2} \circ^2 (Y_9) (\phi3^{999}) \right) (\phi3^{99p'}) + \\
 & \left( \frac{\circ^2}{2} - \frac{1}{2} \circ^2 (Y_9)^2 \right) (\phi3_{p'}^{99p'}) (\phi3^{99p'}) - \frac{1}{4} \circ^2 (Y_{p'}) (Y_{q'}) (\phi3^{99p'}) (\phi3^{99q'}) + \\
 & \frac{1}{2} \circ (Y_9) (\phi3_{p',p'}^{99p'}) - \frac{1}{2} \circ (Y_9) (Y_{p'}) (Y_{q'}) (\phi3^{99p'q'}) - \circ^2 (Y_{p'}) (Y_{p'}) (\phi3_{q'}^{99q'}) (\phi3^{99p'q'}) + \\
 & \left( \frac{\circ^2}{2} - \frac{1}{4} \circ^2 (Y_9)^2 \right) (\phi3_{p',q'}^{99p'q'}) (\phi3^{99p'q'}) - \frac{1}{2} \circ^2 (Y_{p'}) (Y_{q'}) (\phi3_{r,p'}^{99r,p'}) (\phi3^{99q'r'}) + \\
 & \frac{1}{2} \circ (Y_{p'}) (\phi3_{q',p'q'}^{99q',p'q'}) - \frac{1}{6} \circ (Y_{p'}) (Y_{q'}) (Y_{r'}) (\phi3^{99q'r'}) - \frac{1}{2} \circ^2 (Y_9) (Y_{p'}) (\phi3_{q',r'}^{99q',r'}) (\phi3^{99p'q'r'}) + \\
 & \frac{1}{6} \circ^2 (\phi3_{p',q',r'}^{99p',q',r'}) (\phi3^{99p'q'r'}) - \frac{1}{4} \circ^2 (Y_{p'}) (Y_{q'}) (\phi3_{r',s,p'}^{99r',s,p'}) (\phi3^{99q'r's'}) - \\
 & \frac{1}{8} \circ^2 (\phi4^{9999}) - \frac{1}{8} \circ^2 v0^4 (\phi4^{9999}) + \frac{1}{6} \circ^2 v0^3 (Y_9) (\phi4^{9999}) + \frac{1}{4} \circ^2 (Y_9)^2 (\phi4^{9999}) - \\
 & \frac{1}{24} \circ^2 (Y_9)^4 (\phi4^{9999}) + \left( \frac{\circ^2 v0^3}{6} + \frac{1}{2} \circ^2 (Y_9) - \frac{1}{6} \circ^2 (Y_9)^3 \right) (Y_{p'}) (\phi4^{999p'}) + \\
 & \left( -\frac{\circ^2}{4} + \frac{1}{4} \circ^2 (Y_9)^2 \right) (\phi4_{p',p'}^{99p',p'}) + \left( \frac{\circ^2}{4} - \frac{1}{4} \circ^2 (Y_9)^2 \right) (Y_{p'}) (Y_{q'}) (\phi4^{99p'q'}) + \\
 & \frac{1}{2} \circ^2 (Y_9) (Y_{p'}) (\phi4_{q',p'q'}^{99q',p'q'}) - \frac{1}{6} \circ^2 (Y_9) (Y_{p'}) (Y_{q'}) (Y_{r'}) (\phi4^{99p'q'r'}) - \frac{1}{8} \circ^2 (\phi4_{p',q',p'q'}^{99p',q',p'q'}) + \\
 & \frac{1}{4} \circ^2 (Y_{p'}) (Y_{q'}) (\phi4_{r,p'q'r'}^{99r,p'q'r'}) - \frac{1}{24} \circ^2 (Y_{p'}) (Y_{q'}) (Y_{r'}) (Y_{s'}) (\phi4^{99p'q'r's'})
 \end{aligned}$$

foo37 =

$$\begin{aligned}
 & \text{tsimp}[tgeto2[\text{ApplyRules}[\text{foo36} /. \text{ry} \rightarrow \text{se}, \{\text{rule21}, \text{rule22}, \text{rule22b}\}]] + \text{logdetJ}] \\
 & - \frac{v^2}{2} + v v_0 - \frac{v_0^2}{2} - \frac{1}{2} \dim \text{Log}[2 \pi] - \frac{1}{2} (u_{p'}) (u^{p'}) + 2 o v (d_{p', p'}) - 2 o^2 v^2 (d_{p', q'}) (d_{q', p'}) + \\
 & (2 o^2 - 2 o^2 v v_0) (u_{p'}) (u_{q'}) (d_{r', q'}) (d^{p' r'}) - \frac{1}{2} o^2 (u_{p'}) (u_{q'}) (u_{r'}) (u_{s'}) (d^{p' q'}) (d^{r' s'}) + \\
 & 6 o^2 v (u_{p'}) (e_{q', p' q'}) + (-2 o^2 v - o^2 v_0) (u_{p'}) (u_{q'}) (u_{r'}) (e^{p' q' r'}) + \frac{1}{2} o v (\phi_{3^{999}}) - \\
 & \frac{1}{6} o v^3 (\phi_{3^{999}}) + \frac{1}{2} o v v_0^2 (\phi_{3^{999}}) - \frac{1}{3} o v_0^3 (\phi_{3^{999}}) + \frac{1}{6} o^2 (\phi_{3^{999}})^2 - \frac{1}{4} o^2 v^2 (\phi_{3^{999}})^2 + \\
 & (u_{p'}) (u_{q'}) (d^{p' q'}) \left( -o v - o v_0 + \frac{1}{2} o^2 v v_0 (\phi_{3^{999}}) - \frac{1}{2} o^2 v_0^2 (\phi_{3^{999}}) \right) + \\
 & (5 o^2 v - o^2 v^3 + o^2 v v_0^2) (u_{p'}) (d^{p' q'}) (\phi_{3^{99 q'}}) + \\
 & o^2 v (u_{p'}) (d_{q', q'}) (\phi_{3^{99 p'}}) - \frac{3}{2} o^2 v (u_{p'}) (u_{q'}) (u_{r'}) (d^{q' r'}) (\phi_{3^{99 p'}}) + \\
 & (u_{p'}) \left( -\frac{1}{2} o v v_0 + \frac{o v_0^2}{2} - \frac{3}{4} o^2 v (\phi_{3^{999}}) + \frac{1}{4} o^2 v^3 (\phi_{3^{999}}) - \frac{1}{4} o^2 v v_0^2 (\phi_{3^{999}}) \right) (\phi_{3^{99 p'}}) + \\
 & \left( \frac{o^2}{2} - \frac{o^2 v^2}{2} \right) (\phi_{3^{99 p'}}) (\phi_{3^{99 p'}}) + \frac{3}{8} o^2 v v_0 (u_{p'}) (u_{q'}) (\phi_{3^{99 p'}}) (\phi_{3^{99 q'}}) - \frac{1}{2} o v (\phi_{3^9 p', p'}) + \\
 & 2 o^2 v^2 (d_{p', q'}) (\phi_{3^9 q', p'}) + \left( -\frac{3 o^2 v}{2} + \frac{o^2 v^3}{2} - \frac{1}{2} o^2 v v_0^2 \right) (u_{p'}) (\phi_{3^{99 q'}}) (\phi_{3^9 q', p'}) + \\
 & \left( \frac{o^2}{2} - \frac{3 o^2 v^2}{4} \right) (\phi_{3^9 p', q'}) (\phi_{3^9 q', p'}) + \frac{1}{4} o^2 v (u_{p'}) (\phi_{3^{99 p'}}) (\phi_{3^9 q', q'}) - \\
 & 2 o^2 (u_{p'}) (u_{q'}) (d^{q' r'}) (\phi_{3^9 r', p'}) - \frac{1}{2} o^2 (u_{p'}) (u_{q'}) (d^{p' q'}) (\phi_{3^9 r', r'}) + \\
 & \frac{1}{2} o v (u_{p'}) (u_{q'}) (\phi_{3^{99 p' q'}}) + \frac{1}{2} o^2 (u_{p'}) (u_{q'}) (u_{r'}) (u_{s'}) (d^{r' s'}) (\phi_{3^{99 p' q'}}) - \\
 & \frac{1}{4} o^2 v (u_{p'}) (u_{q'}) (u_{r'}) (\phi_{3^{99 r'}}) (\phi_{3^{99 p' q'}}) + \frac{1}{2} o^2 v v_0 (u_{p'}) (u_{q'}) (\phi_{3^9 r', q'}) (\phi_{3^{99 p' r'}}) + \\
 & \frac{1}{2} o (u_{p'}) (\phi_{3^9 p', p' q'}) - 2 o^2 v (u_{p'}) (d_{q', r'}) (\phi_{3^9 r', p' q'}) + \frac{1}{2} o^2 v (u_{p'}) (\phi_{3^9 q', r'}) (\phi_{3^9 r', p' q'}) - \\
 & o^2 v (u_{p'}) (d_{q', p'}) (\phi_{3^9 r', q' r'}) + \frac{1}{2} o^2 v (u_{p'}) (\phi_{3^9 q', p'}) (\phi_{3^9 q', r'}) - \\
 & \frac{1}{6} o (u_{p'}) (u_{q'}) (u_{r'}) (\phi_{3^{99 p' q' r'}}) + \frac{1}{6} o^2 (\phi_{3^9 p', q', r'}) (\phi_{3^{99 p' q' r'}}) + \\
 & o^2 v (u_{p'}) (u_{q'}) (u_{r'}) (d_{s', r'}) (\phi_{3^{99 q' s'}}) - \frac{1}{2} o^2 v (u_{p'}) (u_{q'}) (u_{r'}) (\phi_{3^9 s', r'}) (\phi_{3^{99 q' s'}}) - \\
 & \frac{1}{4} o^2 (u_{p'}) (u_{q'}) (\phi_{3^9 s', p'}) (\phi_{3^{99 r' s'}}) - \frac{1}{8} o^2 (\phi_{4^{9999}}) + \frac{1}{4} o^2 v^2 (\phi_{4^{9999}}) - \frac{1}{24} o^2 v^4 (\phi_{4^{9999}}) + \\
 & \frac{1}{6} o^2 v v_0^3 (\phi_{4^{9999}}) - \frac{1}{8} o^2 v_0^4 (\phi_{4^{9999}}) + \left( \frac{o^2 v}{2} - \frac{o^2 v^3}{6} + \frac{o^2 v_0^3}{6} \right) (u_{p'}) (\phi_{4^{9999 p'}}) + \\
 & \left( -\frac{o^2}{4} + \frac{o^2 v^2}{4} \right) (\phi_{4^{99 p', p'}}) - \frac{1}{4} o^2 v v_0 (u_{p'}) (u_{q'}) (\phi_{4^{99 p' q'}}) - \\
 & \frac{1}{2} o^2 v (u_{p'}) (\phi_{4^9 q', p' q'}) + \frac{1}{3} o^2 v (u_{p'}) (u_{q'}) (u_{r'}) (\phi_{4^{99 p' q' r'}}) - \frac{1}{8} o^2 (\phi_{4^9 p', q', p' q'}) + \\
 & \frac{1}{4} o^2 (u_{p'}) (u_{q'}) (\phi_{4^9 r', p' q' r'}) - \frac{1}{24} o^2 (u_{p'}) (u_{q'}) (u_{r'}) (u_{s'}) (\phi_{4^9 p' q' r' s'})
 \end{aligned}$$

Now we get logdensityuv=foo38=f(u,v|v0).

```
foo38 = Collect[foo37, {o, v, ru[a11] ru[a12] ru[a13] ru[a14],
ru[a11] ru[a12] ru[a13], ru[a11] ru[a12], ru[a11]}];
```

logdensityuv = foo38

$$\begin{aligned}
 & -\frac{v^2}{2} + v v_0 - \frac{v_0^2}{2} - \frac{1}{2} \dim \text{Log}[2 \pi] - \frac{1}{2} (u_{p'}) (u^{p'}) + \\
 & o \left( -v_0 (u_{p'}) (u_{q'}) (d^{p'q'}) - \frac{1}{6} v^3 (\phi_3^{999}) - \frac{1}{3} v_0^3 (\phi_3^{999}) + \right. \\
 & \quad v \left( 2 (d_{p',p'}) + \frac{1}{2} (\phi_3^{999}) + \frac{1}{2} v_0^2 (\phi_3^{999}) - \frac{1}{2} v_0 (u_{p'}) (\phi_3^{99p'}) - \right. \\
 & \quad \quad \left. \frac{1}{2} (\phi_3^{9_{p',p'}}) + (u_{p'}) (u_{q'}) \left( - (d^{p'q'}) + \frac{1}{2} (\phi_3^{9_{p',p'}}) \right) \right) + \\
 & \quad (u_{p'}) \left( \frac{1}{2} v_0^2 (\phi_3^{99p'}) + \frac{1}{2} (\phi_3^{9_{q',p'}}) \right) - \frac{1}{6} (u_{p'}) (u_{q'}) (u_{r'}) (\phi_3^{9_{q',r'}}) + \\
 & o^2 \left( -v_0 (u_{p'}) (u_{q'}) (u_{r'}) (e^{p'q'r'}) + \frac{1}{6} (\phi_3^{999})^2 + \frac{1}{2} (\phi_3^{99_{p'}}) (\phi_3^{99p'}) + \frac{1}{2} (\phi_3^{9_{p',q'}}) (\phi_3^{9_{q',p'}}) + \right. \\
 & \quad \frac{1}{6} (\phi_3^{9_{p',q',r'}}) (\phi_3^{9_{q',r'}}) - \frac{1}{8} (\phi_4^{9999}) - \frac{1}{24} v^4 (\phi_4^{9999}) - \frac{1}{8} v_0^4 (\phi_4^{9999}) + \\
 & \quad v^3 (u_{p'}) \left( - (d^{p'q'}) (\phi_3^{99_{q'}}) + \frac{1}{4} (\phi_3^{999}) (\phi_3^{99p'}) + \frac{1}{2} (\phi_3^{99_{q'}}) (\phi_3^{9_{q',p'}}) - \frac{1}{6} (\phi_4^{999p'}) \right) + \\
 & \quad \frac{1}{6} v_0^3 (u_{p'}) (\phi_4^{999p'}) + v^2 \left( -2 (d_{p',q'}) (d_{q',p'}) - \frac{1}{4} (\phi_3^{999})^2 - \frac{1}{2} (\phi_3^{99_{p'}}) (\phi_3^{99p'}) + \right. \\
 & \quad \quad \left. 2 (d_{p',q'}) (\phi_3^{9_{q',p'}}) - \frac{3}{4} (\phi_3^{9_{p',q'}}) (\phi_3^{9_{q',p'}}) + \frac{1}{4} (\phi_4^{9999}) + \frac{1}{4} (\phi_4^{99_{p',p'}}) \right) - \frac{1}{4} (\phi_4^{99_{p',p'}}) + \\
 & \quad v \left( \frac{1}{6} v_0^3 (\phi_4^{9999}) + (u_{p'}) (u_{q'}) \left( -2 v_0 (d_{r',q'}) (d^{p'r'}) + \frac{1}{2} v_0 (d^{p'q'}) (\phi_3^{999}) + \right. \right. \\
 & \quad \quad \left. \frac{3}{8} v_0 (\phi_3^{99p'}) (\phi_3^{99_{q'}}) + \frac{1}{2} v_0 (\phi_3^{9_{r',q'}}) (\phi_3^{99_{p',r'}}) - \frac{1}{4} v_0 (\phi_4^{99p',q'}) \right) + \\
 & \quad (u_{p'}) \left( 6 (e_{q',p',q'}) + 5 (d^{p'q'}) (\phi_3^{99_{q'}}) + v_0^2 (d^{p'q'}) (\phi_3^{99_{q'}}) + (d_{q',q'}) (\phi_3^{99p'}) - \right. \\
 & \quad \quad \frac{3}{4} (\phi_3^{999}) (\phi_3^{99p'}) - \frac{1}{4} v_0^2 (\phi_3^{999}) (\phi_3^{99p'}) - \frac{3}{2} (\phi_3^{99_{q'}}) (\phi_3^{9_{q',p'}}) - \frac{1}{2} v_0^2 (\phi_3^{99_{q'}}) \\
 & \quad \quad \left. (\phi_3^{9_{q',p'}}) + \frac{1}{4} (\phi_3^{99p'}) (\phi_3^{9_{q',q'}}) - 2 (d_{q',r'}) (\phi_3^{r',p',q'}) + \frac{1}{2} (\phi_3^{9_{q',r'}}) (\phi_3^{r',p',q'}) - \right. \\
 & \quad \quad \left. (d_{q',p'}) (\phi_3^{r',q',r'}) + \frac{1}{2} (\phi_3^{9_{q',p'}}) (\phi_3^{r',q',r'}) + \frac{1}{2} (\phi_4^{9999p'}) - \frac{1}{2} (\phi_4^{9_{q',p',q'}}) \right) + \\
 & \quad (u_{p'}) (u_{q'}) (u_{r'}) \left( -2 (e^{p'q'r'}) - \frac{3}{2} (d^{q'r'}) (\phi_3^{99p'}) - \frac{1}{4} (\phi_3^{99_{r'}}) (\phi_3^{99_{p',q'}}) + \right. \\
 & \quad \quad \left. (d_{s',r'}) (\phi_3^{p',q',s'}) - \frac{1}{2} (\phi_3^{9_{s',r'}}) (\phi_3^{p',q',s'}) + \frac{1}{3} (\phi_4^{99p',q',r'}) \right) - \frac{1}{8} (\phi_4^{p',q',p',q'}) + \\
 & \quad (u_{p'}) (u_{q'}) \left( 2 (d_{r',q'}) (d^{p'r'}) - \frac{1}{2} v_0^2 (d^{p'q'}) (\phi_3^{999}) - 2 (d^{q'r'}) (\phi_3^{9_{r',p'}}) - \right. \\
 & \quad \quad \left. \frac{1}{2} (d^{p'q'}) (\phi_3^{9_{r',r'}}) - \frac{1}{4} (\phi_3^{r',s',p'}) (\phi_3^{q',r',s'}) + \frac{1}{4} (\phi_4^{r',p',q',r'}) \right) + \\
 & \quad (u_{p'}) (u_{q'}) (u_{r'}) (u_{s'}) \left( -\frac{1}{2} (d^{p'q'}) (d^{r's'}) + \frac{1}{2} (d^{r's'}) (\phi_3^{99p',q'}) - \frac{1}{24} (\phi_4^{p',q',r',s'}) \right) \Big)
 \end{aligned}$$

**InputForm[foo38]**

```

-v^2/2 + v*v0 - v0^2/2 - (dim*Log[2*Pi])/2 - (ru[al1]*ru[au1])/2 +
o*(-(v0*ru[al1]*ru[al2]*td[au1, au2]) - (v^3*tp3[9, 9, 9])/6 -
(v0^3*tp3[9, 9, 9])/3 + v*(2*td[al1, au1] + tp3[9, 9, 9])/2 +
(v0^2*tp3[9, 9, 9])/2 - (v0*ru[al1]*tp3[9, 9, au1])/2 -
tp3[9, al1, au1]/2 + ru[al1]*ru[al2]*(-td[au1, au2] +
tp3[9, au1, au2]/2)) + ru[al1]*((v0^2*tp3[9, 9, au1])/2 +
tp3[al2, au1, au2]/2) - (ru[al1]*ru[al2]*ru[al3]*
tp3[au1, au2, au3])/6) +
o^2*(-(v0*ru[al1]*ru[al2]*ru[al3]*te[au1, au2, au3]) +
tp3[9, 9, 9]^2/6 + (tp3[9, 9, al1]*tp3[9, 9, au1])/2 +
(tp3[9, al1, au2]*tp3[9, al2, au1])/2 +
(tp3[al1, al2, al3]*tp3[au1, au2, au3])/6 - tp4[9, 9, 9, 9]/8 -
(v^4*tp4[9, 9, 9, 9])/24 - (v0^4*tp4[9, 9, 9, 9])/8 +
v^3*ru[al1]*(-td[au1, au2]*tp3[9, 9, al2]) +
(tp3[9, 9, 9, 9]*tp3[9, 9, au1])/4 +
(tp3[9, 9, au2]*tp3[9, al2, au1])/2 - tp4[9, 9, 9, au1]/6) +
(v0^3*ru[al1]*tp4[9, 9, 9, au1])/6 +
v^2*(-2*td[al1, au2]*td[al2, au1] - tp3[9, 9, 9]^2/4 -
(tp3[9, 9, al1]*tp3[9, 9, au1])/2 + 2*td[al1, au2]*
tp3[9, al2, au1] - (3*tp3[9, al1, au2]*tp3[9, al2, au1])/4 +
tp4[9, 9, 9, 9, 9]/4 + tp4[9, 9, al1, au1]/4) -
tp4[9, 9, al1, au1]/4 + v*((v0^3*tp4[9, 9, 9, 9])/6 +
ru[al1]*ru[al2]*(-2*v0*td[al3, au2]*td[au1, au3] +
(v0*td[au1, au2]*tp3[9, 9, 9])/2 +
(3*v0*tp3[9, 9, au1]*tp3[9, 9, au2])/8 +
(v0*tp3[9, al3, au2]*tp3[9, au1, au3])/2 -
(v0*tp4[9, 9, au1, au2])/4) +
ru[al1]*(6*te[al2, au1, au2] + 5*td[au1, au2]*tp3[9, 9, al2] +
v0^2*td[au1, au2]*tp3[9, 9, al2] + td[al2, au2]*
tp3[9, 9, au1] - (3*tp3[9, 9, 9]*tp3[9, 9, au1])/4 -
(v0^2*tp3[9, 9, 9]*tp3[9, 9, au1])/4 -
(3*tp3[9, 9, au2]*tp3[9, al2, au1])/2 -
(v0^2*tp3[9, 9, au2]*tp3[9, al2, au1])/2 +
(tp3[9, 9, au1]*tp3[9, al2, au2])/4 - 2*td[al2, au3]*
tp3[al3, au1, au2] + (tp3[9, al2, au3]*tp3[al3, au1, au2])/
2 - td[al2, au1]*tp3[al3, au2, au3] +
(tp3[9, al2, au1]*tp3[al3, au2, au3])/2 +
tp4[9, 9, 9, au1]/2 - tp4[9, al2, au1, au2]/2) +
ru[al1]*ru[al2]*ru[al3]*(-2*te[au1, au2, au3] -
(3*td[au2, au3]*tp3[9, 9, au1])/2 -
(tp3[9, 9, au3]*tp3[9, au1, au2])/4 +
td[al4, au3]*tp3[au1, au2, au4] -
(tp3[9, al4, au3]*tp3[au1, au2, au4])/2 +
tp4[9, au1, au2, au3]/3) - tp4[al1, al2, au1, au2]/8 +
ru[al1]*ru[al2]*(2*td[al3, au2]*td[au1, au3] -
(v0^2*td[au1, au2]*tp3[9, 9, 9])/2 - 2*td[au2, au3]*
tp3[9, al3, au1] - (td[au1, au2]*tp3[9, al3, au3])/2 -
(tp3[al3, al4, au1]*tp3[au2, au3, au4])/4 +
tp4[al3, au1, au2, au3]/4) + ru[al1]*ru[al2]*ru[al3]*ru[al4]*
(-(td[au1, au2]*td[au3, au4])/2 +
(td[au3, au4]*tp3[9, au1, au2])/2 - tp4[au1, au2, au3, au4]/
24)

```

We extract the coefficients for  $u, v$  from the density function  $f(u, v|v_0)$ .

```

foo39 = Collect[CoefficientList[foo38 /. {ru[al_] -> u}, {v, u}],
{o, v0}, tsimp[CanAll[# /. {au1 -> aua, au2 -> aub, au3 -> auc, au4 -> aud,
au5 -> aue, al1 -> ala, al2 -> alb, al3 -> alc, al4 -> ald, al5 -> ale}]] &];

```

**Dimensions[foo39]**

```
{5, 5}
```

**foo40 = foo39;**

$u^0$ -coefficients

$v^0 u^0$

**foo40[[1, 1]]**

$$-\frac{v0^2}{2} - \frac{1}{2} \dim \text{Log}[2 \pi] - \frac{1}{3} \circ v0^3 (\phi3^{999}) +$$

$$\circ^2 \left( \frac{1}{6} (\phi3^{999})^2 + \frac{1}{2} (\phi3^{99}_{p'}) (\phi3^{99}_{p'}) + \frac{1}{2} (\phi3^9_{p,q'}) (\phi3^9_{q',p'}) + \right.$$

$$\left. \frac{1}{6} (\phi3_{p',q',r'}) (\phi3_{p',q',r'}) - \frac{1}{8} (\phi4^{9999}) - \frac{1}{8} v0^4 (\phi4^{9999}) - \frac{1}{4} (\phi4^{99}_{p,p'}) - \frac{1}{8} (\phi4_{p',q',p',q'}) \right)$$

$v^1 u^0$

**foo40[[2, 1]]**

$$v0 + \circ \left( 2 (d_{p,p'}) + \frac{1}{2} (\phi3^{999}) + \frac{1}{2} v0^2 (\phi3^{999}) - \frac{1}{2} (\phi3^9_{p,p'}) \right) + \frac{1}{6} \circ^2 v0^3 (\phi4^{9999})$$

$v^2 u^0$

**foo40[[3, 1]]**

$$-\frac{1}{2} + \circ^2 \left( -2 (d_{p,q'}) (d_{q',p'}) - \frac{1}{4} (\phi3^{999})^2 - \frac{1}{2} (\phi3^9_{p'}) (\phi3^9_{p'}) + \right.$$

$$\left. 2 (d_{p,q'}) (\phi3^9_{q',p'}) - \frac{3}{4} (\phi3^9_{p',q'}) (\phi3^9_{q',p'}) + \frac{1}{4} (\phi4^{9999}) + \frac{1}{4} (\phi4^9_{p,p'}) \right)$$

$v^3 u^0$

**foo40[[4, 1]]**

$$-\frac{1}{6} \circ (\phi3^{999})$$

$v^4 u^0$

**foo40[[5, 1]]**

$$-\frac{1}{24} \circ^2 (\phi4^{9999})$$

$u^1$ -coefficients

$v^0 u^1$

**foo40[[1, 2]]**

$$\circ \left( \frac{1}{2} v0^2 (\phi3^{99a'}) + \frac{1}{2} (\phi3_{p',p',a'}) \right) + \frac{1}{6} \circ^2 v0^3 (\phi4^{999a'})$$

$v^1 u^1$

**foo40[[2, 2]]**

$$-\frac{1}{2} \circ v_0 (\phi_3^{99a'}) + o^2 \left( 6 (e_p, p'a') + 5 (d^{p'a'}) (\phi_3^{99p'}) + (d_{p,p'}) (\phi_3^{99a'}) - \frac{3}{4} (\phi_3^{999}) (\phi_3^{99a'}) + \frac{1}{4} (\phi_3^{99a'}) (\phi_3^9, p') - \frac{3}{2} (\phi_3^{99p'}) (\phi_3^9, a') + v_0^2 \left( (d^{p'a'}) (\phi_3^{99p'}) - \frac{1}{4} (\phi_3^{999}) (\phi_3^{99a'}) - \frac{1}{2} (\phi_3^{99p'}) (\phi_3^9, a') \right) - (d_{p,a'}) (\phi_3^9, p'q') + \frac{1}{2} (\phi_3^9, a') (\phi_3^9, p'q') - 2 (d_{p,q'}) (\phi_3^9, p'a') + \frac{1}{2} (\phi_3^9, q') (\phi_3^9, p'a') + \frac{1}{2} (\phi_4^{999a'}) - \frac{1}{2} (\phi_4^9, p'a') \right)$$

$v^2 u^1$

**foo40[[3, 2]]**

0

$v^3 u^1$

**foo40[[4, 2]]**

$$o^2 \left( - (d^{p'a'}) (\phi_3^{99p'}) + \frac{1}{4} (\phi_3^{999}) (\phi_3^{99a'}) + \frac{1}{2} (\phi_3^{99p'}) (\phi_3^9, a') - \frac{1}{6} (\phi_4^{999a'}) \right)$$

$v^4 u^1$

**foo40[[5, 2]]**

0

$u^2$ -coefficients

$v^0 u^2$

**foo40[[1, 3]]**

$$-\frac{1}{2} - o v_0 (d^{a'b'}) + o^2 \left( 2 (d_{p,b'}) (d^{p'a'}) - \frac{1}{2} v_0^2 (d^{a'b'}) (\phi_3^{999}) - \frac{1}{2} (d^{a'b'}) (\phi_3^9, p') - 2 (d^{p'b'}) (\phi_3^9, a') - \frac{1}{4} (\phi_3^9, q', a') (\phi_3^9, q', b') + \frac{1}{4} (\phi_4^9, p', a', b') \right)$$

$v^1 u^2$

**foo40[[2, 3]]**

$$o \left( - (d^{a'b'}) + \frac{1}{2} (\phi_3^9, a', b') \right) + o^2 v_0 \left( -2 (d_{p,b'}) (d^{p'a'}) + \frac{1}{2} (d^{a'b'}) (\phi_3^{999}) + \frac{3}{8} (\phi_3^{99a'}) (\phi_3^{99b'}) + \frac{1}{2} (\phi_3^9, p', b') (\phi_3^9, p', a') - \frac{1}{4} (\phi_4^9, a', b') \right)$$

$v^2 u^2$

**foo40[[3, 3]]**

0

$v^3 u^2$



**foo40[[4, 3]]**

0

$v^4 u^2$

**foo40[[5, 3]]**

0

$u^3$ -coefficients

$v^0 u^3$

**foo40[[1, 4]]**

$$-o^2 v_0 (e^{a'b'c'}) - \frac{1}{6} o (\phi_3^{a'b'c'})$$

$v^1 u^3$

**foo40[[2, 4]]**

$$o^2 \left( -2 (e^{a'b'c'}) - \frac{3}{2} (d^{b'c'}) (\phi_3^{99a'}) - \frac{1}{4} (\phi_3^{99c'}) (\phi_3^{9a'b'}) + \right. \\ \left. (d_{p'}^{c'}) (\phi_3^{p'a'b'}) - \frac{1}{2} (\phi_3^9_{p'}^{c'}) (\phi_3^{p'a'b'}) + \frac{1}{3} (\phi_4^{9a'b'c'}) \right)$$

$v^2 u^3$

**foo40[[3, 4]]**

0

$v^3 u^3$

**foo40[[4, 4]]**

0

$v^4 u^3$

**foo40[[5, 4]]**

0

$u^4$ -coefficients

$v^0 u^4$

**foo40[[1, 5]]**

$$o^2 \left( -\frac{1}{2} (d^{a'b'}) (d^{c'd'}) + \frac{1}{2} (d^{c'd'}) (\phi_3^{9a'b'}) - \frac{1}{24} (\phi_4^{a'b'c'd'}) \right)$$

$v^1 u^4$

**foo40[[2, 5]]**

0

```

v2 u4

foo40[[3, 5]]
0

v3 u4

foo40[[4, 5]]
0

v4 u4

foo40[[5, 5]]
0

```

### ■ z<sub>c</sub>-formula

We modify the signed distance  $v$  to obtain a modified signed distance specified by  $w = v + \sum_{r=0}^{\infty} \text{cbr}[r] v^r + u_{a'} \sum_{r=0}^{\infty} \text{br}[a', r] v^r$ . The density function of  $w$  and its cumulants are obtained up to  $O(n^{-1})$  terms. The distribution function of  $w$  is calculated by applying the Cornish-Fisher expansion to the cumulants of  $w$ . We would also take account of the scaling by the factor  $\tau$  as well as the local coordinates at the projection in the below.

### ■ modified signed distance $w$

The inverse series of the modified signed distance specifies  $v = w - \sum_{r=0}^{\infty} \text{cr}[r] w^r - u_{a'} \sum_{r=0}^{\infty} \text{br}[a', r] w^r$ . We have assumed that  $\text{cbr}[0]$  and  $\text{cbr}[2]$  are  $O(n^{-1/2})$  and  $\text{cbr}[1]$ ,  $\text{cbr}[3]$ , and all  $\text{br}[a', r]$  are  $O(n^{-1})$ . The other coefficients are  $\text{cbr}[r] = O(n^{-3/2})$  for  $r \geq 4$ . Then the same order applies to  $\text{cr}[r]$ 's. The modified signed distance  $w$  is characterized by the coefficient vector  $c = (\text{cr}[0], \text{cr}[1], \text{cr}[2], \text{cr}[3])$  up to  $O(n^{-1})$  terms, since we can ignore the linear term in  $u$  as explained later. The change of variable is given in "rulevinuw" for  $v$  expressed in terms of  $u$  and  $w$ . The Jacobian is given in  $\text{logjvw} = \log \frac{\partial v}{\partial w}$ . The joint density of  $(u, w)$  is obtained by  $f(u, w | v_0) = f(u, v(w, u) | v_0) J$ , and  $\log f(u, w | v_0)$  is stored in "logdensityuw". We then calculate  $\log f(w | v_0) = \log \int f(u, w | v_0) du$  as an application of "logeexpoly" to  $\text{logdensityuw}$ , and stored in "logdensityw". In fact, the linear term in  $u$ , namely  $u_{a'} \sum_{r=0}^{\infty} \text{br}[a', r] w^r$  does not contribute to the argument for deriving the distribution function of  $w$  as seen in  $\text{logdensityw}$ . By using "logeexpoly" again, we obtain the cumulants of  $w$  as shown in "cumulantw".

### ■ define the modified signed distance as a series of $v$ .

Define  $w = \text{foo45}$  as a function of  $v$  below.

```

foo44 = {o, o2, o, o2};

foo45 = v + Sum[foo44[[i + 1]] cbr[i] vi, {i, 0, 3}]
v + o cbr[0] + o2 v cbr[1] + o v2 cbr[2] + o2 v3 cbr[3]

```

Then consider the inversion  $v = \text{foo46}$  as a function of  $w$  below.

```
foo46 = w - Sum[foo44[[i + 1]] cr[i] wi, {i, 0, 3}]
w - o cr[0] - o2 w cr[1] - o w2 cr[2] - o2 w3 cr[3]
```

The relations between the two sets of the coefficients are given below.

```
func47[cbs_] :=
  Table[gets2[cbs[[i + 1]] - Sum[(i - j + 1) cbs[[i - j + 1 + 1]] cbs[[j + 1]], {j, 0, i}],
    {i, 0, Length[cbs] - 2}]

foo47 = func47[{o cbr[0], o2 cbr[1], o cbr[2], o2 cbr[3], 0}] / foo44
{cbr[0], cbr[1] - 2 cbr[0] cbr[2], cbr[2], -2 cbr[2]2 + cbr[3]}

rule47 = Table[cr[i] → foo47[[i + 1]], {i, 0, 3}]
{cr[0] → cbr[0], cr[1] → cbr[1] - 2 cbr[0] cbr[2],
  cr[2] → cbr[2], cr[3] → -2 cbr[2]2 + cbr[3]}
```

The relation is actually obtained by solving the following coefficients==0.

```
Simplify[CoefficientList[gets2[foo45 /. {v → foo46}], w]]
{o (cbr[0] - cr[0]), 1 + o2 (cbr[1] - 2 cbr[2] cr[0] - cr[1]),
  o (cbr[2] - cr[2]), o2 (cbr[3] - 2 cbr[2] cr[2] - cr[3])}
```

Checking if the relation is correct by seeing the identity.

```
gets2[foo45 /. {v → foo46}] /. rule47]
w
```

Consider the following  $O(n^{-1})$  term.

$$\text{func48}[v\_]=\text{ru}[\text{ala}] o^2 \sum_{r=0}^{\infty} \text{br}[\text{aua}, r] v^r$$

$$o^2 (u_{a^1}) \sum_{r=0}^{\infty} \text{br}[\text{a}^1, r] v^r$$

Since  $v = w + O(n^{-1/2})$ ,  $\text{func48}[v] = \text{func48}[w] + O(n^{-3/2})$ , and we can ignore the difference between  $\text{func48}[v]$  and  $\text{func48}[w]$ . So, if we redefine  $w = \text{foo45} + \text{func48}[v]$ , and  $v = \text{foo46} - \text{func48}[w]$ , the inversion relation still holds. We call "v" as the signed distance, and "w" as a modified signed distance characterized by the coefficients  $\text{cr}[r]$  and  $\text{br}[r]$ .

Jacobian  $J = \frac{\partial v}{\partial w}$  of the transformation from v to w is given below. Here  $D[\text{func48}[w], w]$  is denoted as  $o^2 u_{a^1} \text{dbr}^{a^1}$ .

```
DefineTensor[tDbr, "dbr", {{1}, 1}]
PermWeight::def : Object dbr defined

foo49 = D[foo46, w] - o2 ru[ala] tDbr[aua]
1 - o2 cr[1] - 2 o w cr[2] - 3 o2 w2 cr[3] - o2 (u_{a^1}) (dbr^{a^1})
```

We need the log of the Jacobian for later use.  $\text{logjvw} = \log \frac{\partial v}{\partial w}$ .

$$\log jvw = \text{geto2} \left[ (\text{foo49} - 1) - \frac{1}{2} (\text{foo49} - 1)^2 \right] \\ - 2 \circ w \text{ cr}[2] + o^2 (-\text{cr}[1] - 2 w^2 \text{ cr}[2]^2 - 3 w^2 \text{ cr}[3] - (u_a) (dbr^{a'}) )$$

Similarly, we write  $\text{func48}[w]$  as  $o^2 u_a' br^a$ , and  $\text{vinuw}$  is  $v$  expressed by  $u$  and  $w$ .

```
DefineTensor[tbr, "br", {{1}, 1}]
PermWeight::def : Object br defined

vinuw = CanAll[foo46 - o^2 ru[ala] tbr[aua]]
w - o cr[0] - o^2 w cr[1] - o w^2 cr[2] - o^2 w^3 cr[3] - o^2 (u_p) (br^p)

RuleUnique[rulevinuw, v, vinuw]
```

### ■ density function of w

First, we obtain the joint density of  $(u,w)$  i.e.,  $f(u,w|v0)=f(u,v(w,u)|v0)J$  from the joint density of  $(u,v)$ , the transformation  $v=v(w,u)$ , and the Jacobian.

```
foo50 = tsimpp[tgeto2[ApplyRules[logdensityuv, rulevinuw] + logjvw]];
```

This is the log of the density.  $\text{logdensityuw} = \log f(u,w|v0)$ .

$$\begin{aligned}
 & \text{logdensityuw} = \text{Collect}[\text{foo50}, \{\text{ru}[\text{a11}] \text{ru}[\text{a12}] \text{ru}[\text{a13}] \text{ru}[\text{a14}], \\
 & \quad \text{ru}[\text{a11}] \text{ru}[\text{a12}] \text{ru}[\text{a13}], \text{ru}[\text{a11}] \text{ru}[\text{a12}], \text{ru}[\text{a11}], \text{o}, \text{w}, \text{v0}\}] \\
 & - \frac{\text{v0}^2}{2} + \text{v0 w} - \frac{\text{w}^2}{2} - \frac{1}{2} \dim \text{Log}[2 \pi] + \\
 & \text{o} \left( -\text{v0 cr}[0] - \text{v0 w}^2 \text{cr}[2] + \text{w}^3 \left( \text{cr}[2] - \frac{1}{6} (\phi 3^{999}) \right) - \frac{1}{3} \text{v0}^3 (\phi 3^{999}) + \right. \\
 & \quad \left. \text{w} \left( \text{cr}[0] - 2 \text{cr}[2] + 2 (\text{d}_{\text{p}, \text{p}'}) + \frac{1}{2} (\phi 3^{999}) + \frac{1}{2} \text{v0}^2 (\phi 3^{999}) - \frac{1}{2} (\phi 3^{\text{p}, \text{p}'}) \right) \right) + \\
 & (\text{u}_{\text{p}'}) \left( -\frac{1}{2} (\text{u}_{\text{p}'}) + \text{o} \left( \frac{1}{2} \text{v0}^2 (\phi 3^{99\text{p}'}) - \frac{1}{2} \text{v0 w} (\phi 3^{99\text{p}'}) + \frac{1}{2} (\phi 3_{\text{q}, \text{p}'\text{q}'}) \right) + \right. \\
 & \quad \text{o}^2 \left( -(\text{dbr}^{\text{p}'}) + \frac{1}{2} \text{v0 w}^2 \text{cr}[2] (\phi 3^{99\text{p}'}) + \text{v0} \left( -(\text{br}^{\text{p}'}) + \frac{1}{2} \text{cr}[0] (\phi 3^{99\text{p}'}) \right) + \right. \\
 & \quad \left. \text{w}^3 \left( -(\text{d}^{\text{p}'\text{q}'}) (\phi 3^{99_{\text{q}'}}) + \frac{1}{4} (\phi 3^{999}) (\phi 3^{99\text{p}'}) + \frac{1}{2} (\phi 3^{99\text{q}'}) (\phi 3^{\text{q}, \text{p}'}) - \frac{1}{6} (\phi 4^{999\text{p}'}) \right) + \right. \\
 & \quad \frac{1}{6} \text{v0}^3 (\phi 4^{999\text{p}'}) + \text{w} \left( \text{br}^{\text{p}'} + 6 (\text{e}_{\text{q}, \text{p}'\text{q}'} + 5 (\text{d}^{\text{p}'\text{q}'}) (\phi 3^{99_{\text{q}'}}) + \right. \\
 & \quad (\text{d}_{\text{q}, \text{q}'} (\phi 3^{99\text{p}'}) - \frac{3}{4} (\phi 3^{999}) (\phi 3^{99\text{p}'}) - \frac{3}{2} (\phi 3^{99\text{q}'}) (\phi 3^{\text{q}, \text{p}'}) + \\
 & \quad \left. \text{v0}^2 \left( (\text{d}^{\text{p}'\text{q}'}) (\phi 3^{99_{\text{q}'}}) - \frac{1}{4} (\phi 3^{999}) (\phi 3^{99\text{p}'}) - \frac{1}{2} (\phi 3^{99\text{q}'}) (\phi 3^{\text{q}, \text{p}'}) \right) + \right. \\
 & \quad \frac{1}{4} (\phi 3^{99\text{p}'}) (\phi 3^{\text{q}, \text{q}'} - 2 (\text{d}_{\text{q}, \text{r}'} (\phi 3_{\text{r}, \text{p}'\text{q}'}) + \frac{1}{2} (\phi 3^{\text{q}, \text{r}'} (\phi 3_{\text{r}, \text{p}'\text{q}'}) - \\
 & \quad (\text{d}_{\text{q}, \text{p}'} (\phi 3_{\text{r}, \text{q}'\text{r}'} + \frac{1}{2} (\phi 3^{\text{q}, \text{p}'} (\phi 3_{\text{r}, \text{q}'\text{r}'} + \frac{1}{2} (\phi 4^{999\text{p}'}) - \frac{1}{2} (\phi 4^{\text{q}, \text{p}'\text{q}'}) \left. \left. \right) \right) \right) + \\
 & (\text{u}_{\text{p}'}) (\text{u}_{\text{q}'}) (\text{u}_{\text{r}'} \left( -\frac{1}{6} \text{o} (\phi 3^{\text{p}'\text{q}'\text{r}'} + \text{o}^2 \left( -\text{v0} (\text{e}^{\text{p}'\text{q}'\text{r}'} + \text{w} \left( -2 (\text{e}^{\text{p}'\text{q}'\text{r}'} - \frac{3}{2} (\text{d}^{\text{q}'\text{r}'} (\phi 3^{99\text{p}'}) - \frac{1}{4} \right. \right. \right. \right. \\
 & \quad \left. \left. \left. (\phi 3^{99\text{r}'} (\phi 3^{99\text{q}'}) + (\text{d}_{\text{s}, \text{r}'} (\phi 3^{\text{p}'\text{q}'\text{s}'} - \frac{1}{2} (\phi 3^{\text{q}, \text{r}'} (\phi 3^{\text{p}'\text{q}'\text{s}'} + \frac{1}{3} (\phi 4^{99\text{p}'\text{q}'\text{r}'} \right) \right) \right) \right) + \\
 & \text{o}^2 \left( -\frac{1}{2} \text{cr}[0]^2 - \text{cr}[1] - \text{v0 w}^3 \text{cr}[3] - 2 \text{cr}[0] (\text{d}_{\text{p}, \text{p}'}) - \frac{1}{2} \text{cr}[0] (\phi 3^{999}) - \right. \\
 & \quad \frac{1}{2} \text{v0}^2 \text{cr}[0] (\phi 3^{999}) + \frac{1}{6} (\phi 3^{999})^2 + \\
 & \quad \frac{1}{2} (\phi 3^{\text{p}, \text{p}'} (\phi 3^{99\text{p}'}) + \frac{1}{2} \text{cr}[0] (\phi 3^{\text{p}, \text{p}'}) + \\
 & \quad \frac{1}{2} (\phi 3^{\text{p}, \text{q}'} (\phi 3^{\text{q}, \text{p}'}) + \frac{1}{6} (\phi 3_{\text{p}, \text{q}'\text{r}'} (\phi 3^{\text{p}'\text{q}'\text{r}'} + \\
 & \text{w}^4 \left( -\frac{1}{2} \text{cr}[2]^2 + \text{cr}[3] + \frac{1}{2} \text{cr}[2] (\phi 3^{999}) - \frac{1}{24} (\phi 4^{9999}) \right) - \\
 & \quad \frac{1}{8} (\phi 4^{9999}) - \frac{1}{8} \text{v0}^4 (\phi 4^{9999}) + \text{w} \left( -\text{v0 cr}[1] + \frac{1}{6} \text{v0}^3 (\phi 4^{9999}) \right) + \\
 & \text{w}^2 \left( \text{cr}[1] - \text{cr}[0] \text{cr}[2] - 2 \text{cr}[2]^2 - 3 \text{cr}[3] - 2 \text{cr}[2] (\text{d}_{\text{p}, \text{p}'}) - 2 (\text{d}_{\text{p}, \text{q}'}) (\text{d}_{\text{q}, \text{p}'}) + \right. \\
 & \quad \frac{1}{2} \text{cr}[0] (\phi 3^{999}) - \frac{1}{2} \text{cr}[2] (\phi 3^{999}) - \frac{1}{2} \text{v0}^2 \text{cr}[2] (\phi 3^{999}) - \frac{1}{4} (\phi 3^{999})^2 - \\
 & \quad \frac{1}{2} (\phi 3^{\text{p}, \text{p}'} (\phi 3^{99\text{p}'}) + \frac{1}{2} \text{cr}[2] (\phi 3^{\text{p}, \text{p}'}) + 2 (\text{d}_{\text{p}, \text{q}'}) (\phi 3^{\text{q}, \text{p}'}) - \\
 & \quad \left. \frac{3}{4} (\phi 3^{\text{p}, \text{q}'} (\phi 3^{\text{q}, \text{p}'}) + \frac{1}{4} (\phi 4^{9999}) + \frac{1}{4} (\phi 4^{\text{p}, \text{p}'}) \right) - \frac{1}{4} (\phi 4^{\text{p}, \text{p}'}) - \frac{1}{8} (\phi 4_{\text{p}, \text{q}'\text{p}'\text{q}'} \left. \right) + \\
 & (\text{u}_{\text{p}'}) (\text{u}_{\text{q}'}) \left( \text{o} \left( -\text{v0} (\text{d}^{\text{p}'\text{q}'}) + \text{w} \left( -(\text{d}^{\text{p}'\text{q}'}) + \frac{1}{2} (\phi 3^{\text{p}'\text{q}'}) \right) \right) + \right. \\
 & \quad \text{o}^2 \left( \text{cr}[0] (\text{d}^{\text{p}'\text{q}'}) + 2 (\text{d}_{\text{r}, \text{q}'}) (\text{d}^{\text{p}'\text{r}'} - \frac{1}{2} \text{v0}^2 (\text{d}^{\text{p}'\text{q}'}) (\phi 3^{999}) - 2 (\text{d}^{\text{q}'\text{r}'} (\phi 3^{\text{q}, \text{p}'}) - \right. \\
 & \quad \frac{1}{2} (\text{d}^{\text{p}'\text{q}'}) (\phi 3^{\text{q}, \text{r}'} - \frac{1}{2} \text{cr}[0] (\phi 3^{\text{p}'\text{q}'}) + \text{w}^2 \left( \text{cr}[2] (\text{d}^{\text{p}'\text{q}'}) - \frac{1}{2} \text{cr}[2] (\phi 3^{\text{p}'\text{q}'}) \right) - \\
 & \quad \frac{1}{4} (\phi 3_{\text{r}, \text{s}, \text{p}'} (\phi 3^{\text{q}'\text{r}'\text{s}'} + \text{v0 w} \left( -2 (\text{d}_{\text{r}, \text{q}'}) (\text{d}^{\text{p}'\text{r}'} + \frac{1}{2} (\text{d}^{\text{p}'\text{q}'}) (\phi 3^{999}) + \right. \\
 & \quad \left. \left. \frac{3}{8} (\phi 3^{99\text{p}'}) (\phi 3^{99\text{q}'}) + \frac{1}{2} (\phi 3^{\text{q}, \text{r}'} (\phi 3^{\text{p}'\text{r}'} - \frac{1}{4} (\phi 4^{99\text{p}'\text{q}'}) \right) + \frac{1}{4} (\phi 4_{\text{r}, \text{p}'\text{q}'\text{r}'} \right) \left. \right) + \\
 & \text{o}^2 (\text{u}_{\text{p}'}) (\text{u}_{\text{q}'}) (\text{u}_{\text{r}'} (\text{u}_{\text{s}'} \left( -\frac{1}{2} (\text{d}^{\text{p}'\text{q}'}) (\text{d}^{\text{r}'\text{s}'} + \frac{1}{2} (\text{d}^{\text{r}'\text{s}'} (\phi 3^{\text{p}'\text{q}'}) - \frac{1}{24} (\phi 4^{\text{p}'\text{q}'\text{r}'\text{s}'} \right) \right) \left. \right)
 \end{aligned}$$

This is the log of the standard multivariate normal density in dim-1 dimension.

$$\text{foo51} = -\frac{\text{dim} - 1}{2} \text{Log}[2 \text{Pi}] - \frac{1}{2} \text{ru}[\text{ala}] \text{ru}[\text{aua}]$$

$$\frac{1}{2} (1 - \text{dim}) \text{Log}[2 \pi] - \frac{1}{2} (u_{a'}) (u^{a'})$$

Get the coefficients of the polynomials of  $u_{a'}$  from  $\log f(u, w | v_0) - \text{foo51}$ .

```
foo52 = Collect[CoefficientList[(logdensityw - foo51) /. {ru[al_] -> u}, u], o,
  tsimpp[CanAll[# /. {au1 -> aua, au2 -> aub, au3 -> auc, au4 -> aud, au5 -> aue,
    all -> ala, al2 -> alb, al3 -> alc, al4 -> ald, al5 -> ale}]] &];
```

Dimensions[foo52]

{5}

constant term in terms of u

foo52[[1]]

$$\begin{aligned} & -\frac{v_0^2}{2} + v_0 w - \frac{w^2}{2} - \frac{1}{2} \text{Log}[2 \pi] + \\ & o\left(-v_0 \text{cr}[0] + w \text{cr}[0] - 2 w \text{cr}[2] - v_0 w^2 \text{cr}[2] + w^3 \text{cr}[2] + 2 w (d_{p', p'}) - \right. \\ & \quad \left. \frac{1}{3} v_0^3 (\phi_3^{999}) + \frac{1}{2} w (\phi_3^{999}) + \frac{1}{2} v_0^2 w (\phi_3^{999}) - \frac{1}{6} w^3 (\phi_3^{999}) - \frac{1}{2} w (\phi_3^9_{p', p'})\right) + \\ & o^2\left(-\frac{1}{2} \text{cr}[0]^2 - \text{cr}[1] - v_0 w \text{cr}[1] + w^2 \text{cr}[1] - w^2 \text{cr}[0] \text{cr}[2] - 2 w^2 \text{cr}[2]^2 - \frac{1}{2} w^4 \text{cr}[2]^2 - \right. \\ & \quad 3 w^2 \text{cr}[3] - v_0 w^3 \text{cr}[3] + w^4 \text{cr}[3] + (-2 \text{cr}[0] - 2 w^2 \text{cr}[2]) (d_{p', p'}) - 2 w^2 (d_{p', q'}) (d_{q', p'}) - \\ & \quad \frac{1}{2} \text{cr}[0] (\phi_3^{999}) - \frac{1}{2} v_0^2 \text{cr}[0] (\phi_3^{999}) + \frac{1}{2} w^2 \text{cr}[0] (\phi_3^{999}) - \frac{1}{2} w^2 \text{cr}[2] (\phi_3^{999}) - \\ & \quad \frac{1}{2} v_0^2 w^2 \text{cr}[2] (\phi_3^{999}) + \frac{1}{2} w^4 \text{cr}[2] (\phi_3^{999}) + \frac{1}{6} (\phi_3^{999})^2 - \frac{1}{4} w^2 (\phi_3^{999})^2 + \\ & \quad \left(\frac{1}{2} - \frac{w^2}{2}\right) (\phi_3^9_{p'}) (\phi_3^9_{p'}) + \left(\frac{\text{cr}[0]}{2} + \frac{1}{2} w^2 \text{cr}[2]\right) (\phi_3^9_{p', p'}) + 2 w^2 (d_{p', q'}) (\phi_3^9_{q', p'}) + \\ & \quad \left(\frac{1}{2} - \frac{3 w^2}{4}\right) (\phi_3^9_{p', q'}) (\phi_3^9_{q', p'}) + \frac{1}{6} (\phi_3^9_{p', q', r'}) (\phi_3^9_{p', q', r'}) - \frac{1}{8} (\phi_4^{9999}) - \frac{1}{8} v_0^4 (\phi_4^{9999}) + \\ & \quad \left. \frac{1}{6} v_0^3 w (\phi_4^{9999}) + \frac{1}{4} w^2 (\phi_4^{9999}) - \frac{1}{24} w^4 (\phi_4^{9999}) + \left(-\frac{1}{4} + \frac{w^2}{4}\right) (\phi_4^9_{p', p'}) - \frac{1}{8} (\phi_4^9_{p', q', p', q'})\right) \end{aligned}$$

coefficient of  $u_{a'}$

foo52[[2]]

$$\begin{aligned} & o\left(\left(\frac{v_0^2}{2} - \frac{v_0 w}{2}\right) (\phi_3^{999a'}) + \frac{1}{2} (\phi_3^9_{p', p' a'})\right) + o^2 \\ & \left((-v_0 + w) (b r^{a'}) - d b r^{a'} + 6 w (e_{p', p' a'}) + (5 w + v_0^2 w - w^3) (d^{p' a'}) (\phi_3^9_{p'}) + w (d_{p', p'}) (\phi_3^{999a'}) + \right. \\ & \quad \left(\frac{1}{2} v_0 \text{cr}[0] + \frac{1}{2} v_0 w^2 \text{cr}[2] - \frac{3}{4} w (\phi_3^{999}) - \frac{1}{4} v_0^2 w (\phi_3^{999}) + \frac{1}{4} w^3 (\phi_3^{999})\right) (\phi_3^{999a'}) + \\ & \quad \frac{1}{4} w (\phi_3^{999a'}) (\phi_3^9_{p', p'}) + \left(-\frac{3 w}{2} - \frac{v_0^2 w}{2} + \frac{w^3}{2}\right) (\phi_3^{999p'}) (\phi_3^9_{p', a'}) - \\ & \quad w (d_{p', a'}) (\phi_3^9_{q', p', q'}) + \frac{1}{2} w (\phi_3^9_{p', a'}) (\phi_3^9_{q', p', q'}) - 2 w (d_{p', q'}) (\phi_3^9_{q', p', a'}) + \\ & \quad \left. \frac{1}{2} w (\phi_3^9_{p', q'}) (\phi_3^9_{q', p', a'}) + \left(\frac{v_0^3}{6} + \frac{w}{2} - \frac{w^3}{6}\right) (\phi_4^{9999a'}) - \frac{1}{2} w (\phi_4^9_{p', p' a'})\right) \end{aligned}$$

coefficient of  $u_{a'} u_{b'}$

foo52[[3]]

$$\begin{aligned} & o \left( (-v_0 - w) (d^{a'b'}) + \frac{1}{2} w (\phi_3^{9a'b'}) \right) + \\ & o^2 \left( (2 - 2 v_0 w) (d_p^{b'}) (d^{p'a'}) + (d^{a'b'}) \left( cr[0] + w^2 cr[2] - \frac{1}{2} v_0^2 (\phi_3^{999}) + \frac{1}{2} v_0 w (\phi_3^{999}) \right) + \right. \\ & \quad \frac{3}{8} v_0 w (\phi_3^{99a'}) (\phi_3^{99b'}) - \frac{1}{2} (d^{a'b'}) (\phi_3^9_{p,p'}) - 2 (d^{p'b'}) (\phi_3^9_{p,a'}) + \\ & \quad \frac{1}{2} v_0 w (\phi_3^9_{p,b'}) (\phi_3^{9p'a'}) + \left( -\frac{cr[0]}{2} - \frac{1}{2} w^2 cr[2] \right) (\phi_3^{9a'b'}) - \\ & \quad \left. \frac{1}{4} (\phi_3^9_{p,q'}) (\phi_3^{9p'q'b'}) - \frac{1}{4} v_0 w (\phi_4^{99a'b'}) + \frac{1}{4} (\phi_4^9_{p,p'a'b'}) \right) \end{aligned}$$

coefficient of  $u_a' u_b' u_c'$

foo52[[4]]

$$\begin{aligned} & -\frac{1}{6} o (\phi_3^{a'b'c'}) + \\ & o^2 \left( (-v_0 - 2 w) (e^{a'b'c'}) - \frac{3}{2} w (d^{b'c'}) (\phi_3^{99a'}) - \frac{1}{4} w (\phi_3^{99c'}) (\phi_3^{9a'b'}) + w (d_p^{c'}) (\phi_3^{9p'a'b'}) - \right. \\ & \quad \left. \frac{1}{2} w (\phi_3^9_{p,c'}) (\phi_3^{9p'a'b'}) + \frac{1}{3} w (\phi_4^{9a'b'c'}) \right) \end{aligned}$$

coefficient of  $u_a' u_b' u_c' u_d'$

foo52[[5]]

$$o^2 \left( -\frac{1}{2} (d^{a'b'}) (d^{c'd'}) + \frac{1}{2} (d^{c'd'}) (\phi_3^{9a'b'}) - \frac{1}{24} (\phi_4^{a'b'c'd'}) \right)$$

We now calculate  $\log f(w|v_0) = \log \int f(u, w|v_0) du$  as an application of "logeexppoly" to foo52. It is denoted by logdensityw.

```
foo53 = Collect[foo52 / {1, o, o, o, o^2}, o];
RuleUnique[rule53u0, ta0, foo53[[1]]]
RuleUnique[rule53u1, ta1[aua_], foo53[[2]]]
RuleUnique[rule53u2, ta2[aua_, aub_], tsimp[Symmetrize[foo53[[3]], {aua, aub}]]]
RuleUnique[rule53u3, ta3[aua_, aub_, auc_],
  tsimp[Symmetrize[foo53[[4]], {aua, aub, auc}]]]
RuleUnique[rule53u4, ta4[aua_, aub_, auc_, aud_],
  tsimp[Symmetrize[foo53[[5]], {aua, aub, auc, aud}]]]
foo54 = tgeto2[ApplyRules[logeexppoly /
  {l1 -> a11, u1 -> au1, l2 -> a12, u2 -> au2, l3 -> a13, u3 -> au3, l4 -> a14, u4 -> au4} /
  {sb[la_] -> 0}, {rule53u0, rule53u1, rule53u2, rule53u3, rule53u4}]]];
```

This is  $\log f(w|v_0)$ .

**logdensityw = Collect[foo54, {w, o, v0}, tsimpp]**

$$\begin{aligned}
 & -\frac{v0^2}{2} - \frac{1}{2} \text{Log}[2 \pi] + w^3 \left( -o^2 v0 \text{cr}[3] + o \left( \text{cr}[2] - \frac{1}{6} (\phi3^{999}) \right) \right) + \\
 & o \left( v0 (-\text{cr}[0] - d_{p',p'}) - \frac{1}{3} v0^3 (\phi3^{999}) \right) + \\
 & o^2 w^4 \left( -\frac{1}{2} \text{cr}[2]^2 + \text{cr}[3] + \frac{1}{2} \text{cr}[2] (\phi3^{999}) - \frac{1}{24} (\phi4^{9999}) \right) + \\
 & w \left( v0 + o \left( \text{cr}[0] - 2 \text{cr}[2] + d_{p',p'} + \frac{1}{2} (\phi3^{999}) + \frac{1}{2} v0^2 (\phi3^{999}) \right) + \right. \\
 & \quad o^2 \left( v0^3 \left( -\frac{1}{4} (\phi3^{99}_{p'}) (\phi3^{99}_{p'}) + \frac{1}{6} (\phi4^{9999}) \right) + v0 \left( -\text{cr}[1] + \frac{1}{2} (d_{p',p'}) (\phi3^{999}) + \right. \right. \\
 & \quad \left. \left. \frac{3}{8} (\phi3^{99}_{p'}) (\phi3^{99}_{p'}) - (d^{p',q'}) (\phi3^{99}_{p',q'}) + \frac{1}{2} (\phi3^{99}_{p',q'}) (\phi3^{99}_{q',p'}) - \frac{1}{4} (\phi4^{99}_{p',p'}) \right) \right) \left. \right) + \\
 & w^2 \left( -\frac{1}{2} - o v0 \text{cr}[2] + o^2 \left( \text{cr}[1] - \text{cr}[0] \text{cr}[2] - 2 \text{cr}[2]^2 - 3 \text{cr}[3] - \text{cr}[2] (d_{p',p'}) - \right. \right. \\
 & \quad (d_{p',q'}) (d_{q',p'}) + \frac{1}{2} \text{cr}[0] (\phi3^{999}) - \frac{1}{2} \text{cr}[2] (\phi3^{999}) - \frac{1}{4} (\phi3^{999})^2 - \\
 & \quad \left. \frac{1}{2} (\phi3^{99}_{p'}) (\phi3^{99}_{p'}) + v0^2 \left( -\frac{1}{2} \text{cr}[2] (\phi3^{999}) + \frac{1}{8} (\phi3^{99}_{p'}) (\phi3^{99}_{p'}) \right) + \right. \\
 & \quad \left. (d^{p',q'}) (\phi3^{99}_{p',q'}) - \frac{1}{2} (\phi3^{99}_{p',q'}) (\phi3^{99}_{q',p'}) + \frac{1}{4} (\phi4^{9999}) + \frac{1}{4} (\phi4^{99}_{p',p'}) \right) \left. \right) + \\
 & o^2 \left( -\frac{1}{2} \text{cr}[0]^2 - \text{cr}[1] - \text{cr}[0] (d_{p',p'}) + (d_{p',q'}) (d_{q',p'}) - \frac{1}{2} (d_{p',p'}) (d_{q',q'}) - \frac{1}{2} \text{cr}[0] (\phi3^{999}) + \right. \\
 & \quad \frac{1}{6} (\phi3^{999})^2 + v0^2 \left( (d_{p',q'}) (d^{p',q'}) - \frac{1}{2} \text{cr}[0] (\phi3^{999}) - \frac{1}{2} (d_{p',p'}) (\phi3^{999}) \right) + \\
 & \quad \frac{1}{2} (\phi3^{99}_{p'}) (\phi3^{99}_{p'}) - (d^{p',q'}) (\phi3^{99}_{p',q'}) + \frac{1}{2} (\phi3^{99}_{p',q'}) (\phi3^{99}_{q',p'}) - \\
 & \quad \left. \frac{1}{8} (\phi3_{p',q',q'}) (\phi3_{r',p',r'}) + \frac{1}{8} (\phi3_{p',q',p'}) (\phi3_{r',q',r'}) + \right. \\
 & \quad \left. v0^4 \left( \frac{1}{8} (\phi3^{99}_{p'}) (\phi3^{99}_{p'}) - \frac{1}{8} (\phi4^{9999}) \right) - \frac{1}{8} (\phi4^{9999}) - \frac{1}{4} (\phi4^{99}_{p',p'}) \right)
 \end{aligned}$$



logdensityw // InputForm

```

-v0^2/2 - Log[2*Pi]/2 + w^3*(-(o^2*v0*cr[3]) +
  o*(cr[2] - tp3[9, 9, 9]/6)) +
o*(v0*(-cr[0] - td[al1, au1]) - (v0^3*tp3[9, 9, 9])/3) +
o^2*w^4*(-cr[2]^2/2 + cr[3] + (cr[2]*tp3[9, 9, 9])/2 -
  tp4[9, 9, 9, 9]/24) +
w*(v0 + o*(cr[0] - 2*cr[2] + td[al1, au1] + tp3[9, 9, 9]/2 +
  (v0^2*tp3[9, 9, 9])/2) +
  o^2*(v0^3*(-(tp3[9, 9, al1]*tp3[9, 9, au1])/4 +
    tp4[9, 9, 9, 9]/6) +
    v0*(-cr[1] + (td[al1, au1]*tp3[9, 9, 9])/2 +
      (3*tp3[9, 9, al1]*tp3[9, 9, au1])/8 -
      td[au1, au2]*tp3[9, al1, al2] +
      (tp3[9, al1, au2]*tp3[9, al2, au1])/2 - tp4[9, 9, al1, au1]/
      4)) + w^2*(-1/2 - o*v0*cr[2] +
    o^2*(cr[1] - cr[0]*cr[2] - 2*cr[2]^2 - 3*cr[3] -
      cr[2]*td[al1, au1] - td[al1, au2]*td[al2, au1] +
      (cr[0]*tp3[9, 9, 9])/2 - (cr[2]*tp3[9, 9, 9])/2 -
      tp3[9, 9, 9]^2/4 - (tp3[9, 9, al1]*tp3[9, 9, au1])/2 +
      v0^2*(-(cr[2]*tp3[9, 9, 9])/2 +
        (tp3[9, 9, al1]*tp3[9, 9, au1])/8) +
        td[au1, au2]*tp3[9, al1, al2] -
        (tp3[9, al1, au2]*tp3[9, al2, au1])/2 + tp4[9, 9, 9, 9]/4 +
        tp4[9, 9, 9, al1, au1]/4)) +
    o^2*(-cr[0]^2/2 - cr[1] - cr[0]*td[al1, au1] +
      td[al1, au2]*td[al2, au1] - (td[al1, au1]*td[al2, au2])/2 -
      (cr[0]*tp3[9, 9, 9])/2 + tp3[9, 9, 9]^2/6 +
      v0^2*(td[al1, al2]*td[au1, au2] - (cr[0]*tp3[9, 9, 9])/2 -
        (td[al1, au1]*tp3[9, 9, 9])/2) +
        (tp3[9, 9, al1]*tp3[9, 9, au1])/2 -
        td[au1, au2]*tp3[9, al1, al2] +
        (tp3[9, al1, au2]*tp3[9, al2, au1])/2 -
        (tp3[al1, al2, au2]*tp3[al3, au1, au3])/8 +
        (tp3[al1, al2, au1]*tp3[al3, au2, au3])/8 +
        v0^4*((tp3[9, 9, al1]*tp3[9, 9, au1])/8 - tp4[9, 9, 9, 9]/8) -
        tp4[9, 9, 9, 9]/8 - tp4[9, 9, 9, al1, au1]/4)

```

The coefficients of  $w^i$  in  $\log f(w|v_0)$  are shown below.

```
foo55 = Collect[CoefficientList[logdensityw, w], {o, v0}, tsimp];
```

Coefficient of  $w^0$ .

```
foo55[[1]]
```

$$\begin{aligned}
 & -\frac{v_0^2}{2} - \frac{1}{2} \text{Log}[2\pi] + o\left(v_0(-cr[0] - d_{p,p'}) - \frac{1}{3} v_0^3 (\phi_3^{999})\right) + \\
 & o^2\left(-\frac{1}{2} cr[0]^2 - cr[1] - cr[0](d_{p,p'}) + (d_{p,q'}) (d_{q,p'}) - \frac{1}{2} (d_{p,p'}) (d_{q,q'}) - \frac{1}{2} cr[0] (\phi_3^{999}) + \right. \\
 & \quad \frac{1}{6} (\phi_3^{999})^2 + v_0^2\left((d_{p,q'}) (d_{p',q'}) - \frac{1}{2} cr[0] (\phi_3^{999}) - \frac{1}{2} (d_{p,p'}) (\phi_3^{999})\right) + \\
 & \quad \frac{1}{2} (\phi_3^{99p'}) (\phi_3^{99p'}) - (d_{p',q'}) (\phi_3^{9p',q'}) + \frac{1}{2} (\phi_3^{9p,q'}) (\phi_3^{9q',p'}) - \frac{1}{8} (\phi_{3p',q',q'}) (\phi_{3r',p',r'}) + \frac{1}{8} \\
 & \quad \left. (\phi_{3p',q',p'}) (\phi_{3r',q',r'}) + v_0^4\left(\frac{1}{8} (\phi_3^{99p'}) (\phi_3^{99p'}) - \frac{1}{8} (\phi_4^{9999})\right) - \frac{1}{8} (\phi_4^{9999}) - \frac{1}{4} (\phi_4^{99p,p'})\right)
 \end{aligned}$$

Coefficient of  $w^1$ .

foo55[[2]]

$$v_0 + o \left( cr[0] - 2 cr[2] + d_{p,p'} + \frac{1}{2} (\phi_{3^{999}}) + \frac{1}{2} v_0^2 (\phi_{3^{999}}) \right) +$$

$$o^2 \left( v_0^3 \left( -\frac{1}{4} (\phi_{3^{99p'}}) (\phi_{3^{99p'}}) + \frac{1}{6} (\phi_{4^{9999}}) \right) + v_0 \left( -cr[1] + \frac{1}{2} (d_{p,p'}) (\phi_{3^{999}}) + \right.$$

$$\left. \frac{3}{8} (\phi_{3^{99p'}}) (\phi_{3^{99p'}}) - (d_{p',q'}) (\phi_{3^{9p',q'}}) + \frac{1}{2} (\phi_{3^{9p',q'}}) (\phi_{3^{9q',p'}}) - \frac{1}{4} (\phi_{4^{99p',p'}}) \right) \right)$$

Coefficient of  $w^2$ .

foo55[[3]]

$$-\frac{1}{2} - o v_0 cr[2] + o^2 \left( cr[1] - cr[0] cr[2] - 2 cr[2]^2 - 3 cr[3] - \right.$$

$$cr[2] (d_{p,p'}) - (d_{p',q'}) (d_{q',p'}) + \frac{1}{2} cr[0] (\phi_{3^{999}}) - \frac{1}{2} cr[2] (\phi_{3^{999}}) - \frac{1}{4} (\phi_{3^{999}})^2 -$$

$$\frac{1}{2} (\phi_{3^{99p'}}) (\phi_{3^{99p'}}) + v_0^2 \left( -\frac{1}{2} cr[2] (\phi_{3^{999}}) + \frac{1}{8} (\phi_{3^{99p'}}) (\phi_{3^{99p'}}) \right) +$$

$$\left. (d_{p',q'}) (\phi_{3^{9p',q'}}) - \frac{1}{2} (\phi_{3^{9p',q'}}) (\phi_{3^{9q',p'}}) + \frac{1}{4} (\phi_{4^{9999}}) + \frac{1}{4} (\phi_{4^{99p',p'}}) \right)$$

Coefficient of  $w^3$ .

foo55[[4]]

$$-o^2 v_0 cr[3] + o \left( cr[2] - \frac{1}{6} (\phi_{3^{999}}) \right)$$

Coefficient of  $w^4$ .

foo55[[5]]

$$o^2 \left( -\frac{1}{2} cr[2]^2 + cr[3] + \frac{1}{2} cr[2] (\phi_{3^{999}}) - \frac{1}{24} (\phi_{4^{9999}}) \right)$$

■ **cumulants of w**

Consider the normal density with mean  $v_0+t$  and variance 1 for  $w$ . The log of the density is foo60.

$$foo60 = \frac{-1}{2} \text{Log}[2 \text{Pi}] - \frac{1}{2} (w - (v_0 + t))^2;$$

Then,we define foo61 by  $e^{wt} f(w|v_0) = e^{foo60} \exp(foo61)$ . This foo61 is a polynomial function of  $w$ .

**foo61 = Collect[w t + logdensityw - foo60, {w, o}, Simplify]**

$$\begin{aligned} & \frac{1}{2} t (t + 2 v_0) + w^3 \left( -o^2 v_0 \text{cr}[3] + o \left( \text{cr}[2] - \frac{1}{6} (\phi_3^{999}) \right) \right) - \\ & \frac{1}{3} o v_0 (3 \text{cr}[0] + 3 (d_{p,p'}) + v_0^2 (\phi_3^{999})) + \\ & o^2 w^4 \left( -\frac{1}{2} \text{cr}[2]^2 + \text{cr}[3] + \frac{1}{2} \text{cr}[2] (\phi_3^{999}) - \frac{1}{24} (\phi_4^{9999}) \right) + \\ & \frac{1}{24} o^2 \left( -12 \text{cr}[0]^2 - 24 \text{cr}[1] + 24 (d_{p,q'}) (d_{q,p'}) + 24 v_0^2 (d_{p,q'}) (d^{p'q'}) - 12 \text{cr}[0] (\phi_3^{999}) - \right. \\ & \quad 12 v_0^2 \text{cr}[0] (\phi_3^{999}) + 4 (\phi_3^{999})^2 - 12 (d_{p,p'}) (2 \text{cr}[0] + d_{q,q'} + v_0^2 (\phi_3^{999})) + \\ & \quad 12 (\phi_3^{99p'}) (\phi_3^{99p'}) + 3 v_0^4 (\phi_3^{99p'}) (\phi_3^{99p'}) - 24 (d^{p'q'}) (\phi_3^{9p,q'}) + 12 (\phi_3^{9p,q'}) (\phi_3^{9q,p'}) - \\ & \quad \left. 3 (\phi_{3p,q'}) (\phi_{3r,p'r'}) + 3 (\phi_{3p,q'}) (\phi_{3r,q'r'}) - 3 (\phi_4^{9999}) - 3 v_0^4 (\phi_4^{9999}) - 6 (\phi_4^{99p,p'}) \right) + \\ & w^2 \left( -o v_0 \text{cr}[2] + \frac{1}{8} o^2 (8 \text{cr}[1] - 8 \text{cr}[0] \text{cr}[2] - 16 \text{cr}[2]^2 - 24 \text{cr}[3] - \right. \\ & \quad 8 \text{cr}[2] (d_{p,p'}) - 8 (d_{p,q'}) (d_{q,p'}) + 4 \text{cr}[0] (\phi_3^{999}) - 4 \text{cr}[2] (\phi_3^{999}) - \\ & \quad 4 v_0^2 \text{cr}[2] (\phi_3^{999}) - 2 (\phi_3^{999})^2 - 4 (\phi_3^{99p'}) (\phi_3^{99p'}) + v_0^2 (\phi_3^{99p'}) (\phi_3^{99p'}) + \\ & \quad \left. 8 (d^{p'q'}) (\phi_3^{9p,q'}) - 4 (\phi_3^{9p,q'}) (\phi_3^{9q,p'}) + 2 (\phi_4^{9999}) + 2 (\phi_4^{99p,p'}) \right) + \\ & w \left( o (d_{p,p'} + \frac{1}{2} (2 \text{cr}[0] - 4 \text{cr}[2] + (1 + v_0^2) (\phi_3^{999}))) - \right. \\ & \quad \frac{1}{24} o^2 v_0 (24 \text{cr}[1] - 12 (d_{p,p'}) (\phi_3^{999}) + 3 (-3 + 2 v_0^2) (\phi_3^{99p'}) (\phi_3^{99p'}) + \\ & \quad \left. 24 (d^{p'q'}) (\phi_3^{9p,q'}) - 12 (\phi_3^{9p,q'}) (\phi_3^{9q,p'}) - 4 v_0^2 (\phi_4^{9999}) + 6 (\phi_4^{99p,p'}) \right) \end{aligned}$$

Get the coefficients of  $w^i$ 's for foo61, and store them in foo62 below.

**foo62 = Collect[CoefficientList[foo61, w], {o, v0}, tsimp];**

**Length[foo62]**

5

**foo62[[1]]**

$$\begin{aligned} & \frac{t^2}{2} + t v_0 + o \left( v_0 (-\text{cr}[0] - d_{p,p'}) - \frac{1}{3} v_0^3 (\phi_3^{999}) \right) + \\ & o^2 \left( -\frac{1}{2} \text{cr}[0]^2 - \text{cr}[1] - \text{cr}[0] (d_{p,p'}) + (d_{p,q'}) (d_{q,p'}) - \frac{1}{2} (d_{p,p'}) (d_{q,q'}) - \frac{1}{2} \text{cr}[0] (\phi_3^{999}) + \right. \\ & \quad \frac{1}{6} (\phi_3^{999})^2 + v_0^2 \left( (d_{p,q'}) (d^{p'q'}) - \frac{1}{2} \text{cr}[0] (\phi_3^{999}) - \frac{1}{2} (d_{p,p'}) (\phi_3^{999}) \right) + \\ & \quad \frac{1}{2} (\phi_3^{99p'}) (\phi_3^{99p'}) - (d^{p'q'}) (\phi_3^{9p,q'}) + \frac{1}{2} (\phi_3^{9p,q'}) (\phi_3^{9q,p'}) - \frac{1}{8} (\phi_{3p,q'}) (\phi_{3r,p'r'}) + \frac{1}{8} \\ & \quad \left. (\phi_{3p,q'}) (\phi_{3r,q'r'}) + v_0^4 \left( \frac{1}{8} (\phi_3^{99p'}) (\phi_3^{99p'}) - \frac{1}{8} (\phi_4^{9999}) \right) - \frac{1}{8} (\phi_4^{9999}) - \frac{1}{4} (\phi_4^{99p,p'}) \right) \end{aligned}$$

**foo62[[2]]**

$$\begin{aligned} & o \left( \text{cr}[0] - 2 \text{cr}[2] + d_{p,p'} + \frac{1}{2} (\phi_3^{999}) + \frac{1}{2} v_0^2 (\phi_3^{999}) \right) + \\ & o^2 \left( v_0^3 \left( -\frac{1}{4} (\phi_3^{99p'}) (\phi_3^{99p'}) + \frac{1}{6} (\phi_4^{9999}) \right) + v_0 \left( -\text{cr}[1] + \frac{1}{2} (d_{p,p'}) (\phi_3^{999}) + \right. \right. \\ & \quad \left. \left. \frac{3}{8} (\phi_3^{99p'}) (\phi_3^{99p'}) - (d^{p'q'}) (\phi_3^{9p,q'}) + \frac{1}{2} (\phi_3^{9p,q'}) (\phi_3^{9q,p'}) - \frac{1}{4} (\phi_4^{99p,p'}) \right) \right) \end{aligned}$$

foo62[[3]]

$$-o v0 cr[2] + o^2 \left( cr[1] - cr[0] cr[2] - 2 cr[2]^2 - 3 cr[3] - cr[2] (d_p, p') - (d_p, q') (d_q, p') + \frac{1}{2} cr[0] (\phi_3^{999}) - \frac{1}{2} cr[2] (\phi_3^{999}) - \frac{1}{4} (\phi_3^{999})^2 - \frac{1}{2} (\phi_3^{99 p'}) (\phi_3^{99 p'}) + v0^2 \left( -\frac{1}{2} cr[2] (\phi_3^{999}) + \frac{1}{8} (\phi_3^{99 p'}) (\phi_3^{99 p'}) \right) + (d^{p' q'}) (\phi_3^{9 p' q'}) - \frac{1}{2} (\phi_3^{9 p' q'}) (\phi_3^{9 q' p'}) + \frac{1}{4} (\phi_4^{9999}) + \frac{1}{4} (\phi_4^{99 p' p'}) \right)$$

foo62[[4]]

$$-o^2 v0 cr[3] + o \left( cr[2] - \frac{1}{6} (\phi_3^{999}) \right)$$

foo62[[5]]

$$o^2 \left( -\frac{1}{2} cr[2]^2 + cr[3] + \frac{1}{2} cr[2] (\phi_3^{999}) - \frac{1}{24} (\phi_4^{9999}) \right)$$

Apply "logeexpoly" to foo62. We get foo64 =  $\log \int_{-\infty}^{\infty} e^{wt} f(w|v0) dw = \log \int_{-\infty}^{\infty} e^{foo60} \exp(foo61) dw$ .

foo63 = Simplify[foo62 / {1, o, o, o, o^2}];

RuleUnique[rule63u0, ta0, foo63[[1]]]

RuleUnique[rule63u1, ta1[aua\_], foo63[[2]]]

RuleUnique[rule63u2, ta2[aua\_, aub\_], foo63[[3]]]

RuleUnique[rule63u3, ta3[aua\_, aub\_, auc\_], foo63[[4]]]

RuleUnique[rule63u4, ta4[aua\_, aub\_, auc\_, aud\_], foo63[[5]]]

foo64 = tgeto2[ApplyRules[logeexpoly /. {sb[la\_] -> v0 + t}, {rule63u0, rule63u1, rule63u2, rule63u3, rule63u4}]];

Get the coefficients of  $t^i$ ,  $i = 0, 1, 2, 3, 4$ , and multiply  $i!$  so that we get  $\kappa_i$ .

foo65 = Collect[CoefficientList[foo64, t] \* {1, 1, 2, 6, 24}, {o, v0}, tsimpp];

Length[foo65]

5

$\kappa_0$  should be zero.

foo65[[1]]

$$o^2 \left( -\frac{1}{8} (\phi_3^{9 p' q'}) (\phi_3^{9 r' p' r'}) + \frac{1}{8} (\phi_3^{9 p' q'}) (\phi_3^{9 r' q' r'}) \right)$$

foo65[[1]] = CanAll[% /. {a11 -> alc, au1 -> auc, a12 -> alb, au2 -> aub}]

0

$\kappa_1$

**foo65[[2]]**

$$v0 + o \left( cr[0] + cr[2] + v0^2 cr[2] + d_{p,p'} \right) +$$

$$o^2 \left( v0^3 (2 cr[2]^2 + cr[3]) + v0 \left( cr[1] + 2 cr[0] cr[2] + 6 cr[2]^2 + \right.$$

$$3 cr[3] - 2 (d_{p,q'}) (d_{q,p'}) + (d_{p,p'}) \left( 2 cr[2] - \frac{1}{2} (\phi^{3^{999}}) \right) - cr[2] (\phi^{3^{999}}) -$$

$$\left. \frac{5}{8} (\phi^{3^{99}_{p'}}) (\phi^{3^{99}_{p'}}) + (d^{p',q'}) (\phi^{3^{99}_{p',q'}}) - \frac{1}{2} (\phi^{3^{99}_{p',q'}}) (\phi^{3^{99}_{q',p'}}) + \frac{1}{4} (\phi^{4^{99}_{p,p'}}) \right) \Big)$$

$K_2$

**foo65[[3]]**

$$1 + o v0 (4 cr[2] - \phi^{3^{999}}) +$$

$$o^2 \left( 2 cr[1] + 4 cr[0] cr[2] + 14 cr[2]^2 + 6 cr[3] - 2 (d_{p,q'}) (d_{q,p'}) + (d_{p,p'}) (4 cr[2] - \phi^{3^{999}}) - \right.$$

$$2 cr[2] (\phi^{3^{999}}) - (\phi^{3^{99}_{p'}}) (\phi^{3^{99}_{p'}}) + 2 (d^{p',q'}) (\phi^{3^{99}_{p',q'}}) - (\phi^{3^{99}_{p',q'}}) (\phi^{3^{99}_{q',p'}}) +$$

$$v0^2 \left( 16 cr[2]^2 + 6 cr[3] - 4 cr[2] (\phi^{3^{999}}) + (\phi^{3^{999}})^2 + \frac{1}{4} (\phi^{3^{99}_{p'}}) (\phi^{3^{99}_{p'}}) - \frac{1}{2} (\phi^{4^{999}}) \right) +$$

$$\left. \frac{1}{2} (\phi^{4^{99}_{p,p'}}) \right)$$

$K_3$

**foo65[[4]]**

$$o (6 cr[2] - \phi^{3^{999}}) + o^2 v0 (60 cr[2]^2 + 18 cr[3] - 18 cr[2] (\phi^{3^{999}}) + 3 (\phi^{3^{999}})^2 - \phi^{4^{999}})$$

$K_4$

**foo65[[5]]**

$$o^2 (96 cr[2]^2 + 24 cr[3] - 24 cr[2] (\phi^{3^{999}}) + 3 (\phi^{3^{999}})^2 - \phi^{4^{999}})$$

**cumulantw = Drop[foo65, 1];**

**cumulantw // InputForm**

$$\{v0 + o*(cr[0] + cr[2] + v0^2*cr[2] + td[al1, au1]) +$$

$$o^2*(v0^3*(2*cr[2]^2 + cr[3]) + v0*(cr[1] + 2*cr[0]*cr[2] +$$

$$6*cr[2]^2 + 3*cr[3] - 2*td[al1, au2]*td[al2, au1] +$$

$$td[al1, au1]*(2*cr[2] - tp3[9, 9, 9]/2) -$$

$$cr[2]*tp3[9, 9, 9] - (5*tp3[9, 9, al1]*tp3[9, 9, au1])/8 +$$

$$td[au1, au2]*tp3[9, al1, al2] -$$

$$(tp3[9, al1, au2]*tp3[9, al2, au1])/2 + tp4[9, 9, al1, au1]/$$

$$4), 1 + o*v0*(4*cr[2] - tp3[9, 9, 9]) +$$

$$o^2*(2*cr[1] + 4*cr[0]*cr[2] + 14*cr[2]^2 + 6*cr[3] -$$

$$2*td[al1, au2]*td[al2, au1] + td[al1, au1]*$$

$$(4*cr[2] - tp3[9, 9, 9]) - 2*cr[2]*tp3[9, 9, 9] -$$

$$tp3[9, 9, al1]*tp3[9, 9, au1] + 2*td[au1, au2]*$$

$$tp3[9, al1, al2] - tp3[9, al1, au2]*tp3[9, al2, au1] +$$

$$v0^2*(16*cr[2]^2 + 6*cr[3] - 4*cr[2]*tp3[9, 9, 9] +$$

$$tp3[9, 9, 9]^2 + (tp3[9, 9, al1]*tp3[9, 9, au1])/4 -$$

$$tp4[9, 9, 9, 9]/2) + tp4[9, 9, al1, au1]/2),$$

$$o*(6*cr[2] - tp3[9, 9, 9]) + o^2*v0*(60*cr[2]^2 + 18*cr[3] -$$

$$18*cr[2]*tp3[9, 9, 9] + 3*tp3[9, 9, 9]^2 - tp4[9, 9, 9, 9]),$$

$$o^2*(96*cr[2]^2 + 24*cr[3] - 24*cr[2]*tp3[9, 9, 9] +$$

$$3*tp3[9, 9, 9]^2 - tp4[9, 9, 9, 9])\}$$

### ■ distribution function of w

The Cornish-Fisher expansion for the standardized random variable is taken from Johnson and Kotz (1994) as shown in "cfexpw" below. We first obtain the same expansion for nonstandardized variable as shown in "cfexpw", and apply it to the cumulants of w. This gives the distribution function of w, and we obtain zformula =  $\Phi^{-1}(\Pr\{W \leq w | v0\})$ , where  $\Phi^{-1}$  is the quantile function of the standard normal distribution. The same expression, but without MathTensor notation, is also given in "zform". Finally, the scaling by the factor "tau" is applied to these results, and zc-formula is stored in "zformulatau" as well as in "zformtau".

### ■ Cornish-Fisher expansion (p.66 of Johnson and Kotz 1994).

cfexpw =  $U(X_a)$  in p.66 of JK94 is for the standardized distribution. We assume the cumulants are  $kx1 = 0, kx2 = 1, kx3 = O(n^{-1/2}), kx4 = O(n^{-1}), kx5, kx6, \dots = O(n^{-3/2})$ . The following expression is defined by  $\Pr\{X \leq x\} = \Phi(\text{cfexpw})$ , or  $\text{cfexpw} = \Phi^{-1}(\Pr\{X \leq x\})$ .

$$\text{cfexpw} = x - \frac{1}{6} (x^2 - 1) kx[3] - \frac{1}{24} (x^3 - 3x) kx[4] + \frac{1}{36} (4x^3 - 7x) kx[3]^2;$$

For w, the cumulants are  $kw1 = O(1), kw2 = 1 + O(n^{-1/2}), kw3 = O(n^{-1/2}), kw4 = O(n^{-1})$ . We first standardize w and apply cfexpw to the standardized w to get cfexpw =  $\Phi^{-1}(\Pr\{W \leq w\})$ .

```
rule70 = {x -> (w - kw[1]) / Sqrt[kw[2]]};
rule71 = {kx[1] -> 0, kx[2] -> 1, kx[3] -> kw[3] / kw[2]^(3/2), kx[4] -> kw[4] / kw[2]^2};
rule72 = {kw[1] -> aw1, kw[2] -> 1 + o aw2, kw[3] -> o aw3, kw[4] -> o^2 aw4};
rule73 = Simplify[Solve[(x /. rule70) == w, w][[1]]]
{w -> kw[1] + x Sqrt[kw[2]]}
cfexpw = gets2[cfexpw /. Join[rule70, rule71] /. rule72]
-aw1 + 1/6 o (aw3 (1 - (aw1 - w)^2) + 3 aw2 (aw1 - w)) + w +
1/72 o^2 (27 aw2^2 (-aw1 + w) + 6 aw2 aw3 (-3 + 5 aw1^2 - 10 aw1 w + 5 w^2) +
3 aw4 ((aw1 - w)^3 + 3 (-aw1 + w)) + 2 aw3^2 (7 (aw1 - w) + 4 (-aw1 + w)^3))
```

### ■ Cornish-Fisher expansion of w

We apply cfexpw to cumulantw.

```
aw = Simplify[(cumulantw - {0, 1, 0, 0}) / {1, o, o, o^2}];
RuleUnique[rulecumaw1, aw1, aw[[1]]]
RuleUnique[rulecumaw2, aw2, aw[[2]]]
RuleUnique[rulecumaw3, aw3, aw[[3]]]
RuleUnique[rulecumaw4, aw4, aw[[4]]]
```

```
func75[exp_, rule_] := tgeto2[ApplyRules[exp, rule]]
foo75 = func75[
  func75[func75[func75[cfexpw, rulecumaw1], rulecumaw2], rulecumaw3], rulecumaw4];
```

The following zformula is defined as  $zformula = \Phi^{-1}(\Pr\{W \leq w\})$ .

```
zformula = Collect[foo75, {o, w, v0}, tsimpp]
-v0 + w +
o (-cr[0] - dp',p' + w2 (-cr[2] +  $\frac{1}{6} (\phi_{3^{999}})$ ) -  $\frac{1}{6} (\phi_{3^{999}})$  -  $\frac{1}{3} v0^2 (\phi_{3^{999}})$  +  $\frac{1}{6} v0 w (\phi_{3^{999}})$ ) +
o2 (v03 ( $\frac{1}{18} (\phi_{3^{999}})^2$  +  $\frac{1}{8} (\phi_{3^{99p'}}) (\phi_{3^{99p'}})$  -  $\frac{1}{8} (\phi_{4^{9999}})$ ) +
v0 ((dp',q') (dq',p') -  $\frac{1}{6} cr[0] (\phi_{3^{999}})$  -  $\frac{1}{6} (d_{p',p'}) (\phi_{3^{999}})$  +  $\frac{5}{72} (\phi_{3^{999}})^2$  +  $\frac{1}{8} (\phi_{3^{99p'}})$ 
( $\phi_{3^{99p'}})$  -  $\frac{1}{24} (\phi_{4^{9999}})$ ) + v0 w2 (- $\frac{1}{6} cr[2] (\phi_{3^{999}})$  -  $\frac{1}{24} (\phi_{3^{999}})^2$  +  $\frac{1}{24} (\phi_{4^{9999}})$ ) +
w3 (-cr[3] -  $\frac{1}{3} cr[2] (\phi_{3^{999}})$  -  $\frac{1}{72} (\phi_{3^{999}})^2$  +  $\frac{1}{24} (\phi_{4^{9999}})$ ) +
w (-cr[1] + (dp',q') (dq',p') -  $\frac{1}{3} cr[0] (\phi_{3^{999}})$  +  $\frac{1}{6} (d_{p',p'}) (\phi_{3^{999}})$  +
 $\frac{13}{72} (\phi_{3^{999}})^2$  +  $\frac{1}{2} (\phi_{3^{99p'}}) (\phi_{3^{99p'}})$  - (dp',q') (φ39p',q') +  $\frac{1}{2} (\phi_{3^9_{p',q'}}) (\phi_{3^9_{q',p'}})$  +
v02 (- $\frac{1}{8} (\phi_{3^{99p'}}) (\phi_{3^{99p'}})$  +  $\frac{1}{24} (\phi_{4^{9999}})$ ) -  $\frac{1}{8} (\phi_{4^{9999}})$  -  $\frac{1}{4} (\phi_{4^{99p',p'}})$ ))
```

```
zformula // InputForm
```

```
-v0 + w + o*(-cr[0] - td[all, au1] +
w2*(-cr[2] + tp3[9, 9, 9]/6) - tp3[9, 9, 9]/6 -
(v02*tp3[9, 9, 9])/3 + (v0*w*tp3[9, 9, 9])/6) +
o2*(v03*(tp3[9, 9, 9]2/18 + (tp3[9, 9, all]*tp3[9, 9, au1])/8 -
tp4[9, 9, 9, 9]/8) + v0*(td[all, au2]*td[al2, au1] -
(cr[0]*tp3[9, 9, 9])/6 - (td[all, au1]*tp3[9, 9, 9])/6 +
(5*tp3[9, 9, 9]2)/72 + (tp3[9, 9, all]*tp3[9, 9, au1])/8 -
tp4[9, 9, 9, 9]/24) + v0*w2*((-cr[2]*tp3[9, 9, 9])/6 -
tp3[9, 9, 9]2/24 + tp4[9, 9, 9, 9]/24) +
w3*(-cr[3] - (cr[2]*tp3[9, 9, 9])/3 - tp3[9, 9, 9]2/72 +
tp4[9, 9, 9, 9]/24) + w*(-cr[1] + td[all, au2]*td[al2, au1] -
(cr[0]*tp3[9, 9, 9])/3 + (td[all, au1]*tp3[9, 9, 9])/6 +
(13*tp3[9, 9, 9]2)/72 + (tp3[9, 9, all]*tp3[9, 9, au1])/2 -
td[au1, au2]*tp3[9, all, al2] +
(tp3[9, all, au2]*tp3[9, al2, au1])/2 +
v02*(-(tp3[9, 9, all]*tp3[9, 9, au1])/8 +
tp4[9, 9, 9, 9]/24) - tp4[9, 9, 9, 9]/8 -
tp4[9, 9, all, au1]/4))
```

Get the coefficients of  $w^i v0^j$  for zformula.

```
foo76 = Collect[CoefficientList[zformula, {w, v0}], o, tsimpp];
```

```
Dimensions[foo76]
```

```
{4, 4}
```

$w^0 v0^0$

```
foo76[[1, 1]]
```

```
o (-cr[0] - dp',p' -  $\frac{1}{6} (\phi_{3^{999}})$ )
```

$w^0 v0^1$

**foo76[[1, 2]]**

$$-1 + o^2 \left( (d_{p',q'}) (d_{q',p'}) - \frac{1}{6} \text{cr}[0] (\phi3^{999}) - \frac{1}{6} (d_{p',p'}) (\phi3^{999}) + \frac{5}{72} (\phi3^{999})^2 + \frac{1}{8} (\phi3^{99}_{p'}) (\phi3^{99p'}) - \frac{1}{24} (\phi4^{9999}) \right)$$

$w^0 v0^2$

**foo76[[1, 3]]**

$$-\frac{1}{3} o (\phi3^{999})$$

$w^0 v0^3$

**foo76[[1, 4]]**

$$o^2 \left( \frac{1}{18} (\phi3^{999})^2 + \frac{1}{8} (\phi3^{99}_{p'}) (\phi3^{99p'}) - \frac{1}{8} (\phi4^{9999}) \right)$$

$w^1 v0^0$

**foo76[[2, 1]]**

$$1 + o^2 \left( -\text{cr}[1] + (d_{p',q'}) (d_{q',p'}) - \frac{1}{3} \text{cr}[0] (\phi3^{999}) + \frac{1}{6} (d_{p',p'}) (\phi3^{999}) + \frac{13}{72} (\phi3^{999})^2 + \frac{1}{2} (\phi3^{99}_{p'}) (\phi3^{99p'}) - (d^{p'q'}) (\phi3^9_{p'q'}) + \frac{1}{2} (\phi3^9_{p,q'}) (\phi3^9_{q',p'}) - \frac{1}{8} (\phi4^{9999}) - \frac{1}{4} (\phi4^{99}_{p',p'}) \right)$$

$w^1 v0^1$

**foo76[[2, 2]]**

$$\frac{1}{6} o (\phi3^{999})$$

$w^1 v0^2$

**foo76[[2, 3]]**

$$o^2 \left( -\frac{1}{8} (\phi3^{99}_{p'}) (\phi3^{99p'}) + \frac{1}{24} (\phi4^{9999}) \right)$$

$w^1 v0^3$

**foo76[[2, 4]]**

$$0$$

$w^2 v0^0$

**foo76[[3, 1]]**

$$o \left( -\text{cr}[2] + \frac{1}{6} (\phi3^{999}) \right)$$

$w^2 v0^1$



foo76[[3, 2]]

$$o^2 \left( -\frac{1}{6} \text{cr}[2] (\phi^{3^{999}}) - \frac{1}{24} (\phi^{3^{999}})^2 + \frac{1}{24} (\phi^{4^{999}}) \right)$$

$w^2 v^0^2$

foo76[[3, 3]]

0

$w^2 v^0^3$

foo76[[3, 4]]

0

$w^3 v^0^0$

foo76[[4, 1]]

$$o^2 \left( -\text{cr}[3] - \frac{1}{3} \text{cr}[2] (\phi^{3^{999}}) - \frac{1}{72} (\phi^{3^{999}})^2 + \frac{1}{24} (\phi^{4^{999}}) \right)$$

$w^3 v^0^1$

foo76[[4, 2]]

0

$w^3 v^0^2$

foo76[[4, 3]]

0

$w^3 v^0^3$

foo76[[4, 4]]

0

### ■ zc-formula using a simplified notation

In the below, the tensor symbols are replaced by regular symbols.

RuleUnique[rule80a, td[a11\_, au1\_], Daa, PairaQ[a11, au1]]

RuleUnique[rule80b, td[a11\_, au2\_] td[a12\_, au1\_],  
Dab2, PairaQ[{a11, a12}, {au1, au2}]]

RuleUnique[rule80c, tp3[9, 9, 9], P999]

RuleUnique[rule80d, tp4[9, 9, 9, 9], P9999]

RuleUnique[rule80e, tp3[9, 9, a11\_] tp3[9, 9, au1\_], P99a2, PairaQ[a11, au1]]

RuleUnique[rule80f, td[au1\_, au2\_] tp3[9, a11\_, a12\_],  
DabP9ab, PairaQ[{a11, a12}, {au1, au2}]]

```

RuleUnique[rule80g, tp3[9, a11_, au2_] tp3[9, a12_, au1_],
  P9ab2, PairaQ[{a11, a12}, {au1, au2}]]

RuleUnique[rule80h, tp4[9, 9, a11_, au1_], P99aa, PairaQ[a11, au1]]

rule81 = {cr[0] → c0, cr[1] → c1, cr[2] → c2, cr[3] → c3};

```

The following expression of "zform" is equivalent to "zformula", but without the tensor symbols so that we can use it without MathTensor.

```

zform = Collect[ApplyRules[zformula, {rule80a, rule80b, rule80c,
  rule80d, rule80e, rule80f, rule80g, rule80h}] /. rule81, {o, w, v0}]

-v0 + w + o ( -c0 - Daa - P999/6 - P999 v0^2/3 + P999 v0 w/6 + (-c2 + P999/6) w^2 ) +
o^2 ( ( Dab2 - c0 P999/6 - Daa P999/6 + 5 P999^2/72 - P9999/24 + P99a2/8 ) v0 +
( P999^2/18 - P9999/8 + P99a2/8 ) v0^3 + ( -c1 + Dab2 - DabP9ab - c0 P999/3 + Daa P999/6 +
13 P999^2/72 - P9999/8 + P99a2/2 - P99aa/4 + P9ab2/2 + ( P9999/24 - P99a2/8 ) v0^2 ) w +
( -c2 P999/6 - P999^2/24 + P9999/24 ) v0 w^2 + ( -c3 - c2 P999/3 - P999^2/72 + P9999/24 ) w^3 )

```

**zform // InputForm**

```

-v0 + w + o*(-c0 - Daa - P999/6 - (P999*v0^2)/3 + (P999*v0*w)/6 +
(-c2 + P999/6)*w^2) +
o^2*((Dab2 - (c0*P999)/6 - (Daa*P999)/6 + (5*P999^2)/72 -
P9999/24 + P99a2/8)*v0 + (P999^2/18 - P9999/8 + P99a2/8)*
v0^3 + (-c1 + Dab2 - DabP9ab - (c0*P999)/3 + (Daa*P999)/6 +
(13*P999^2)/72 - P9999/8 + P99a2/2 - P99aa/4 + P9ab2/2 +
(P9999/24 - P99a2/8)*v0^2)*w +
(-(c2*P999)/6 - P999^2/24 + P9999/24)*v0*w^2 +
(-c3 - (c2*P999)/3 - P999^2/72 + P9999/24)*w^3)

```

■ scaling by the factor "tau".

When scaling the problem by the factor  $\tau$ , the expression of the z-formula changes. First, the  $O(1)$  term such as  $w$  and  $v0$  are multiplied by  $\tau^{-1}$ . On the other hand,  $O(n^{-1/2})$  terms such as  $\phi^{ijk}$  and  $d^{ab}$  are multiplied by  $\tau$ ,  $O(n^{-1})$  terms such as  $\phi^{ijkl}$  and  $e^{abc}$  are by  $\tau^2$ . The  $cr[r]$  coefficient for modified signed distance is multiplied by  $\tau^{r-1}$ .

```

rule85a = {w → w / tau, v0 → v0 / tau};

rule85b =
  {tp3[ala_, alb_, alc_] → tau tp3[ala, alb, alc], td[ala_, alb_] → tau td[ala, alb]};

rule85c = {tp4[ala_, alb_, alc_, ald_] → tau^2 tp4[ala, alb, alc, ald],
  te[ala_, alb_, alc_] → tau^2 te[ala, alb, alc]};

rule85d = {cr[r_] → cr[r] tau^{r-1}};

rule85 = Join[rule85a, rule85b, rule85c, rule85d];

```

**zformulatau = Collect[zformula /. rule85, {tau, o, w, v0}]**

$$\begin{aligned} & \frac{1}{\tau} \left( -v_0 + w + o \left( -cr[0] + w^2 \left( -cr[2] + \frac{1}{6} (\phi_3^{999}) \right) - \frac{1}{3} v_0^2 (\phi_3^{999}) + \frac{1}{6} v_0 w (\phi_3^{999}) \right) + \right. \\ & \quad o^2 \left( -\frac{1}{6} v_0 cr[0] (\phi_3^{999}) + \right. \\ & \quad \quad w \left( -cr[1] - \frac{1}{3} cr[0] (\phi_3^{999}) + v_0^2 \left( -\frac{1}{8} (\phi_3^{999}_{p'}) (\phi_3^{999}_{p'}) + \frac{1}{24} (\phi_4^{9999}) \right) \right) + \\ & \quad \quad v_0^3 \left( \frac{1}{18} (\phi_3^{999})^2 + \frac{1}{8} (\phi_3^{999}_{p'}) (\phi_3^{999}_{p'}) - \frac{1}{8} (\phi_4^{9999}) \right) + \\ & \quad \quad v_0 w^2 \left( -\frac{1}{6} cr[2] (\phi_3^{999}) - \frac{1}{24} (\phi_3^{999})^2 + \frac{1}{24} (\phi_4^{9999}) \right) + \\ & \quad \quad \left. \left. w^3 \left( -cr[3] - \frac{1}{3} cr[2] (\phi_3^{999}) - \frac{1}{72} (\phi_3^{999})^2 + \frac{1}{24} (\phi_4^{9999}) \right) \right) \right) + \\ & \tau \left( o \left( - (d_{p,p'}) - \frac{1}{6} (\phi_3^{999}) \right) + o^2 \left( v_0 \left( (d_{p,q'}) (d_{q,p'}) - \frac{1}{6} (d_{p,p'}) (\phi_3^{999}) + \right. \right. \right. \\ & \quad \quad \left. \left. \frac{5}{72} (\phi_3^{999})^2 + \frac{1}{8} (\phi_3^{999}_{p'}) (\phi_3^{999}_{p'}) - \frac{1}{24} (\phi_4^{9999}) \right) + \right. \\ & \quad \quad \left. w \left( (d_{p,q'}) (d_{q,p'}) + \frac{1}{6} (d_{p,p'}) (\phi_3^{999}) + \frac{13}{72} (\phi_3^{999})^2 + \frac{1}{2} (\phi_3^{999}_{p'}) (\phi_3^{999}_{p'}) - \right. \right. \\ & \quad \quad \left. \left. (d^{p,q'}) (\phi_3^{999}_{p',q'}) + \frac{1}{2} (\phi_3^{999}_{p',q'}) (\phi_3^{999}_{q',p'}) - \frac{1}{8} (\phi_4^{9999}) - \frac{1}{4} (\phi_4^{999}_{p',p'}) \right) \right) \end{aligned}$$

**zformulatau // InputForm**

$$\begin{aligned} & (-v_0 + w + o*(-cr[0] + w^2*(-cr[2] + tp3[9, 9, 9]/6) - \\ & \quad (v_0^2*tp3[9, 9, 9])/3 + (v_0*w*tp3[9, 9, 9])/6) + \\ & \quad o^2*(-(v_0*cr[0]*tp3[9, 9, 9])/6 + \\ & \quad \quad w*(-cr[1] - (cr[0]*tp3[9, 9, 9])/3 + \\ & \quad \quad v_0^2*(-(tp3[9, 9, all]*tp3[9, 9, aul])/8 + \\ & \quad \quad \quad tp4[9, 9, 9, 9]/24)) + v_0^3*(tp3[9, 9, 9]^2/18 + \\ & \quad \quad \quad (tp3[9, 9, all]*tp3[9, 9, aul])/8 - tp4[9, 9, 9, 9]/8) + \\ & \quad \quad v_0*w^2*(-(cr[2]*tp3[9, 9, 9])/6 - tp3[9, 9, 9]^2/24 + \\ & \quad \quad \quad tp4[9, 9, 9, 9]/24) + w^3*(-cr[3] - (cr[2]*tp3[9, 9, 9])/3 - \\ & \quad \quad \quad tp3[9, 9, 9]^2/72 + tp4[9, 9, 9, 9]/24))/tau + \\ & \tau*(o*(-td[all, aul] - tp3[9, 9, 9]/6) + \\ & \quad o^2*(v_0*(td[all, au2]*td[al2, aul] - (td[all, aul]*tp3[9, 9, 9])/ \\ & \quad \quad 6 + (5*tp3[9, 9, 9]^2)/72 + (tp3[9, 9, all]*tp3[9, 9, aul])/ \\ & \quad \quad 8 - tp4[9, 9, 9, 9]/24) + w*(td[all, au2]*td[al2, aul] + \\ & \quad \quad (td[all, aul]*tp3[9, 9, 9])/6 + (13*tp3[9, 9, 9]^2)/72 + \\ & \quad \quad (tp3[9, 9, all]*tp3[9, 9, aul])/2 - td[aul, au2]* \\ & \quad \quad tp3[9, all, al2] + (tp3[9, all, au2]*tp3[9, al2, au1])/2 - \\ & \quad \quad tp4[9, 9, 9, 9]/8 - tp4[9, 9, all, aul]/4)) \end{aligned}$$

**zformtau =**

**Collect[ApplyRules[zformulatau, {rule80a, rule80b, rule80c, rule80d, rule80e, rule80f, rule80g, rule80h}] /. rule81, {tau, o, w, v0}]**

$$\begin{aligned} & \tau \left( o \left( -Daa - \frac{P999}{6} \right) + o^2 \left( \left( Dab2 - \frac{Daa P999}{6} + \frac{5 P999^2}{72} - \frac{P9999}{24} + \frac{P99a2}{8} \right) v_0 + \right. \\ & \quad \left. \left( Dab2 - DabP9ab + \frac{Daa P999}{6} + \frac{13 P999^2}{72} - \frac{P9999}{8} + \frac{P99a2}{2} - \frac{P99aa}{4} + \frac{P9ab2}{2} \right) w \right) \right) + \\ & \frac{1}{\tau} \left( -v_0 + w + o \left( -c_0 - \frac{P999 v_0^2}{3} + \frac{P999 v_0 w}{6} + \left( -c_2 + \frac{P999}{6} \right) w^2 \right) + o^2 \left( -\frac{1}{6} c_0 P999 v_0 + \right. \right. \\ & \quad \left( \frac{P999^2}{18} - \frac{P9999}{8} + \frac{P99a2}{8} \right) v_0^3 + \left( -c_1 - \frac{c_0 P999}{3} + \left( \frac{P9999}{24} - \frac{P99a2}{8} \right) v_0^2 \right) w + \\ & \quad \left. \left( -\frac{c_2 P999}{6} - \frac{P999^2}{24} + \frac{P9999}{24} \right) v_0 w^2 + \left( -c_3 - \frac{c_2 P999}{3} - \frac{P999^2}{72} + \frac{P9999}{24} \right) w^3 \right) \end{aligned}$$

**zformtau // InputForm**

```
tau*(o*(-Daa - P999/6) +
  o^2*((Dab2 - (Daa*P999)/6 + (5*P999^2)/72 - P9999/24 + P99a2/8)*
    v0 + (Dab2 - DabP9ab + (Daa*P999)/6 + (13*P999^2)/72 -
      P9999/8 + P99a2/2 - P99aa/4 + P9ab2/2)*w)) +
(-v0 + w + o*(-c0 - (P999*v0^2)/3 + (P999*v0*w)/6 +
  (-c2 + P999/6)*w^2) + o^2*(-(c0*P999*v0)/6 +
  (P999^2/18 - P9999/8 + P99a2/8)*v0^3 +
  (-c1 - (c0*P999)/3 + (P9999/24 - P99a2/8)*v0^2)*w +
  (-c2*P999)/6 - P999^2/24 + P9999/24)*v0*w^2 +
  (-c3 - (c2*P999)/3 - P999^2/72 + P9999/24)*w^3))/tau
```

### ■ local coordinates at the projection

We consider a local coordinate  $\Delta\eta$  around a point  $\eta(u_0,0)$  on the surface, where  $u_0$  indicates any specified value of  $u$ . This will be used for  $u_0$  specifying the projection of  $y$  onto the surface. The change of variable  $\eta \leftrightarrow \Delta\eta$  is specified by  $\eta_a = \eta_a(u_0, 0) + B_a^b(u_0) \Delta\eta_b$  for each  $u_0$ . The expression for  $\eta_a$  is given in "rule93", and that for  $\eta_9$  is in "rule94". The surface is expressed as  $\Delta\eta_{\text{dim}} = -\hat{d}^{a'b'} \Delta\eta_a \Delta\eta_{b'} - \hat{e}^{a'b'c'} \Delta\eta_a \Delta\eta_{b'} \Delta\eta_{c'}$ , where the coefficients are shown in foo101 and foo102. Next, the expression for  $\frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta=\eta(u_0)+B\Delta\eta}$   $B_p^a(u_0) B_q^b(u_0)$  is obtained and stored in foo114[ua,ub]. This is equated with  $\hat{\phi}^{ab} + \hat{\phi}^{abc} \Delta\eta_c + \frac{1}{2} \hat{\phi}^{abcd} \Delta\eta_c \Delta\eta_d$ , and the coefficients  $\hat{\phi}^{ab}$ ,  $\hat{\phi}^{abc}$ , and  $\hat{\phi}^{abcd}$  are obtained in foo121. The inverse of the metric  $\hat{\phi}_{a'b'} = (\hat{\phi}^{a'b'})^{-1}$  is in rule131, which is used for foo132  $= \hat{\phi}_{a'b'} \hat{d}^{a'b'}$ . These conversion rules are summarized in "rulesproj". zc-formula evaluated at  $\eta(u_0,0)$  is shown in zformulau0, and that for scaling tau is in zformulatauu0.

### ■ the expression for the surface in the local coordinates

We use  $u_0^a$  for the  $u_a$ -coordinate of the projection.

```
DefineTensor[ru0, "u0", {{1}, 1}]
PermWeight::def : Object u0 defined
```

Define local coordinates at the projection, and denote  $\Delta\eta_a$ . The local coordinate  $\Delta\eta_a$  is in the  $B^a$  direction.

```
DefineTensor[re, "Delta eta", {{1}, 1}]
PermWeight::def : Object Delta eta defined
```

First, separate the type-a and 9 indices in the local parametrization at the projection.  $\eta_a$  in foo90 indicates the projection point, whereas foo90 itself indicates the  $\eta_a$ -coordinates for a general point.

```
se[1a] + tB[1a, ub] re[1b]
eta_a + (Delta eta_b) (B_a^b)
foo90 = CanAll[sepa[se[1a] + tB[1a, ub] re[1b], 1b]]
eta_a + (Delta eta_9) (B_a^9) + (Delta eta_p) (B_a^p)
```

foo91 is foo90 for  $a=a'$ .

```
foo91 = ApplyRules[foo90 /. {la -> ala}, rule1]
(Kdeltaa, p') (up') + (Δη9) (Ba, 9) + (Δηp') (Ba, p')
```

foo92 is foo90 for a=9.

```
foo92 = ApplyRules[foo90 /. {la -> -9}, rule2]
(Δη9) (B9) + (Δηp') (B9, p') - o (up') (uq') (dp'q') - o2 (up') (uq') (ur') (ep'q'r')
```

Then,  $B^a$  is expanded by its expression.  $u_{a'}$  is now substituted by  $u0_{a'}$  to change the origin to the projection. Here we obtain foo93 =  $\eta_{a'}$  and foo94 =  $\eta_9$ .

```
foo93 = ApplyRules[foo91, {rule3, rule4, rule15, rule16}] /. ru -> ru0
(Kdeltaa, p') (Δηp') + (Kdeltaa, p') (u0p') + 2 o (Δη9) (u0p') (da, p') +
3 o2 (Δη9) (u0p') (u0q') (ea, p'q') + o2 (Δη9) (u0p') (u0q') (dp'q') (φ399a) +
o2 (Δη9) (u0p') (u0q') (da, q') (φ399p') - o (Δη9) (u0p') (φ39a, p') +
1/2 o2 (Δη9) (u0p') (u0q') (φ399q') (φ39a, p') - 2 o2 (Δη9) (u0p') (u0q') (dr, q') (φ3a, p'r') +
o2 (Δη9) (u0p') (u0q') (φ39r, q') (φ3a, p'r') - 1/2 o2 (Δη9) (u0p') (u0q') (φ49a, p'q')
```

```
RuleUnique[rule93, se[ala_], foo93, IndexaQ[ala]]
```

```
foo94 = ApplyRules[foo92, {rule3, rule4, rule15, rule16}] /. ru -> ru0
```

```
Δη9 - 2 o (Δηp') (u0q') (dp'q') - o (u0p') (u0q') (dp'q') -
2 o2 (Δη9) (u0p') (u0q') (dr, q') (dp'r') - 3 o2 (Δηp') (u0q') (u0r') (ep'q'r') -
o2 (u0p') (u0q') (u0r') (ep'q'r') + 1/2 o2 (Δη9) (u0p') (u0q') (dp'q') (φ3999) -
1/2 o (Δη9) (u0p') (φ399p') + 3/8 o2 (Δη9) (u0p') (u0q') (φ399p') (φ399q') +
1/2 o2 (Δη9) (u0p') (u0q') (φ39r, q') (φ39p'r') - 1/4 o2 (Δη9) (u0p') (u0q') (φ499p'q')
```

```
RuleUnique[rule94, se[-9], foo94]
```

We will equate foo93 with foo95, and foo94 with foo96 below to derive the expression of the surface in the local coordinates. foo95 and foo96 define the surface with the origin at 0. First we consider  $\eta_{a'}$  direction.

```
foo95 = tsimpp[ApplyRules[se[ala], rule1]]
ua'
```

Thus,  $u_{a'}$  = foo93 as a function of  $\Delta\eta_{a'}$ . We make it rule95.

```
RuleUnique[rule95, ru[ala_], foo93]
```

Consider  $\eta_9$  direction.

```
foo96 = ApplyRules[se[-9], rule2]
-o (up') (uq') (dp'q') - o2 (up') (uq') (ur') (ep'q'r')
```

Using the rule95, we get an expression of foo96 in terms of  $\Delta\eta_{a'}$ 's.

**foo97 = tgeto2[ApplyRules[foo96, rule95]]**

$$\begin{aligned} & \circ (- (\Delta\eta_{p'}) (\Delta\eta_{q'}) (d^{p'q'}) - 2 (\Delta\eta_{p'}) (u_{0q'}) (d^{p'q'}) - (u_{0p'}) (u_{0q'}) (d^{p'q'}) + \\ & \quad o^2 (-4 (\Delta\eta_{\theta}) (\Delta\eta_{p'}) (u_{0q'}) (d_{r'}^{q'}) (d^{p'r'}) - 4 (\Delta\eta_{\theta}) (u_{0p'}) (u_{0q'}) (d_{r'}^{q'}) (d^{p'r'}) - \\ & \quad (\Delta\eta_{p'}) (\Delta\eta_{q'}) (\Delta\eta_{r'}) (e^{p'q'r'}) - 3 (\Delta\eta_{p'}) (\Delta\eta_{q'}) (u_{0r'}) (e^{p'q'r'}) - \\ & \quad 3 (\Delta\eta_{p'}) (u_{0q'}) (u_{0r'}) (e^{p'q'r'}) - (u_{0p'}) (u_{0q'}) (u_{0r'}) (e^{p'q'r'}) + \\ & \quad 2 (\Delta\eta_{\theta}) (\Delta\eta_{p'}) (u_{0q'}) (d^{p'r'}) (\phi_{r'}^{9q'}) + 2 (\Delta\eta_{\theta}) (u_{0p'}) (u_{0q'}) (d^{p'r'}) (\phi_{r'}^{9q'}) \end{aligned}$$

Equate foo94==foo97 to solve the expression of  $\Delta\eta_{\theta}$  in terms of  $\Delta\eta_{q'}$ .

**foo98 = CoefficientList[tsimpp[foo94 - foo97], re[-9]];**

**Length[foo98]**

2

**foo98[[1]]**

$$\circ (\Delta\eta_{p'}) (\Delta\eta_{q'}) (d^{p'q'}) + o^2 (\Delta\eta_{p'}) (\Delta\eta_{q'}) (\Delta\eta_{r'}) (e^{p'q'r'}) + 3 o^2 (\Delta\eta_{p'}) (\Delta\eta_{q'}) (u_{0r'}) (e^{p'q'r'})$$

**foo98[[2]]**

$$\begin{aligned} & 1 + 4 o^2 (\Delta\eta_{p'}) (u_{0q'}) (d_{r'}^{q'}) (d^{p'r'}) + 2 o^2 (u_{0p'}) (u_{0q'}) (d_{r'}^{q'}) (d^{p'r'}) + \\ & \quad \frac{1}{2} o^2 (u_{0p'}) (u_{0q'}) (d^{p'q'}) (\phi_3^{999}) - \frac{1}{2} o (u_{0p'}) (\phi_3^{99p'}) + \frac{3}{8} o^2 (u_{0p'}) (u_{0q'}) (\phi_3^{99p'}) (\phi_3^{99q'}) - \\ & \quad 2 o^2 (\Delta\eta_{p'}) (u_{0q'}) (d^{p'r'}) (\phi_3^{9r',q'}) - 2 o^2 (u_{0p'}) (u_{0q'}) (d^{p'r'}) (\phi_3^{9r',q'}) + \\ & \quad \frac{1}{2} o^2 (u_{0p'}) (u_{0q'}) (\phi_3^{9r',q'}) (\phi_3^{99p'r'}) - \frac{1}{4} o^2 (u_{0p'}) (u_{0q'}) (\phi_4^{99p'q'}) \end{aligned}$$

The following foo99 gives an expression of  $\Delta\eta_{\theta}$  in terms of  $\Delta\eta_{q'}$ .

**foo99 = Collect[tgets2[-x/y, x, foo98[[1]], y, foo98[[2]]],  
{re[al1] re[al2] re[al3], re[al1] re[al2], ru0[al3]}**

$$\begin{aligned} & -o^2 (\Delta\eta_{p'}) (\Delta\eta_{q'}) (\Delta\eta_{r'}) (e^{p'q'r'}) + \\ & \quad (\Delta\eta_{p'}) (\Delta\eta_{q'}) \left( -o (d^{p'q'}) + (u_{0r'}) \left( -3 o^2 (e^{p'q'r'}) - \frac{1}{2} o^2 (d^{p'q'}) (\phi_3^{99r'}) \right) \right) \end{aligned}$$

get the coefficients of  $\Delta\eta_{a'}$ ,  $\Delta\eta_{b'}$  and  $\Delta\eta_{a'}\Delta\eta_{b'}\Delta\eta_{c'}$  for  $\Delta\eta_{\theta}$ .

**foo100 = Collect[CoefficientList[foo99 /. re[ala\_] -> x, x] /. {au1 -> aua, au2 -> aub,  
au3 -> auc, au4 -> aud, al1 -> ala, al2 -> alb, al3 -> alc, al4 -> ald}, o, tsimpp]**

$$\left\{ 0, 0, -o (d^{a'b'}) + o^2 \left( -3 (u_{0p'}) (e^{p'a'b'}) - \frac{1}{2} (u_{0p'}) (d^{a'b'}) (\phi_3^{99p'}) \right), -o^2 (e^{a'b'c'}) \right\}$$

This is  $d^{a'b'}$  at the projection. We denote it  $\hat{d}^{a'b'} = \text{foo101}$ .

**foo101 = Collect[Simplify[-foo100[[3]] / o], {ru0[al1], o}, tsimp]**

$$d^{a'b'} + o (u_{0p'}) \left( 3 (e^{p'a'b'}) + \frac{1}{2} (d^{a'b'}) (\phi_3^{99p'}) \right)$$

**RuleUnique[rule101, td[aua, aub], foo101]**

This is  $e^{a'b'c'}$  at the projection. We denote it  $\hat{e}^{a'b'c'} = \text{foo102}$ .

**foo102 = Simplify[-foo100[[4]] / o^2]**

$$e^{a'b'c'}$$

Now the surface is expressed in the local coordinates as  $\Delta\eta_9 = -\hat{d}^{a'b'} \Delta\eta_a \Delta\eta_{b'} - \hat{e}^{a'b'c'} \Delta\eta_a \Delta\eta_{b'} \Delta\eta_{c'}$ .

## ■ the expressions for the potential derivatives

the metric

```
DefineTensor[tp2, "φ2", {{2, 1}, 1}]
PermWeight::sym : Symmetries of φ2 assigned
PermWeight::def : Object φ2 defined
```

the inverse of the metric

```
DefineTensor[tr2, "iφ2", {{2, 1}, 1}]
PermWeight::sym : Symmetries of iφ2 assigned
PermWeight::def : Object iφ2 defined
```

$\text{phi2eta} = \frac{\partial^2 \phi(\eta)}{\partial \eta_a \partial \eta_b}$  is derived earlier.

**phi2eta**

$$\text{Kdelta}^{ab} + o(\eta_p) (\phi_3^{pab}) + \frac{1}{2} o^2(\eta_p) (\eta_q) (\phi_4^{pqab})$$

$\text{foo110} = \text{phi2eta}$  but  $\eta_p$  is separated into  $\eta_{p'}$  and  $\eta_9$  in the summation.

**foo110 = CanAll[sepa[sepa[phi2eta, 11], 12]]**

$$\text{Kdelta}^{ab} + o(\eta_9) (\phi_3^{9ab}) + o(\eta_{p'}) (\phi_3^{p'ab}) + \frac{1}{2} o^2(\eta_9)^2 (\phi_4^{99ab}) + o^2(\eta_9) (\eta_{p'}) (\phi_4^{9p'ab}) + \frac{1}{2} o^2(\eta_{p'}) (\eta_{q'}) (\phi_4^{p'q'ab})$$

$\text{foo111} = \text{foo110}$  but  $\eta_{p'}$  and  $\eta_9$  are substituted by their expressions in the local coordinates.

**foo111 = tgeto2[ApplyRules[foo110, {rule93, rule94}]]**

$$\begin{aligned} & \text{Kdelta}^{ab} + o((\Delta\eta_9) (\phi_3^{9ab}) + (\Delta\eta_{p'}) (\phi_3^{p'ab}) + (u_{0p'}) (\phi_3^{p'ab})) + \\ & o^2 \left( -2 (\Delta\eta_{p'}) (u_{0q'}) (d^{p'q'}) (\phi_3^{9ab}) - (u_{0p'}) (u_{0q'}) (d^{p'q'}) (\phi_3^{9ab}) - \right. \\ & \quad \frac{1}{2} (\Delta\eta_9) (u_{0p'}) (\phi_3^{99p'}) (\phi_3^{9ab}) + 2 (\Delta\eta_9) (u_{0p'}) (d_{q'}^{p'}) (\phi_3^{q'ab}) - (\Delta\eta_9) (u_{0p'}) (\phi_3^{9_{q'}p'}) \\ & \quad (\phi_3^{q'ab}) + \frac{1}{2} (\Delta\eta_9)^2 (\phi_4^{99ab}) + (\Delta\eta_9) (\Delta\eta_{p'}) (\phi_4^{9p'ab}) + (\Delta\eta_9) (u_{0p'}) (\phi_4^{9p'ab}) + \\ & \quad \left. \frac{1}{2} (\Delta\eta_{p'}) (\Delta\eta_{q'}) (\phi_4^{p'q'ab}) + (\Delta\eta_{p'}) (u_{0q'}) (\phi_4^{p'q'ab}) + \frac{1}{2} (u_{0p'}) (u_{0q'}) (\phi_4^{p'q'ab}) \right) \end{aligned}$$

$\text{foo112} = \frac{\partial^2 \phi(\eta)}{\partial \eta_a \partial \eta_b} \Big|_{\eta=\eta(u_0)+B\Delta\eta} B_a^c(u_0) B_b^d(u_0)$

**foo112 = foo111 tB[1a, uc] tB[1b, ud]**

$$\begin{aligned}
 & (B_a^c) (B_b^d) \left( K\delta\epsilon^{ab} + o \left( (\Delta\eta_9) (\phi_3^{9ab}) + (\Delta\eta_{p'}) (\phi_3^{p'ab}) + (u_{0p'}) (\phi_3^{p'ab}) \right) + \right. \\
 & o^2 \left( -2 (\Delta\eta_{p'}) (u_{0q'}) (\bar{d}^{p'q'}) (\phi_3^{9ab}) - (u_{0p'}) (u_{0q'}) (\bar{d}^{p'q'}) (\phi_3^{9ab}) - \frac{1}{2} (\Delta\eta_9) (u_{0p'}) \right. \\
 & \quad \left. (\phi_3^{99p'}) (\phi_3^{9ab}) + 2 (\Delta\eta_9) (u_{0p'}) (\bar{d}_{q'}^{p'}) (\phi_3^{q'ab}) - (\Delta\eta_9) (u_{0p'}) (\phi_3^{9_{q'}p'}) (\phi_3^{q'ab}) + \right. \\
 & \quad \left. \frac{1}{2} (\Delta\eta_9)^2 (\phi_4^{99ab}) + (\Delta\eta_9) (\Delta\eta_{p'}) (\phi_4^{9p'ab}) + (\Delta\eta_9) (u_{0p'}) (\phi_4^{9p'ab}) + \right. \\
 & \quad \left. \frac{1}{2} (\Delta\eta_{p'}) (\Delta\eta_{q'}) (\phi_4^{p'q'ab}) + (\Delta\eta_{p'}) (u_{0q'}) (\phi_4^{p'q'ab}) + \frac{1}{2} (u_{0p'}) (u_{0q'}) (\phi_4^{p'q'ab}) \right) \left. \right)
 \end{aligned}$$

Separate the regular indices a and b for the summation into type-a indexes and 9's.

**foo113 = CanAll[sepa[sepa[foo112, 1a], 1b]];**

foo114[ua,ub]=  $\frac{\partial^2 \phi(\eta)}{\partial \eta_p \partial \eta_q} \Big|_{\eta=\eta(u_0)+B\Delta\eta} B_p^a(u_0) B_q^b(u_0)$  is the same as foo112, but the subscripts are changed. In the below, we substitute  $B^a$ 's by their expressions at the projection.



foo114[ua\_, ub\_] = foo113 /. {uc → ua, ud → ub}

$$\begin{aligned}
 & (B_9^a) (B_9^b) + (Kdelta^{9p'}) (B_9^b) (B_{p'}^a) + (Kdelta^{9p'}) (B_9^a) (B_{p'}^b) + (Kdelta^{p'q'}) (B_{p'}^a) (B_{q'}^b) + \\
 & o(\Delta\eta_9) (B_9^a) (B_9^b) (\phi 3^{999}) - 2 o^2(\Delta\eta_{p'}) (u0_{q'}) (B_9^a) (B_9^b) (d^{p'q'}) (\phi 3^{999}) - \\
 & o^2(u0_{p'}) (u0_{q'}) (B_9^a) (B_9^b) (d^{p'q'}) (\phi 3^{999}) + o(\Delta\eta_{p'}) (B_9^a) (B_9^b) (\phi 3^{99p'}) + \\
 & o(u0_{p'}) (B_9^a) (B_9^b) (\phi 3^{99p'}) + o(\Delta\eta_9) (B_9^b) (B_{p'}^a) (\phi 3^{99p'}) + o(\Delta\eta_9) (B_9^a) (B_{p'}^b) (\phi 3^{99p'}) - \\
 & \frac{1}{2} o^2(\Delta\eta_9) (u0_{p'}) (B_9^a) (B_9^b) (\phi 3^{999}) (\phi 3^{99p'}) + 2 o^2(\Delta\eta_9) (u0_{p'}) (B_9^a) (B_9^b) (d_{q'}^{p'}) (\phi 3^{99q'}) - \\
 & \frac{1}{2} o^2(\Delta\eta_9) (u0_{p'}) (B_9^b) (B_{q'}^a) (\phi 3^{99p'}) (\phi 3^{99q'}) - \\
 & \frac{1}{2} o^2(\Delta\eta_9) (u0_{p'}) (B_9^a) (B_{q'}^b) (\phi 3^{99p'}) (\phi 3^{99q'}) - \\
 & 2 o^2(\Delta\eta_{p'}) (u0_{q'}) (B_9^b) (B_{r'}^a) (d^{p'q'}) (\phi 3^{99r'}) - \\
 & o^2(u0_{p'}) (u0_{q'}) (B_9^b) (B_{r'}^a) (d^{p'q'}) (\phi 3^{99r'}) - 2 o^2(\Delta\eta_{p'}) (u0_{q'}) (B_9^a) (B_{r'}^b) (d^{p'q'}) (\phi 3^{99r'}) - \\
 & o^2(u0_{p'}) (u0_{q'}) (B_9^a) (B_{r'}^b) (d^{p'q'}) (\phi 3^{99r'}) - o^2(\Delta\eta_9) (u0_{p'}) (B_9^a) (B_9^b) (\phi 3^{99q'}) (\phi 3_{q'}^{9p'}) + \\
 & o(\Delta\eta_{p'}) (B_9^b) (B_{q'}^a) (\phi 3^{99p'q'}) + o(u0_{p'}) (B_9^b) (B_{q'}^a) (\phi 3^{99p'q'}) + \\
 & o(\Delta\eta_{p'}) (B_9^a) (B_{q'}^b) (\phi 3^{99p'q'}) + o(u0_{p'}) (B_9^a) (B_{q'}^b) (\phi 3^{99p'q'}) + \\
 & o(\Delta\eta_9) (B_{p'}^a) (B_{q'}^b) (\phi 3^{99p'q'}) + 2 o^2(\Delta\eta_9) (u0_{p'}) (B_9^b) (B_{q'}^a) (d_{r'}^{p'}) (\phi 3^{99q'r'}) + \\
 & 2 o^2(\Delta\eta_9) (u0_{p'}) (B_9^a) (B_{q'}^b) (d_{r'}^{p'}) (\phi 3^{99q'r'}) - \\
 & \frac{1}{2} o^2(\Delta\eta_9) (u0_{p'}) (B_{q'}^a) (B_{r'}^b) (\phi 3^{99p'}) (\phi 3^{99q'r'}) - \\
 & o^2(\Delta\eta_9) (u0_{p'}) (B_9^b) (B_{q'}^a) (\phi 3_{r'}^{9p'}) (\phi 3^{99q'r'}) - \\
 & o^2(\Delta\eta_9) (u0_{p'}) (B_9^a) (B_{q'}^b) (\phi 3_{r'}^{9p'}) (\phi 3^{99q'r'}) - \\
 & 2 o^2(\Delta\eta_{p'}) (u0_{q'}) (B_{r'}^a) (B_{s'}^b) (d^{p'q'}) (\phi 3^{99r's'}) - \\
 & o^2(u0_{p'}) (u0_{q'}) (B_{r'}^a) (B_{s'}^b) (d^{p'q'}) (\phi 3^{99r's'}) + o(\Delta\eta_{p'}) (B_{q'}^a) (B_{r'}^b) (\phi 3^{p'q'r'}) + \\
 & o(u0_{p'}) (B_{q'}^a) (B_{r'}^b) (\phi 3^{p'q'r'}) + 2 o^2(\Delta\eta_9) (u0_{p'}) (B_{q'}^a) (B_{r'}^b) (d_{s'}^{p'}) (\phi 3^{q'r's'}) - \\
 & o^2(\Delta\eta_9) (u0_{p'}) (B_{q'}^a) (B_{r'}^b) (\phi 3_{s'}^{9p'}) (\phi 3^{q'r's'}) + \\
 & \frac{1}{2} o^2(\Delta\eta_9)^2 (B_9^a) (B_9^b) (\phi 4^{9999}) + o^2(\Delta\eta_9) (\Delta\eta_{p'}) (B_9^a) (B_9^b) (\phi 4^{999p'}) + \\
 & o^2(\Delta\eta_9) (u0_{p'}) (B_9^a) (B_9^b) (\phi 4^{999p'}) + \frac{1}{2} o^2(\Delta\eta_9)^2 (B_9^b) (B_{p'}^a) (\phi 4^{999p'}) + \\
 & \frac{1}{2} o^2(\Delta\eta_9)^2 (B_9^a) (B_{p'}^b) (\phi 4^{999p'}) + \frac{1}{2} o^2(\Delta\eta_{p'}) (\Delta\eta_{q'}) (B_9^a) (B_9^b) (\phi 4^{99p'q'}) + \\
 & o^2(\Delta\eta_{p'}) (u0_{q'}) (B_9^a) (B_9^b) (\phi 4^{99p'q'}) + \frac{1}{2} o^2(u0_{p'}) (u0_{q'}) (B_9^a) (B_9^b) (\phi 4^{99p'q'}) + \\
 & o^2(\Delta\eta_9) (\Delta\eta_{p'}) (B_9^b) (B_{q'}^a) (\phi 4^{99p'q'}) + o^2(\Delta\eta_9) (u0_{p'}) (B_9^b) (B_{q'}^a) (\phi 4^{99p'q'}) + \\
 & o^2(\Delta\eta_9) (\Delta\eta_{p'}) (B_9^a) (B_{q'}^b) (\phi 4^{99p'q'}) + o^2(\Delta\eta_9) (u0_{p'}) (B_9^a) (B_{q'}^b) (\phi 4^{99p'q'}) + \\
 & \frac{1}{2} o^2(\Delta\eta_9)^2 (B_{p'}^a) (B_{q'}^b) (\phi 4^{99p'q'}) + \frac{1}{2} o^2(\Delta\eta_{p'}) (\Delta\eta_{q'}) (B_9^b) (B_{r'}^a) (\phi 4^{99p'q'r'}) + \\
 & o^2(\Delta\eta_{p'}) (u0_{q'}) (B_9^b) (B_{r'}^a) (\phi 4^{99p'q'r'}) + \frac{1}{2} o^2(u0_{p'}) (u0_{q'}) (B_9^b) (B_{r'}^a) (\phi 4^{99p'q'r'}) + \\
 & \frac{1}{2} o^2(\Delta\eta_{p'}) (\Delta\eta_{q'}) (B_9^a) (B_{r'}^b) (\phi 4^{99p'q'r'}) + o^2(\Delta\eta_{p'}) (u0_{q'}) (B_9^a) (B_{r'}^b) (\phi 4^{99p'q'r'}) + \\
 & \frac{1}{2} o^2(u0_{p'}) (u0_{q'}) (B_9^a) (B_{r'}^b) (\phi 4^{99p'q'r'}) + o^2(\Delta\eta_9) (\Delta\eta_{p'}) (B_{q'}^a) (B_{r'}^b) (\phi 4^{99p'q'r'}) + \\
 & o^2(\Delta\eta_9) (u0_{p'}) (B_{q'}^a) (B_{r'}^b) (\phi 4^{99p'q'r'}) + \frac{1}{2} o^2(\Delta\eta_{p'}) (\Delta\eta_{q'}) (B_{r'}^a) (B_{s'}^b) (\phi 4^{p'q'r's'}) + \\
 & o^2(\Delta\eta_{p'}) (u0_{q'}) (B_{r'}^a) (B_{s'}^b) (\phi 4^{p'q'r's'}) + \frac{1}{2} o^2(u0_{p'}) (u0_{q'}) (B_{r'}^a) (B_{s'}^b) (\phi 4^{p'q'r's'})
 \end{aligned}$$

foo115=foo114[aua,aub]

$$\begin{aligned}
 & \text{foo115} = \\
 & \text{tgeto2[ApplyRules[foo114[aua, aub], {rule3, rule4, rule15, rule16}] /. ru \to ru0]} \\
 & \text{Kdelta}^{a'b'} + o((\Delta\eta_g)(\phi_3^{9a'b'}) + (\Delta\eta_{p'}) (\phi_3^{p'a'b'}) + (u_{0p'}) (\phi_3^{p'a'b'}) + \\
 & o^2 \left( 4 (u_{0p'}) (u_{0q'}) (d^{p'a'}) (d^{q'b'}) - 2 (\Delta\eta_g) (u_{0p'}) (d^{p'b'}) (\phi_3^{99a'}) - \right. \\
 & \quad 2 (\Delta\eta_g) (u_{0p'}) (d^{p'a'}) (\phi_3^{99b'}) - 2 (\Delta\eta_{p'}) (u_{0q'}) (d^{q'b'}) (\phi_3^{99p'a'}) - \\
 & \quad 2 (\Delta\eta_{p'}) (u_{0q'}) (d^{q'a'}) (\phi_3^{99p'b'}) - 2 (u_{0p'}) (u_{0q'}) (d^{p'b'}) (\phi_3^{99q'a'}) - \\
 & \quad 2 (u_{0p'}) (u_{0q'}) (d^{p'a'}) (\phi_3^{99q'b'}) - 2 (\Delta\eta_{p'}) (u_{0q'}) (d^{p'q'}) (\phi_3^{9a'b'}) - \\
 & \quad (u_{0p'}) (u_{0q'}) (d^{p'q'}) (\phi_3^{9a'b'}) - \frac{1}{2} (\Delta\eta_g) (u_{0p'}) (\phi_3^{99p'}) (\phi_3^{9a'b'}) + \\
 & \quad 2 (\Delta\eta_g) (u_{0p'}) (d_{q,p'}) (\phi_3^{q'a'b'}) - (\Delta\eta_g) (u_{0p'}) (\phi_3^9_{q,p'}) (\phi_3^{q'a'b'}) + \\
 & \quad \frac{1}{2} (\Delta\eta_g)^2 (\phi_4^{99a'b'}) + (\Delta\eta_g) (\Delta\eta_{p'}) (\phi_4^{99p'a'b'}) + (\Delta\eta_g) (u_{0p'}) (\phi_4^{99p'a'b'}) + \\
 & \quad \left. \frac{1}{2} (\Delta\eta_{p'}) (\Delta\eta_{q'}) (\phi_4^{p'q'a'b'}) + (\Delta\eta_{p'}) (u_{0q'}) (\phi_4^{p'q'a'b'}) + \frac{1}{2} (u_{0p'}) (u_{0q'}) (\phi_4^{p'q'a'b'}) \right)
 \end{aligned}$$

check if foo115 is consistent with ph2bu obtained earlier.

$$\text{tsimp[tsimp[foo115 /. {re[la_] \to 0, ru0 \to ru}] - phi2bu]}$$

0

foo116=foo114[9,aua]

$$\begin{aligned}
 & \text{foo116} = \text{tgeto2[ApplyRules[foo114[9, aua], {rule3, rule4, rule15, rule16}] /. ru \to ru0]} \\
 & o((\Delta\eta_g)(\phi_3^{99a'}) + (\Delta\eta_{p'}) (\phi_3^{99p'a'})) + \\
 & o^2 \left( -2 (\Delta\eta_g) (u_{0p'}) (d^{p'a'}) (\phi_3^{999}) - 2 (\Delta\eta_{p'}) (u_{0q'}) (d^{q'a'}) (\phi_3^{99p'}) + \right. \\
 & \quad 2 (u_{0p'}) (u_{0q'}) (d^{q'a'}) (\phi_3^{99p'}) - 2 (u_{0p'}) (u_{0q'}) (d^{p'a'}) (\phi_3^{99q'}) - \\
 & \quad 2 (\Delta\eta_{p'}) (u_{0q'}) (d^{p'q'}) (\phi_3^{99a'}) - (\Delta\eta_g) (u_{0p'}) (\phi_3^{99p'}) (\phi_3^{99a'}) - \\
 & \quad \frac{1}{2} (\Delta\eta_{p'}) (u_{0q'}) (\phi_3^{99q'}) (\phi_3^{99p'a'}) + \frac{1}{2} (u_{0p'}) (u_{0q'}) (\phi_3^{99q'}) (\phi_3^{99p'a'}) + \\
 & \quad 4 (\Delta\eta_g) (u_{0p'}) (d_{q,p'}) (\phi_3^{9q'a'}) - \frac{1}{2} (u_{0p'}) (u_{0q'}) (\phi_3^{99p'}) (\phi_3^{9q'a'}) - \\
 & \quad 2 (\Delta\eta_g) (u_{0p'}) (\phi_3^9_{q,p'}) (\phi_3^{9q'a'}) + 2 (\Delta\eta_{p'}) (u_{0q'}) (d_{r,q'}) (\phi_3^{p'r'a'}) - \\
 & \quad 2 (u_{0p'}) (u_{0q'}) (d_{r,q'}) (\phi_3^{p'r'a'}) - (\Delta\eta_{p'}) (u_{0q'}) (\phi_3^9_{r,q'}) (\phi_3^{p'r'a'}) + \\
 & \quad (u_{0p'}) (u_{0q'}) (\phi_3^9_{r,q'}) (\phi_3^{p'r'a'}) + 2 (u_{0p'}) (u_{0q'}) (d_{r,p'}) (\phi_3^{q'r'a'}) - \\
 & \quad (u_{0p'}) (u_{0q'}) (\phi_3^9_{r,p'}) (\phi_3^{q'r'a'}) + \frac{1}{2} (\Delta\eta_g)^2 (\phi_4^{999a'}) + (\Delta\eta_g) (\Delta\eta_{p'}) (\phi_4^{99p'a'}) + \\
 & \quad \left. (\Delta\eta_g) (u_{0p'}) (\phi_4^{99p'a'}) + \frac{1}{2} (\Delta\eta_{p'}) (\Delta\eta_{q'}) (\phi_4^{99p'q'a'}) + (\Delta\eta_{p'}) (u_{0q'}) (\phi_4^{99p'q'a'}) \right)
 \end{aligned}$$

foo117=foo114[9,9]

$$\begin{aligned}
 & \text{foo117} = \text{tgeto2[ApplyRules[foo114[9, 9], {rule3, rule4, rule15, rule16}] /. ru \to ru0]} \\
 & 1 + o((\Delta\eta_g)(\phi_3^{999}) + (\Delta\eta_{p'}) (\phi_3^{99p'})) + \\
 & o^2 \left( -2 (\Delta\eta_{p'}) (u_{0q'}) (d^{p'q'}) (\phi_3^{999}) - \frac{3}{2} (\Delta\eta_g) (u_{0p'}) (\phi_3^{999}) (\phi_3^{99p'}) + \right. \\
 & \quad 6 (\Delta\eta_g) (u_{0p'}) (d_{q,p'}) (\phi_3^{99q'}) - (\Delta\eta_{p'}) (u_{0q'}) (\phi_3^{99p'}) (\phi_3^{99q'}) - \\
 & \quad 3 (\Delta\eta_g) (u_{0p'}) (\phi_3^{99q'}) (\phi_3^9_{q,p'}) - 2 (u_{0p'}) (u_{0q'}) (d^{p'r'}) (\phi_3^9_{r,q'}) + \\
 & \quad 4 (\Delta\eta_{p'}) (u_{0q'}) (d_{r,q'}) (\phi_3^{99p'r'}) - 2 (u_{0p'}) (u_{0q'}) (d_{r,q'}) (\phi_3^{99p'r'}) - \\
 & \quad 2 (\Delta\eta_{p'}) (u_{0q'}) (\phi_3^9_{r,q'}) (\phi_3^{99p'r'}) + 2 (u_{0p'}) (u_{0q'}) (\phi_3^9_{r,q'}) (\phi_3^{99p'r'}) + \\
 & \quad 4 (u_{0p'}) (u_{0q'}) (d_{r,p'}) (\phi_3^{9q'r'}) - 2 (u_{0p'}) (u_{0q'}) (\phi_3^9_{r,p'}) (\phi_3^{9q'r'}) + \\
 & \quad \frac{1}{2} (\Delta\eta_g)^2 (\phi_4^{9999}) + (\Delta\eta_g) (\Delta\eta_{p'}) (\phi_4^{999p'}) + (\Delta\eta_g) (u_{0p'}) (\phi_4^{999p'}) + \\
 & \quad \left. \frac{1}{2} (\Delta\eta_{p'}) (\Delta\eta_{q'}) (\phi_4^{99p'q'}) + (\Delta\eta_{p'}) (u_{0q'}) (\phi_4^{99p'q'}) \right)
 \end{aligned}$$

Now obtain the coefficients in terms of  $\Delta\eta_a$  for foo115,foo116,foo117.

```
goo118 = {{1, 1 / o, 2 / o^2}, {1 / o, 1 / o^2, 2 / o^3}, {2 / o^2, 2 / o^3, 4 / o^4}};
```

```
goo118 // MatrixForm
```

$$\begin{pmatrix} 1 & \frac{1}{o} & \frac{2}{o^2} \\ \frac{1}{o} & \frac{1}{o^2} & \frac{2}{o^3} \\ \frac{2}{o^2} & \frac{2}{o^3} & \frac{4}{o^4} \end{pmatrix}$$

```
foo118 =
```

```
Collect[CoefficientList[foo115 /. {re[-9] → D9, re[ala_] → DA}, {DA, D9}] * goo118,
o, tsimpp[CanAll[# /. {au1 → auc, au2 → aud, au3 → aue, au4 → auf,
au5 → aug, al1 → alc, al2 → ald, al3 → ale, al4 → alf, al5 → alg}]] &];
```

Symmetries may be inconsistent.

```
foo119 =
```

```
Collect[CoefficientList[foo116 /. {re[-9] → D9, re[ala_] → DA}, {DA, D9}] * goo118,
o, tsimpp[CanAll[# /. {au1 → auc, au2 → aud, au3 → aue, au4 → auf,
au5 → aug, al1 → alc, al2 → ald, al3 → ale, al4 → alf, al5 → alg}]] &];
```

```
foo120 =
```

```
Collect[CoefficientList[foo117 /. {re[-9] → D9, re[ala_] → DA}, {DA, D9}] * goo118,
o, tsimpp[CanAll[# /. {au1 → auc, au2 → aud, au3 → aue, au4 → auf,
au5 → aug, al1 → alc, al2 → ald, al3 → ale, al4 → alf, al5 → alg}]] &];
```

```
Dimensions[foo118]
```

```
{3, 3}
```

```
Dimensions[foo119]
```

```
{3, 3}
```

```
Dimensions[foo120]
```

```
{3, 3}
```

```
foo121 = {foo118, foo119, foo120};
```

### ■ Geometric quantities at the projection

$\hat{\phi}^{a'b'}$

```
foo121[[1, 1, 1]]
```

$$\begin{aligned} & \text{Kdelta}^{a'b'} + o(u_{0p'}) (\phi^{3p'a'b'}) + \\ & o^2 \left( 4 (u_{0p'}) (u_{0q'}) (d^{p'a'}) (d^{q'b'}) - 2 (u_{0p'}) (u_{0q'}) (d^{p'b'}) (\phi^{3^9q'a'}) - 2 (u_{0p'}) (u_{0q'}) \right. \\ & \left. (d^{p'a'}) (\phi^{3^9q'b'}) - (u_{0p'}) (u_{0q'}) (d^{p'q'}) (\phi^{3^9a'b'}) + \frac{1}{2} (u_{0p'}) (u_{0q'}) (\phi^{4p'q'a'b'}) \right) \end{aligned}$$

```
RuleUnique[rule121Pab, tp2[aua_, aub_], foo121[[1, 1, 1]]]
```

$\hat{\phi}^{9a'}$

foo121[[2, 1, 1]]

0

RuleUnique[rule121P9a, tp2[9, aua\_], foo121[[2, 1, 1]]]

$\hat{\phi}^{99}$

foo121[[3, 1, 1]]

1

RuleUnique[rule121P99, tp2[9, 9], foo121[[3, 1, 1]]]

$\hat{\phi}^{a'b'c'}$

foo121[[1, 2, 1]]

$$\phi_3^{a'b'c'} + o\left(-2(u_{0p'}) (d^{p'c'}) (\phi_3^{9a'b'}) - 2(u_{0p'}) (d^{p'b'}) (\phi_3^{9a'c'}) - 2(u_{0p'}) (d^{p'a'}) (\phi_3^{9b'c'}) + (u_{0p'}) (\phi_4^{p'a'b'c'})\right)$$

RuleUnique[rule121Pabc, tp3[aua\_, aub\_, auc\_], foo121[[1, 2, 1]]]

$\hat{\phi}^{9a'b'}$

foo121[[1, 1, 2]]

$$\phi_3^{9a'b'} + o\left(-2(u_{0p'}) (d^{p'b'}) (\phi_3^{99a'}) - 2(u_{0p'}) (d^{p'a'}) (\phi_3^{99b'}) - \frac{1}{2}(u_{0p'}) (\phi_3^{99p'}) (\phi_3^{9a'b'}) + 2(u_{0p'}) (d_{q'}^{p'}) (\phi_3^{9q'a'b'}) - (u_{0p'}) (\phi_3^{9q,p'}) (\phi_3^{9q'a'b'}) + (u_{0p'}) (\phi_4^{9p'a'b'})\right)$$

(foo121[[2, 2, 1]] /. auc → aub) - foo121[[1, 1, 2]]

0

RuleUnique[rule121P9ab, tp3[9, aua\_, aub\_], foo121[[1, 1, 2]]]

$\hat{\phi}^{99a'}$

foo121[[2, 1, 2]]

$$\phi_3^{99a'} + o\left(-2(u_{0p'}) (d^{p'a'}) (\phi_3^{999}) - (u_{0p'}) (\phi_3^{99p'}) (\phi_3^{99a'}) + 4(u_{0p'}) (d_{q'}^{p'}) (\phi_3^{99q'a'}) - 2(u_{0p'}) (\phi_3^{9q,p'}) (\phi_3^{9q'a'}) + (u_{0p'}) (\phi_4^{99p'a'})\right)$$

(foo121[[3, 2, 1]] /. auc → aua) - foo121[[2, 1, 2]]

0

RuleUnique[rule121P99a, tp3[9, 9, aua\_], foo121[[2, 1, 2]]]

$\hat{\phi}^{999}$

foo121[[3, 1, 2]]

$$\phi_3^{999} + o\left(-\frac{3}{2}(u_{0p'}) (\phi_3^{999}) (\phi_3^{99p'}) + 6(u_{0p'}) (d_{q'}^{p'}) (\phi_3^{99q'}) - 3(u_{0p'}) (\phi_3^{99q'}) (\phi_3^{9q,p'}) + (u_{0p'}) (\phi_4^{999p'})\right)$$

RuleUnique[rule121P999, tp3[9, 9, 9], foo121[[3, 1, 2]]]

$\hat{\phi}^{a'b'c'd'}$ 

foo121[[1, 3, 1]]

 $\phi_4^{a'b'c'd'}$ 

RuleUnique[rule121Pabcd, tp4[aua\_, aub\_, auc\_, aud\_], foo121[[1, 3, 1]]]

 $\hat{\phi}^{9a'b'c'}$ 

foo121[[1, 2, 2]]

 $\phi_4^{9a'b'c'}$ 

foo121[[2, 3, 1]] /. {auc → aub, aud → auc}

 $\phi_4^{9a'b'c'}$ 

RuleUnique[rule121P9abc, tp4[9, aua\_, aub\_, auc\_], foo121[[1, 2, 2]]]

 $\hat{\phi}^{99a'b'}$ 

foo121[[1, 1, 3]]

 $\phi_4^{99a'b'}$ 

foo121[[2, 2, 2]] /. {auc → aub}

 $\phi_4^{99a'b'}$ 

foo121[[3, 3, 1]] /. {auc → aua, aud → aub}

 $\phi_4^{99a'b'}$ 

RuleUnique[rule121Pabcd, tp4[9, 9, aua\_, aub\_], foo121[[1, 1, 3]]]

 $\hat{\phi}^{999a'}$ 

foo121[[2, 1, 3]]

 $\phi_4^{999a'}$ 

foo121[[3, 2, 2]] /. auc → aua

 $\phi_4^{999a'}$ 

RuleUnique[rule121P999a, tp4[9, 9, 9, aua\_], foo121[[2, 1, 3]]]

 $\hat{\phi}^{9999}$ 

foo121[[3, 1, 3]]

 $\phi_4^{9999}$ 

RuleUnique[rule121P9999, tp4[9, 9, 9, 9], foo121[[3, 1, 3]]]

zero terms

```
{foo121[[1, 3, 2]], foo121[[1, 2, 3]], foo121[[1, 3, 3]]}
{0, 0, 0}

{foo121[[2, 3, 2]], foo121[[2, 2, 3]], foo121[[2, 3, 3]]}
{0, 0, 0}

{foo121[[3, 3, 2]], foo121[[3, 2, 3]], foo121[[3, 3, 3]]}
{0, 0, 0}
```

$$A = \hat{\phi}^{a'b'} - \delta^{a'b'}$$

```
DefineTensor[t125, "A", {{2, 1}, 1}]
```

```
PermWeight::sym : Symmetries of A assigned
```

```
PermWeight::def : Object A defined
```

```
foo125 = ApplyRules[tp2[aua, aub], rule121Pab] - Kdelta[aua, aub]
```

$$4 \, \sigma^2 (u_{0p'}) (u_{0q'}) (d^{p'a'}) (d^{q'b'}) - 2 \, \sigma^2 (u_{0p'}) (u_{0q'}) (d^{p'b'}) (\phi^{3^9 q' a'}) -$$

$$2 \, \sigma^2 (u_{0p'}) (u_{0q'}) (d^{p'a'}) (\phi^{3^9 q' b'}) - \sigma^2 (u_{0p'}) (u_{0q'}) (d^{p'q'}) (\phi^{3^9 a' b'}) +$$

$$0 (u_{0p'}) (\phi^{3^9 p' a' b'}) + \frac{1}{2} \, \sigma^2 (u_{0p'}) (u_{0q'}) (\phi^{4^9 p' q' a' b'})$$

```
RuleUnique[rule125, t125[aua_, aub_], foo125]
```

$$\text{foo130} = A^2$$

```
foo130 = tgeto2[ApplyRules[t125[aua, auc] Kdelta[alc, ald] t125[aud, aub], rule125]] /.
{aua -> ala, aub -> alb}
```

$$\sigma^2 (u_{0p'}) (u_{0q'}) (\phi_{3r'a, p'}) (\phi_{3b, q'r'})$$

$$\text{foo131} = (I + A)^{-1} = I - A + A^2 = \text{the inverse of the metric} = \hat{\phi}_{a'b'} = (\hat{\phi}^{a'b'})^{-1}$$

```
foo131 =
```

```
Collect[Kdelta[ala, alb] - ApplyRules[t125[ala, alb], rule125] + foo130, o, tsimpp]
```

```
Symmetries may be inconsistent.
```

$$Kdelta_{a'b'} - \sigma (u_{0p'}) (\phi_{3a'b, p'}) +$$

$$\sigma^2 \left( -4 (u_{0p'}) (u_{0q'}) (d_{a, p'}) (d_{b, q'}) + (u_{0p'}) (u_{0q'}) (d^{p'q'}) (\phi_{3^9 a'b'}) + \right.$$

$$2 (u_{0p'}) (u_{0q'}) (d_{b, p'}) (\phi_{3^9 a, q'}) + 2 (u_{0p'}) (u_{0q'}) (d_{a, p'}) (\phi_{3^9 b, q'}) +$$

$$\left. (u_{0p'}) (u_{0q'}) (\phi_{3r'a, p'}) (\phi_{3b, q'r'}) - \frac{1}{2} (u_{0p'}) (u_{0q'}) (\phi_{4a'b, p'q'}) \right)$$

```
RuleUnique[rule131, tr2[ala_, alb_], foo131]
```

$$\text{foo132} = i\phi_{a'b'} \hat{d}^{a'b'} \text{ substitutes } \delta_{a'b'} d^{a'b'} \text{ at the projection.}$$

```
tr2[ala, alb] td[aua, aub]
```

$$(d^{a'b'}) (i\phi_{a'b'})$$

```

foo132 =
  tsimpp[tgeto2[ApplyRules[o tr2[ala, alb] td[aua, aub], {rule101, rule131}]] / o]
dp, p' + 3 o (u0, p') (eq, p' q') +  $\frac{1}{2}$  o (u0, p') (dq, q') (φ399p') - o (u0, p') (dq' r') (φ3q', r', p')

RuleUnique[rule132, td[ala_, aua_], foo132, PairaQ[ala, aua]]

```

Here we summarize the substitution rules for the projection for the derivatives. Here only discuss  $O(n^{-1/2})$  terms. This includes  $\phi^{999}$ ,  $d^{a' a'}$ .

```
rulesproj = {rule121P999, rule132};
```

■ **zc-formula**

```

zformulau0 = Collect[tgeto2[ApplyRules[zformula, rulesproj]], {o, ru0[all], w, v0}]
-v0 + w +
o (-cr[0] - dp, p' + w2 (-cr[2] +  $\frac{1}{6}$  (φ3999)) -  $\frac{1}{6}$  (φ3999) -  $\frac{1}{3}$  v02 (φ3999) +  $\frac{1}{6}$  v0 w (φ3999)) +
o2 (v03 ( $\frac{1}{18}$  (φ3999)2 +  $\frac{1}{8}$  (φ399p') (φ399p') -  $\frac{1}{8}$  (φ49999)) +
v0 ((dp, q') (dq, p') -  $\frac{1}{6}$  cr[0] (φ3999) -  $\frac{1}{6}$  (dp, p') (φ3999) +  $\frac{5}{72}$  (φ3999)2 +  $\frac{1}{8}$  (φ399p')
(φ399p') -  $\frac{1}{24}$  (φ49999)) + v0 w2 (- $\frac{1}{6}$  cr[2] (φ3999) -  $\frac{1}{24}$  (φ3999)2 +  $\frac{1}{24}$  (φ49999)) +
w3 (-cr[3] -  $\frac{1}{3}$  cr[2] (φ3999) -  $\frac{1}{72}$  (φ3999)2 +  $\frac{1}{24}$  (φ49999)) +
(u0p') (-3 (eq, p' q') -  $\frac{1}{2}$  (dq, q') (φ399p') +  $\frac{1}{4}$  (φ3999) (φ399p') -
(dq, p') (φ399q') +  $\frac{1}{2}$  (φ399q') (φ39q', p') + (dq' r') (φ3q', r', p') +
v02 ( $\frac{1}{2}$  (φ3999) (φ399p') - 2 (dq, p') (φ399q') + (φ399q') (φ39q', p') -  $\frac{1}{3}$  (φ4999p')) +
v0 w (- $\frac{1}{4}$  (φ3999) (φ399p') + (dq, p') (φ399q') -  $\frac{1}{2}$  (φ399q') (φ39q', p') +  $\frac{1}{6}$  (φ4999p')) +
w2 (- $\frac{1}{4}$  (φ3999) (φ399p') + (dq, p') (φ399q') -  $\frac{1}{2}$  (φ399q') (φ39q', p') +  $\frac{1}{6}$  (φ4999p')) -
 $\frac{1}{6}$  (φ4999p')) + w (-cr[1] + (dp, q') (dq, p') -  $\frac{1}{3}$  cr[0] (φ3999) +  $\frac{1}{6}$  (dp, p') (φ3999) +
 $\frac{13}{72}$  (φ3999)2 +  $\frac{1}{2}$  (φ399p') (φ399p') - (dp' q') (φ39p', q') +  $\frac{1}{2}$  (φ39p', q') (φ39q', p') +
v02 (- $\frac{1}{8}$  (φ399p') (φ399p') +  $\frac{1}{24}$  (φ49999)) -  $\frac{1}{8}$  (φ49999) -  $\frac{1}{4}$  (φ499p', p'))

```

**zformulatau0 =**

**Collect[tgeto2[ApplyRules[zformulatau, rulesproj]], {tau, o, ru0[all], w, v0}]**

$$\begin{aligned}
 & \frac{1}{\text{tau}} \left( -v_0 + w + o \left( -\text{cr}[0] + w^2 \left( -\text{cr}[2] + \frac{1}{6} (\phi_3^{999}) \right) - \frac{1}{3} v_0^2 (\phi_3^{999}) + \frac{1}{6} v_0 w (\phi_3^{999}) \right) + \right. \\
 & \quad o^2 \left( -\frac{1}{6} v_0 \text{cr}[0] (\phi_3^{999}) + \right. \\
 & \quad \left. w \left( -\text{cr}[1] - \frac{1}{3} \text{cr}[0] (\phi_3^{999}) + v_0^2 \left( -\frac{1}{8} (\phi_3^{99}{}_{p'}) (\phi_3^{99}{}_{p'}) + \frac{1}{24} (\phi_4^{9999}) \right) \right) + \\
 & \quad v_0^3 \left( \frac{1}{18} (\phi_3^{999})^2 + \frac{1}{8} (\phi_3^{99}{}_{p'}) (\phi_3^{99}{}_{p'}) - \frac{1}{8} (\phi_4^{9999}) \right) + \\
 & \quad v_0 w^2 \left( -\frac{1}{6} \text{cr}[2] (\phi_3^{999}) - \frac{1}{24} (\phi_3^{999})^2 + \frac{1}{24} (\phi_4^{9999}) \right) + \\
 & \quad w^3 \left( -\text{cr}[3] - \frac{1}{3} \text{cr}[2] (\phi_3^{999}) - \frac{1}{72} (\phi_3^{999})^2 + \frac{1}{24} (\phi_4^{9999}) \right) + \\
 & \quad (u_0{}_{p'}) \left( v_0^2 \left( \frac{1}{2} (\phi_3^{999}) (\phi_3^{99}{}_{p'}) - 2 (d_{q'}{}_{p'}) (\phi_3^{99}{}_{q'}) + (\phi_3^{99}{}_{q'}) (\phi_3^9{}_{q'}{}_{p'}) - \frac{1}{3} (\phi_4^{999}{}_{p'}) \right) + \right. \\
 & \quad \left. v_0 w \left( -\frac{1}{4} (\phi_3^{999}) (\phi_3^{99}{}_{p'}) + (d_{q'}{}_{p'}) (\phi_3^{99}{}_{q'}) - \frac{1}{2} (\phi_3^{99}{}_{q'}) (\phi_3^9{}_{q'}{}_{p'}) + \frac{1}{6} (\phi_4^{999}{}_{p'}) \right) + \right. \\
 & \quad \left. w^2 \left( -\frac{1}{4} (\phi_3^{999}) (\phi_3^{99}{}_{p'}) + (d_{q'}{}_{p'}) (\phi_3^{99}{}_{q'}) - \frac{1}{2} (\phi_3^{99}{}_{q'}) (\phi_3^9{}_{q'}{}_{p'}) + \frac{1}{6} (\phi_4^{999}{}_{p'}) \right) \right) \Big) + \\
 & \text{tau} \left( o \left( - (d_p{}_{p'}) - \frac{1}{6} (\phi_3^{999}) \right) + o^2 \left( v_0 \left( (d_p{}_{q'}) (d_{q'}{}_{p'}) - \frac{1}{6} (d_p{}_{p'}) (\phi_3^{999}) + \right. \right. \right. \\
 & \quad \left. \left. \frac{5}{72} (\phi_3^{999})^2 + \frac{1}{8} (\phi_3^{99}{}_{p'}) (\phi_3^{99}{}_{p'}) - \frac{1}{24} (\phi_4^{9999}) \right) + \right. \\
 & \quad (u_0{}_{p'}) \left( -3 (e_{q'}{}_{p'}{}_{q'}) - \frac{1}{2} (d_{q'}{}_{q'}) (\phi_3^{99}{}_{p'}) + \frac{1}{4} (\phi_3^{999}) (\phi_3^{99}{}_{p'}) - (d_{q'}{}_{p'}) (\phi_3^{99}{}_{q'}) + \right. \\
 & \quad \left. \frac{1}{2} (\phi_3^{99}{}_{q'}) (\phi_3^9{}_{q'}{}_{p'}) + (d^{q'}{}_{r'}) (\phi_3{}_{q'}{}_{r'}{}_{p'}) - \frac{1}{6} (\phi_4^{999}{}_{p'}) \right) + \\
 & \quad \left. w \left( (d_p{}_{q'}) (d_{q'}{}_{p'}) + \frac{1}{6} (d_p{}_{p'}) (\phi_3^{999}) + \frac{13}{72} (\phi_3^{999})^2 + \frac{1}{2} (\phi_3^{99}{}_{p'}) (\phi_3^{99}{}_{p'}) - \right. \right. \\
 & \quad \left. \left. (d^{p'}{}_{q'}) (\phi_3^9{}_{p'}{}_{q'}) + \frac{1}{2} (\phi_3^9{}_{p'}{}_{q'}) (\phi_3^9{}_{q'}{}_{p'}) - \frac{1}{8} (\phi_4^{9999}) - \frac{1}{4} (\phi_4^{99}{}_{p'}{}_{p'}) \right) \right) \Big)
 \end{aligned}$$



**InputForm[zformulatauu0]**

```
(-v0 + w + o*(-cr[0] + w^2*(-cr[2] + tp3[9, 9, 9]/6) -
(v0^2*tp3[9, 9, 9])/3 + (v0*w*tp3[9, 9, 9])/6) +
o^2*(-(v0*cr[0]*tp3[9, 9, 9])/6 +
w*(-cr[1] - (cr[0]*tp3[9, 9, 9])/3 +
v0^2*(-(tp3[9, 9, a11]*tp3[9, 9, au1])/8 +
tp4[9, 9, 9, 9]/24)) + v0^3*(tp3[9, 9, 9]^2/18 +
(tp3[9, 9, a11]*tp3[9, 9, au1])/8 - tp4[9, 9, 9, 9]/8) +
v0*w^2*(-(cr[2]*tp3[9, 9, 9])/6 - tp3[9, 9, 9]^2/24 +
tp4[9, 9, 9, 9]/24) + w^3*(-cr[3] - (cr[2]*tp3[9, 9, 9])/3 -
tp3[9, 9, 9]^2/72 + tp4[9, 9, 9, 9]/24) +
ru0[a11]*(v0^2*((tp3[9, 9, 9]*tp3[9, 9, au1])/2 -
2*td[a12, au1]*tp3[9, 9, au2] + tp3[9, 9, au2]*
tp3[9, a12, au1] - tp4[9, 9, 9, au1]/3) +
v0*w*(-(tp3[9, 9, 9]*tp3[9, 9, au1])/4 +
td[a12, au1]*tp3[9, 9, au2] -
(tp3[9, 9, au2]*tp3[9, a12, au1])/2 + tp4[9, 9, 9, au1]/
6) + w^2*(-(tp3[9, 9, 9]*tp3[9, 9, au1])/4 +
td[a12, au1]*tp3[9, 9, au2] -
(tp3[9, 9, au2]*tp3[9, a12, au1])/2 + tp4[9, 9, 9, au1]/
6))))/tau + tau*(o*(-td[a11, au1] - tp3[9, 9, 9]/6) +
o^2*(v0*(td[a11, au2]*td[a12, au1] - (td[a11, au1]*tp3[9, 9, 9])/
6 + (5*tp3[9, 9, 9]^2)/72 + (tp3[9, 9, a11]*tp3[9, 9, au1])/
8 - tp4[9, 9, 9, 9]/24) + ru0[a11]*(-3*te[a12, au1, au2] -
(td[a12, au2]*tp3[9, 9, au1])/2 +
(tp3[9, 9, 9]*tp3[9, 9, au1])/4 - td[a12, au1]*
tp3[9, 9, au2] + (tp3[9, 9, au2]*tp3[9, a12, au1])/2 +
td[au2, au3]*tp3[a12, a13, au1] - tp4[9, 9, 9, au1]/6) +
w*(td[a11, au2]*td[a12, au1] + (td[a11, au1]*tp3[9, 9, 9])/6 +
(13*tp3[9, 9, 9]^2)/72 + (tp3[9, 9, a11]*tp3[9, 9, au1])/2 -
td[au1, au2]*tp3[9, a11, a12] +
(tp3[9, a11, au2]*tp3[9, a12, au1])/2 - tp4[9, 9, 9, 9]/8 -
tp4[9, 9, a11, au1]/4)))
```

We confirm that zformula depends on  $u0_{a'}$  only linearly, and the term is only  $O(n^{-1})$ .

**Collect[Coefficient[zformulatauu0, ru0[a11]], {o, tau}]**

$$o^2 \left( \tau \left( -3 (e_{q', p' q'}) - \frac{1}{2} (d_{q', q'}) (\phi_{3^{99p'}}) + \frac{1}{4} (\phi_{3^{999}}) (\phi_{3^{99p'}}) - \right. \right. \\ \left. \left. (d_{q', p'}) (\phi_{3^{99q'}}) + \frac{1}{2} (\phi_{3^{99q'}}) (\phi_{3^9_{q', p'}}) + (d^{q' r'}) (\phi_{3_{q', r', p'}}) - \frac{1}{6} (\phi_{4^{999p'}}) \right) + \right. \\ \left. \frac{1}{\tau} \left( \frac{1}{2} v_0^2 (\phi_{3^{999}}) (\phi_{3^{99p'}}) - \frac{1}{4} v_0 w (\phi_{3^{999}}) (\phi_{3^{99p'}}) - \frac{1}{4} w^2 (\phi_{3^{999}}) (\phi_{3^{99p'}}) - \right. \right. \\ \left. \left. 2 v_0^2 (d_{q', p'}) (\phi_{3^{99q'}}) + v_0 w (d_{q', p'}) (\phi_{3^{99q'}}) + w^2 (d_{q', p'}) (\phi_{3^{99q'}}) + \right. \right. \\ \left. \left. v_0^2 (\phi_{3^{99q'}}) (\phi_{3^9_{q', p'}}) - \frac{1}{2} v_0 w (\phi_{3^{99q'}}) (\phi_{3^9_{q', p'}}) - \frac{1}{2} w^2 (\phi_{3^{99q'}}) (\phi_{3^9_{q', p'}}) - \right. \right. \\ \left. \left. \frac{1}{3} v_0^2 (\phi_{4^{999p'}}) + \frac{1}{6} v_0 w (\phi_{4^{999p'}}) + \frac{1}{6} w^2 (\phi_{4^{999p'}}) \right) \right)$$

## Bootstrap Methods

In this part, the asymptotic accuracies of several bootstrap methods are discussed. We use the zc-formula obtained in the previous part.

### ■ Startup

This section initializes the *Mathematica* session.

## ■ packages

```
<< Statistics`ContinuousDistributions`
```

## ■ error messages

```
Off[General::spell1]
```

## ■ distribution functions

```
gammadist[x_, m_, α_] := PDF[GammaDistribution[m, α], x]
Gammadist[x_, m_, α_] := CDF[GammaDistribution[m, α], x]
f[x_] := PDF[NormalDistribution[0, 1], x]
F[x_] := CDF[NormalDistribution[0, 1], x]
Q[x_] := Quantile[NormalDistribution[0, 1], x]
Chidist[x_, {di_, nc_}] := CDF[NoncentralChiSquareDistribution[di, nc], x]
```

# ■ Asymptotic Analysis of Bootstrap Methods

This section calculates the distribution functions of several bootstrap methods for showing their asymptotic accuracies in terms of the unbiasedness of hypothesis testing of the region  $R$ . The calculations are based on the  $z_c$ -formula obtained in the previous part. We first define a pivot statistic and shows its third-order accuracy. The bootstrap probability is first-order accurate, the double bootstrap is second-order accurate, and the two-level bootstrap is second-order accurate.

## ■ preliminary

The  $z_c$ -formula is given in  $z_c[w, cc, v_0, \tau] = z_{\text{form}\tau} = z_c(w; v_0, \tau) = \Phi^{-1}[\Pr\{W \leq w; v_0, \tau\}]$ , where  $cc = \{c_0, c_1, c_2, c_3\}$  specifies the modified signed distance  $w$ . The signed distance  $v$  is expressed in terms of  $w$  by  $v = w - \sum_{r=0}^3 c_r w^r$ , or in the inverse series  $w = v - \sum_{r=0}^3 cb_r v^r$ . We write the coefficients  $cb_0 = cb_0$ ,  $cb_1 = cb_1$ , or  $c_0 = c_0$ ,  $c_1 = c_1$ , etc. The rule to calculate  $\{c_0, c_1, c_2, c_3\}$  in terms of  $\{cb_0, cb_1, cb_2, cb_3\}$  is given in "rulecc2cb" or in  $cb2cc$  function. The function  $zq2cc[\text{exp}]$  calculates the  $\{c_0, c_1, c_2, c_3\}$  from the polynomial of  $w$  in terms of  $v$ .

## ■ simplification functions

Ignore  $O(n^{-3/2})$  terms for scalar

```
geto2[exp_] := Sum[Simplify[Coefficient[exp, o, i]] oi, {i, -1, 2}]
```

Series expansion for scalar ignoring  $O(n^{-3/2})$  terms.

```
gets2[exp_] := geto2[Series[exp, {o, 0, 2}]]
```

```
geto[exp_, n_] := Sum[Simplify[Coefficient[exp, o, i]] oi, {i, -1, n}]
```

```
gets[exp_, n_] := geto[Series[exp, {o, 0, n}], n]
```

■ **zc-formula**

zc[w,cc,v0,tau]=zformtau is  $z_c(w; v_0, \tau) = \Phi^{-1}[\Pr\{W \leq w; v_0, \tau\}]$ , where  $u_{0a}$  is assumed zero. The coefficients  $cc=\{c_0,c_1,c_2,c_3\}$  specify the modified signed distance  $w$ . We do not need to use the more general  $zformtauu_0$  in which  $u_{0a} \neq 0$ , because the  $u_0$  terms contribute only  $O(n^{-3/2})$  in our calculation below.

$$\begin{aligned} & \text{zc}[w_, \{c0_, c1_, c2_, c3_\}, v0_, tau_] = \\ & \text{tau} * (\text{o} * (-\text{Daa} - \text{P999} / 6) + \text{o}^2 * ((\text{Dab2} - (\text{Daa} * \text{P999}) / 6 + (5 * \text{P999}^2) / 72 - \\ & \quad \text{P9999} / 24 + \text{P99a2} / 8) * v0 + (\text{Dab2} - \text{DabP9ab} + (\text{Daa} * \text{P999}) / 6 + \\ & \quad (13 * \text{P999}^2) / 72 - \text{P9999} / 8 + \text{P99a2} / 2 - \text{P99aa} / 4 + \text{P9ab2} / 2) * w)) + \\ & (-v0 + w + \text{o} * (-c0 - (\text{P999} * v0^2) / 3 + (\text{P999} * v0 * w) / 6 + (-c2 + \text{P999} / 6) * w^2) + \\ & \quad \text{o}^2 * (-c0 * \text{P999} * v0) / 6 + (\text{P999}^2 / 18 - \text{P9999} / 8 + \text{P99a2} / 8) * v0^3 + \\ & \quad (-c1 - (c0 * \text{P999}) / 3 + (\text{P9999} / 24 - \text{P99a2} / 8) * v0^2) * w + \\ & \quad (-c2 * \text{P999}) / 6 - \text{P999}^2 / 24 + \text{P9999} / 24) * v0 * w^2 + \\ & \quad (-c3 - (c2 * \text{P999}) / 3 - \text{P999}^2 / 72 + \text{P9999} / 24) * w^3) / \text{tau} \\ & \text{tau} \left( \text{o} \left( -\text{Daa} - \frac{\text{P999}}{6} \right) + \text{o}^2 \left( \left( \text{Dab2} - \frac{\text{Daa} \text{P999}}{6} + \frac{5 \text{P999}^2}{72} - \frac{\text{P9999}}{24} + \frac{\text{P99a2}}{8} \right) v0 + \right. \right. \\ & \quad \left. \left( \text{Dab2} - \text{DabP9ab} + \frac{\text{Daa} \text{P999}}{6} + \frac{13 \text{P999}^2}{72} - \frac{\text{P9999}}{8} + \frac{\text{P99a2}}{2} - \frac{\text{P99aa}}{4} + \frac{\text{P9ab2}}{2} \right) w \right) \right) + \\ & \frac{1}{\text{tau}} \left( -v0 + w + \text{o} \left( -c0 - \frac{\text{P999} v0^2}{3} + \frac{\text{P999} v0 w}{6} + \left( -c2 + \frac{\text{P999}}{6} \right) w^2 \right) + \text{o}^2 \left( -\frac{1}{6} c0 \text{P999} v0 + \right. \right. \\ & \quad \left. \left( \frac{\text{P999}^2}{18} - \frac{\text{P9999}}{8} + \frac{\text{P99a2}}{8} \right) v0^3 + \left( -c1 - \frac{c0 \text{P999}}{3} + \left( \frac{\text{P9999}}{24} - \frac{\text{P99a2}}{8} \right) v0^2 \right) w + \right. \\ & \quad \left. \left( -\frac{c2 \text{P999}}{6} - \frac{\text{P999}^2}{24} + \frac{\text{P9999}}{24} \right) v0 w^2 + \left( -c3 - \frac{c2 \text{P999}}{3} - \frac{\text{P999}^2}{72} + \frac{\text{P9999}}{24} \right) w^3 \right) \end{aligned}$$

■ **modified signed distance**

$\{c_0,c_1,c_2,c_3\}$  are represented by  $\{cb_0,cb_1,cb_2,cb_3\}$

```
rulecc2cb = {c0 -> cb0, c1 -> cb1 - 2 cb0 cb2, c2 -> cb2, c3 -> -2 cb2^2 + cb3};
coef2cb[coef_] := Expand[Simplify[(coef - {0, 1, 0, 0}) / {o, o^2, o, o^2}]]
cb2cc[{cb0_, cb1_, cb2_, cb3_}] :=
  Expand[Simplify[{cb0, cb1 - 2 cb0 cb2, cb2, -2 cb2^2 + cb3}]];
zq2cc[exp_] := cb2cc[coef2cb[PadRight[CoefficientList[exp, v], 4]]]
```

■ **the pivot and some existing bootstrap methods**

The pivot is defined as  $z_8[v]=\hat{z}_\infty(0, v) = -\Phi^{-1}(\Pr\{V \geq v; v_0 = 0\})=z_c[v, \{0,0,0,0\}, 0, 1]$ .  $cb_r$ 's and  $c_r$ 's are in  $cbz_8$  and  $ccz_8$  respectively for  $z_8[v]$ . We define  $z_q[v]=\hat{z}_q(0, v)=z_8[v] + q_0 + q_1 v + q_2 v^2 + q_3 v^3$ , where the coefficients  $qq=\{q_0,q_1,q_2,q_3\}$  specify the  $z_q[v]$ .  $zq2qq$  calculates  $qq$  from any  $z$ -value.  $cb_r$ 's and  $c_r$ 's are in  $cbz_q$  and  $ccz_q$  respectively for  $z_q[v]$ . The distribution function of  $z_q$  is obtained as  $\Pr\{z_q[V] \leq w; v_0, \tau\}=\Phi\{zfqzq[w, \{q_0,q_1,q_2,q_3\}, v_0, \tau]\}$ . We observe that  $zfqzq[w, \{0,0,0,0\}, 0, 1]=w$ , and thus the distribution function of  $z_8$  under  $v_0=0$  is  $\Pr\{Z_8 \leq w; 0, 1\}=\Phi(w)$ .

The bootstrap probability is  $\tilde{\alpha}_1(0, v, \tau_1) = \Pr\{V \leq 0; v_0 = v, \tau_1\}$  for  $y=\eta(0, v)$ , and the corresponding  $z$ -value is  $z_1[v, \tau_1]=\hat{z}_1(0, v, \tau_1) = -\Phi^{-1}(\tilde{\alpha}_1(0, v, \tau_1))=z_c[0, \{0,0,0,0\}, v, \tau_1]$ . For  $\tau_1=1$ , we define  $\hat{z}_0 = z_0[v]=z_1[v, 1]$ , which can be regarded as another  $w$ . For general  $\tau_1$ ,  $w_1=\tau_1 z_1[v, \tau_1]$  is regarded as another  $w$  with  $cb_r$ 's being

cbw1 and  $c_r$ 's being ccw1, and the distribution function is expressed as  $\Pr\{W1 \leq w; v0, \tau\} = \Phi(zfw1)$ . For  $\tau=1$  and  $\tau_1=1$ , we have  $\Pr\{\hat{Z}_0 \leq w; v0, \tau = 1\} = \Phi\{zfv0[w, v0]\}$ , which becomes  $zfv0[w, 0] = w + O(n^{-1/2})$  under  $v0=0$ , showing the first-order accuracy of  $z0[v]$ .

The z-value of the double bootstrap probability is  $zd[v] = -\Phi^{-1}[\Pr\{\hat{Z}_0 \leq \hat{z}_0(v); v0 = 0\}]$ , and we observe that  $z8[v]=zd[v]$ , showing the double bootstrap asymptotically equivalent to the third-order accurate pivot statistic up to  $O(n^{-1})$  terms.

The ABC formula is given in abcformula[v,ac]. The z-value of the two-level bootstrap method is calculated in za[v]. Its  $q_i$ 's are in qqza. The distribution function of za[v] under  $\tau=1$  is  $\Pr\{za[V] \leq w; v0, 1\} = \Phi\{zfvq[w, qqza, v0, 1]\}$ . This becomes  $w + O(n^{-1})$  for  $v0=0$ , showing the second-order accuracy of the two-level bootstrap.

### ■ pivot statistic

We define  $\hat{\alpha}_\infty(0, v) = \Pr\{V \geq v; v0 = 0\}$ , and the corresponding z-value  $\hat{z}_\infty(0, v) = -\Phi^{-1}(\hat{\alpha}_\infty(0, v))$ . We denote this z-value as  $z8[v]=zc[v, \{0,0,0,0\}, 0, 1]$ .

```

z8[v_] = Collect[zc[v, {0, 0, 0, 0}, 0, 1], {o, v}]

v + o (-Daa -  $\frac{P999}{6} + \frac{P999 v^2}{6}$ ) +
o^2 ( (Dab2 - DabP9ab +  $\frac{Daa P999}{6} + \frac{13 P999^2}{72} - \frac{P9999}{8} + \frac{P99a2}{2} - \frac{P99aa}{4} + \frac{P9ab2}{2}$ ) v +
(  $-\frac{P999^2}{72} + \frac{P9999}{24}$ ) v^3 )

cbz8 = coef2cb[CoefficientList[z8[v], v]]

{-Daa -  $\frac{P999}{6}$ , Dab2 - DabP9ab +  $\frac{Daa P999}{6} + \frac{13 P999^2}{72} - \frac{P9999}{8} + \frac{P99a2}{2} - \frac{P99aa}{4} + \frac{P9ab2}{2}$ ,
 $\frac{P999}{6}$ ,  $-\frac{P999^2}{72} + \frac{P9999}{24}$  }

ccz8 = cb2cc[cbz8]

{-Daa -  $\frac{P999}{6}$ , Dab2 - DabP9ab +  $\frac{Daa P999}{2} + \frac{17 P999^2}{72} - \frac{P9999}{8} + \frac{P99a2}{2} - \frac{P99aa}{4} + \frac{P9ab2}{2}$ ,
 $\frac{P999}{6}$ ,  $-\frac{5 P999^2}{72} + \frac{P9999}{24}$  }

```

We slightly alter  $z8[v]$  and denoted  $zq[v]=\hat{z}_q(0, v)$  below.

```

zq[v_, {q0_, q1_, q2_, q3_}] = z8[v] + o q0 + o^2 q1 v + o q2 v^2 + o^2 q3 v^3;

```

Here we define a function to collect  $q_i$ 's for later use

```

zq2qq[zz_] :=
Expand[Simplify[PadRight[CoefficientList[zz - z8[v], v], 4] / {o, o^2, o, o^2}]]

```

check if this is correct.

```

zq2qq[zq[v, {q0, q1, q2, q3}]]
{q0, q1, q2, q3}

```

Now we continue to calculate the distribution function of  $zq[v]$

$$\mathbf{cbzq} = \mathbf{coef2cb}[\mathbf{CoefficientList}[\mathbf{zq}[\mathbf{v}, \{\mathbf{q0}, \mathbf{q1}, \mathbf{q2}, \mathbf{q3}\}], \mathbf{v}]]$$

$$\left\{ -\text{Daa} - \frac{\text{P999}}{6} + \mathbf{q0}, \right. \\ \left. \text{Dab2} - \text{DabP9ab} + \frac{\text{Daa P999}}{6} + \frac{13 \text{P999}^2}{72} - \frac{\text{P9999}}{8} + \frac{\text{P99a2}}{2} - \frac{\text{P99aa}}{4} + \frac{\text{P9ab2}}{2} + \mathbf{q1}, \right. \\ \left. \frac{\text{P999}}{6} + \mathbf{q2}, -\frac{\text{P999}^2}{72} + \frac{\text{P9999}}{24} + \mathbf{q3} \right\}$$

$$\mathbf{cczq} = \mathbf{cb2cc}[\mathbf{cbzq}]$$

$$\left\{ -\text{Daa} - \frac{\text{P999}}{6} + \mathbf{q0}, \text{Dab2} - \text{DabP9ab} + \frac{\text{Daa P999}}{2} + \frac{17 \text{P999}^2}{72} - \frac{\text{P9999}}{8} + \right. \\ \left. \frac{\text{P99a2}}{2} - \frac{\text{P99aa}}{4} + \frac{\text{P9ab2}}{2} - \frac{\text{P999 q0}}{3} + \mathbf{q1} + 2 \text{Daa q2} + \frac{\text{P999 q2}}{3} - 2 \mathbf{q0 q2}, \right. \\ \left. \frac{\text{P999}}{6} + \mathbf{q2}, -\frac{5 \text{P999}^2}{72} + \frac{\text{P9999}}{24} - \frac{2 \text{P999 q2}}{3} - 2 \mathbf{q2}^2 + \mathbf{q3} \right\}$$

The distribution function of zq is obtained here.  $\Pr\{zq[V] \leq w; v0, \tau\} = \Phi\{zfq[w, \{q0, q1, q2, q3\}, v0, \tau]\}$ .

$$\mathbf{zfq}[\mathbf{w}_, \{\mathbf{q0}_, \mathbf{q1}_, \mathbf{q2}_, \mathbf{q3}_\}, \mathbf{v0}_, \mathbf{\tau}_] =$$

$$\mathbf{Collect}[\mathbf{zc}[\mathbf{w}, \mathbf{cczq}, \mathbf{v0}, \mathbf{\tau}], \{\mathbf{o}, \mathbf{w}, \mathbf{v0}\}, \mathbf{Expand}]$$

$$-\frac{\mathbf{v0}}{\mathbf{\tau}} + \frac{\mathbf{w}}{\mathbf{\tau}} + \mathbf{o} \left( \frac{\text{Daa}}{\mathbf{\tau}} + \frac{\text{P999}}{6 \mathbf{\tau}} - \frac{\mathbf{q0}}{\mathbf{\tau}} - \text{Daa } \mathbf{\tau} - \frac{\text{P999 } \mathbf{\tau}}{6} - \frac{\text{P999 } \mathbf{v0}^2}{3 \mathbf{\tau}} + \frac{\text{P999 } \mathbf{v0} \mathbf{w}}{6 \mathbf{\tau}} - \frac{\mathbf{q2} \mathbf{w}^2}{\mathbf{\tau}} \right) + \\ \mathbf{o}^2 \left( \left( \frac{\text{Daa P999}}{6 \mathbf{\tau}} + \frac{\text{P999}^2}{36 \mathbf{\tau}} - \frac{\text{P999 q0}}{6 \mathbf{\tau}} + \text{Dab2 } \mathbf{\tau} - \frac{\text{Daa P999 } \mathbf{\tau}}{6} + \right. \right. \\ \left. \left. \frac{5 \text{P999}^2 \mathbf{\tau}}{72} - \frac{\text{P9999 } \mathbf{\tau}}{24} + \frac{\text{P99a2 } \mathbf{\tau}}{8} \right) \mathbf{v0} + \left( \frac{\text{P999}^2}{18 \mathbf{\tau}} - \frac{\text{P9999}}{8 \mathbf{\tau}} + \frac{\text{P99a2}}{8 \mathbf{\tau}} \right) \mathbf{v0}^3 + \right. \\ \left( -\frac{\text{Dab2}}{\mathbf{\tau}} + \frac{\text{DabP9ab}}{\mathbf{\tau}} - \frac{\text{Daa P999}}{6 \mathbf{\tau}} - \frac{13 \text{P999}^2}{72 \mathbf{\tau}} + \frac{\text{P9999}}{8 \mathbf{\tau}} - \frac{\text{P99a2}}{2 \mathbf{\tau}} + \frac{\text{P99aa}}{4 \mathbf{\tau}} - \frac{\text{P9ab2}}{2 \mathbf{\tau}} - \frac{\mathbf{q1}}{\mathbf{\tau}} - \right. \\ \left. \frac{2 \text{Daa q2}}{\mathbf{\tau}} - \frac{\text{P999 q2}}{3 \mathbf{\tau}} + \frac{2 \mathbf{q0 q2}}{\mathbf{\tau}} + \text{Dab2 } \mathbf{\tau} - \text{DabP9ab } \mathbf{\tau} + \frac{\text{Daa P999 } \mathbf{\tau}}{6} + \frac{13 \text{P999}^2 \mathbf{\tau}}{72} \right. \\ \left. \frac{\text{P9999 } \mathbf{\tau}}{8} + \frac{\text{P99a2 } \mathbf{\tau}}{2} - \frac{\text{P99aa } \mathbf{\tau}}{4} + \frac{\text{P9ab2 } \mathbf{\tau}}{2} + \left( \frac{\text{P9999}}{24 \mathbf{\tau}} - \frac{\text{P99a2}}{8 \mathbf{\tau}} \right) \mathbf{v0}^2 \right) \mathbf{w} + \\ \left( -\frac{5 \text{P999}^2}{72 \mathbf{\tau}} + \frac{\text{P9999}}{24 \mathbf{\tau}} - \frac{\text{P999 q2}}{6 \mathbf{\tau}} \right) \mathbf{v0} \mathbf{w}^2 + \left( \frac{\text{P999 q2}}{3 \mathbf{\tau}} + \frac{2 \mathbf{q2}^2}{\mathbf{\tau}} - \frac{\mathbf{q3}}{\mathbf{\tau}} \right) \mathbf{w}^3 \Big)$$

For tau=1, zfq becomes

$$\mathbf{zfq}[\mathbf{w}, \{\mathbf{q0}, \mathbf{q1}, \mathbf{q2}, \mathbf{q3}\}, \mathbf{v0}, 1]$$

$$-\mathbf{v0} + \mathbf{w} + \mathbf{o} \left( -\mathbf{q0} - \frac{\text{P999 } \mathbf{v0}^2}{3} + \frac{\text{P999 } \mathbf{v0} \mathbf{w}}{6} - \mathbf{q2} \mathbf{w}^2 \right) + \\ \mathbf{o}^2 \left( \left( \text{Dab2} + \frac{7 \text{P999}^2}{72} - \frac{\text{P9999}}{24} + \frac{\text{P99a2}}{8} - \frac{\text{P999 q0}}{6} \right) \mathbf{v0} + \left( \frac{\text{P999}^2}{18} - \frac{\text{P9999}}{8} + \frac{\text{P99a2}}{8} \right) \mathbf{v0}^3 + \right. \\ \left( -\mathbf{q1} - 2 \text{Daa q2} - \frac{\text{P999 q2}}{3} + 2 \mathbf{q0 q2} + \left( \frac{\text{P9999}}{24} - \frac{\text{P99a2}}{8} \right) \mathbf{v0}^2 \right) \mathbf{w} + \\ \left( -\frac{5 \text{P999}^2}{72} + \frac{\text{P9999}}{24} - \frac{\text{P999 q2}}{6} \right) \mathbf{v0} \mathbf{w}^2 + \left( \frac{\text{P999 q2}}{3} + 2 \mathbf{q2}^2 - \mathbf{q3} \right) \mathbf{w}^3 \Big)$$

When v0=0, tau=1, zfq becomes

$$\mathbf{zfq}[\mathbf{w}, \{\mathbf{q0}, \mathbf{q1}, \mathbf{q2}, \mathbf{q3}\}, 0, 1]$$

$$\mathbf{w} + \mathbf{o} \left( -\mathbf{q0} - \mathbf{q2} \mathbf{w}^2 \right) + \mathbf{o}^2 \left( \left( -\mathbf{q1} - 2 \text{Daa q2} - \frac{\text{P999 q2}}{3} + 2 \mathbf{q0 q2} \right) \mathbf{w} + \left( \frac{\text{P999 q2}}{3} + 2 \mathbf{q2}^2 - \mathbf{q3} \right) \mathbf{w}^3 \right)$$

In particular, the distribution function of z8 under v0=0 is  $\Pr\{Z8 \leq w; 0, 1\} = \Phi(w)$ .

zfq[w, {0, 0, 0, 0}, 0, 1]

w

■ bootstrap probability

We define  $\tilde{\alpha}_1(0, v, \tau) = \Pr\{V \leq 0; v_0 = v, \tau\}$ . This is the bootstrap probability for  $y=\eta(0,v)$ . The z-value is  $\tilde{z}_1(0, v, \tau) = -\Phi^{-1}(\tilde{\alpha}_1(0, v, \tau))$ . This becomes  $z1[v,\tau]=zc[0,\{0,0,0,0\},v,\tau]$ . For a general  $y=\eta(u,v)$  with  $u \neq 0$ , the expression changes only by the linear term in u and the difference is only  $O(n^{-1})$ .

z1[v\_, tau\_] = Collect[-zc[0, {0, 0, 0, 0}, v, tau], {tau, o, v}, Expand]

$$\tau \left( o \left( Daa + \frac{P999}{6} \right) + o^2 \left( -Dab2 + \frac{Daa P999}{6} - \frac{5 P999^2}{72} + \frac{P9999}{24} - \frac{P99a2}{8} \right) v \right) + \frac{v + \frac{1}{3} o P999 v^2 + o^2 \left( -\frac{P999^2}{18} + \frac{P9999}{8} - \frac{P99a2}{8} \right) v^3}{\tau}$$

The following  $w1=\tau z1[v,\tau]$  is regarded as another w.

w1[v\_, tau\_] = Collect[tau z1[v, tau], {o, v, tau}]

$$v + o \left( \left( Daa + \frac{P999}{6} \right) \tau^2 + \frac{P999 v^2}{3} \right) + o^2 \left( \left( -Dab2 + \frac{Daa P999}{6} - \frac{5 P999^2}{72} + \frac{P9999}{24} - \frac{P99a2}{8} \right) \tau^2 v + \left( -\frac{P999^2}{18} + \frac{P9999}{8} - \frac{P99a2}{8} \right) v^3 \right)$$

Here we obtain the coefficients cc for w1. The scale tau is specified instead of tau.

cbw1 = coef2cb[CoefficientList[w1[v, tau], v]]

$$\left\{ Daa \tau^2 + \frac{P999 \tau^2}{6}, -Dab2 \tau^2 + \frac{1}{6} Daa P999 \tau^2 - \frac{5 P999^2 \tau^2}{72} + \frac{P9999 \tau^2}{24} - \frac{P99a2 \tau^2}{8}, \frac{P999}{3}, -\frac{P999^2}{18} + \frac{P9999}{8} - \frac{P99a2}{8} \right\}$$

ccw1 = cb2cc[cbw1]

$$\left\{ Daa \tau^2 + \frac{P999 \tau^2}{6}, -Dab2 \tau^2 - \frac{1}{2} Daa P999 \tau^2 - \frac{13 P999^2 \tau^2}{72} + \frac{P9999 \tau^2}{24} - \frac{P99a2 \tau^2}{8}, \frac{P999}{3}, -\frac{5 P999^2}{18} + \frac{P9999}{8} - \frac{P99a2}{8} \right\}$$

The distribution function of w1 under v0 and scale tau is  $\Pr\{W1 \leq w; v_0, \tau\} = \Phi(zfw1)$ .

$$\begin{aligned}
 \text{zfw1}[w_, \text{tau1}_, v0_, \text{tau}_] &= \text{Collect}[\text{zc}[w, \text{ccw1}, v0, \text{tau}], \{o, w, \text{tau1}, v0, \text{tau}\}, \text{Expand}] \\
 &= \frac{v0}{\text{tau}} + \frac{w}{\text{tau}} + o \left( \left( -\text{Daa} - \frac{\text{P999}}{6} \right) \text{tau} + \frac{(-\text{Daa} - \frac{\text{P999}}{6}) \text{tau1}^2}{\text{tau}} - \frac{\text{P999} v0^2}{3 \text{tau}} + \frac{\text{P999} v0 w}{6 \text{tau}} - \frac{\text{P999} w^2}{6 \text{tau}} \right) + \\
 &o^2 \left( \left( \text{Dab2} - \frac{\text{Daa} \text{P999}}{6} + \frac{5 \text{P999}^2}{72} - \frac{\text{P9999}}{24} + \frac{\text{P99a2}}{8} \right) \text{tau} v0 + \right. \\
 &\quad \left. \frac{(-\frac{\text{Daa} \text{P999}}{6} - \frac{\text{P999}^2}{36}) \text{tau1}^2 v0}{\text{tau}} + \frac{(\frac{\text{P999}^2}{18} - \frac{\text{P9999}}{8} + \frac{\text{P99a2}}{8}) v0^3}{\text{tau}} + \right. \\
 &\quad \left( \left( \text{Dab2} - \text{DabP9ab} + \frac{\text{Daa} \text{P999}}{6} + \frac{13 \text{P999}^2}{72} - \frac{\text{P9999}}{8} + \frac{\text{P99a2}}{2} - \frac{\text{P99aa}}{4} + \frac{\text{P9ab2}}{2} \right) \text{tau} + \right. \\
 &\quad \left. \frac{(\text{Dab2} + \frac{\text{Daa} \text{P999}}{6} + \frac{\text{P999}^2}{8} - \frac{\text{P9999}}{24} + \frac{\text{P99a2}}{8}) \text{tau1}^2}{\text{tau}} + \frac{(\frac{\text{P9999}}{24} - \frac{\text{P99a2}}{8}) v0^2}{\text{tau}} \right) w + \\
 &\quad \left. \frac{(-\frac{7 \text{P999}^2}{72} + \frac{\text{P9999}}{24}) v0 w^2}{\text{tau}} + \frac{(\frac{11 \text{P999}^2}{72} - \frac{\text{P9999}}{12} + \frac{\text{P99a2}}{8}) w^3}{\text{tau}} \right)
 \end{aligned}$$

We can use the function `zq2cc` to obtain `ccw1` directly from `w1[v]`.

$$\begin{aligned}
 \text{zq2cc}[w1[v, \text{tau1}]] - \text{ccw1} \\
 \{0, 0, 0, 0\}
 \end{aligned}$$

We can do the same as above in another way though `zq`.

$$\begin{aligned}
 \text{qqw1} &= \text{zq2qq}[w1[v, \text{tau1}]] \\
 &\left\{ \text{Daa} + \frac{\text{P999}}{6} + \text{Daa} \text{tau1}^2 + \frac{\text{P999} \text{tau1}^2}{6}, -\text{Dab2} + \text{DabP9ab} - \frac{\text{Daa} \text{P999}}{6} - \right. \\
 &\quad \left. \frac{13 \text{P999}^2}{72} + \frac{\text{P9999}}{8} - \frac{\text{P99a2}}{2} + \frac{\text{P99aa}}{4} - \frac{\text{P9ab2}}{2} - \text{Dab2} \text{tau1}^2 + \frac{1}{6} \text{Daa} \text{P999} \text{tau1}^2 - \right. \\
 &\quad \left. \frac{5 \text{P999}^2 \text{tau1}^2}{72} + \frac{\text{P9999} \text{tau1}^2}{24} - \frac{\text{P99a2} \text{tau1}^2}{8}, \frac{\text{P999}}{6}, -\frac{\text{P999}^2}{24} + \frac{\text{P9999}}{12} - \frac{\text{P99a2}}{8} \right\}
 \end{aligned}$$

$$\begin{aligned}
 \text{Collect}[\text{zfqzq}[w, \text{qqw1}, v0, \text{tau}], \{o, w, \text{tau1}, v0, \text{tau}\}, \text{Expand}] - \text{zfw1}[w, \text{tau1}, v0, \text{tau}] \\
 0
 \end{aligned}$$

The usual bootstrap probability is defined from  $\tilde{\alpha}_1(0, v, \text{tau})$  with  $\text{tau}=1$ . We denote it as  $\hat{\alpha}_0(0, v) = \tilde{\alpha}_1(0, v, 1)$ . The corresponding z-value is denoted by  $\hat{z}_0(0, v)$ .

$$\begin{aligned}
 \text{z0}[v_] &= \text{z1}[v, 1] \\
 &= o \left( \text{Daa} + \frac{\text{P999}}{6} \right) + v + o^2 \left( -\text{Dab2} + \frac{\text{Daa} \text{P999}}{6} - \frac{5 \text{P999}^2}{72} + \frac{\text{P9999}}{24} - \frac{\text{P99a2}}{8} \right) v + \\
 &\quad \frac{1}{3} o \text{P999} v^2 + o^2 \left( -\frac{\text{P999}^2}{18} + \frac{\text{P9999}}{8} - \frac{\text{P99a2}}{8} \right) v^3
 \end{aligned}$$

The distribution function of  $\hat{z}_0(u, v)$  is denoted by  $\text{Pr} \{ \hat{Z}_0 \leq w; v0, \text{tau} = 1 \} = \Phi \{ \text{zfqz0}[w, v0] \}$ .

$$\begin{aligned}
 \mathbf{zfv0}[\mathbf{w}_-, \mathbf{v0}_-] &= \text{Collect}[\mathbf{zfv1}[\mathbf{w}, 1, \mathbf{v0}, 1], \{\mathbf{o}, \mathbf{w}, \mathbf{v0}\}] \\
 &= -\mathbf{v0} + \mathbf{w} + \mathbf{o} \left( -2 \text{Daa} - \frac{\text{P999}}{3} - \frac{\text{P999} \mathbf{v0}^2}{3} + \frac{\text{P999} \mathbf{v0} \mathbf{w}}{6} - \frac{\text{P999} \mathbf{w}^2}{6} \right) + \\
 &\quad \mathbf{o}^2 \left( \left( \text{Dab2} - \frac{\text{Daa} \text{P999}}{3} + \frac{\text{P999}^2}{24} - \frac{\text{P9999}}{24} + \frac{\text{P99a2}}{8} \right) \mathbf{v0} + \right. \\
 &\quad \left( \frac{\text{P999}^2}{18} - \frac{\text{P9999}}{8} + \frac{\text{P99a2}}{8} \right) \mathbf{v0}^3 + \left( 2 \text{Dab2} - \text{DabP9ab} + \frac{\text{Daa} \text{P999}}{3} + \frac{11 \text{P999}^2}{36} - \right. \\
 &\quad \left. \frac{\text{P9999}}{6} + \frac{5 \text{P99a2}}{8} - \frac{\text{P99aa}}{4} + \frac{\text{P9ab2}}{2} + \left( \frac{\text{P9999}}{24} - \frac{\text{P99a2}}{8} \right) \mathbf{v0}^2 \right) \mathbf{w} + \\
 &\quad \left. \left( -\frac{7 \text{P999}^2}{72} + \frac{\text{P9999}}{24} \right) \mathbf{v0} \mathbf{w}^2 + \left( \frac{11 \text{P999}^2}{72} - \frac{\text{P9999}}{12} + \frac{\text{P99a2}}{8} \right) \mathbf{w}^3 \right)
 \end{aligned}$$

Under  $\mathbf{v0}=0$ ,  $\mathbf{zfv0}$  becomes

$$\begin{aligned}
 \mathbf{zfv0}[\mathbf{w}, 0] &= \mathbf{w} + \mathbf{o} \left( -2 \text{Daa} - \frac{\text{P999}}{3} - \frac{\text{P999} \mathbf{w}^2}{6} \right) + \\
 &\quad \mathbf{o}^2 \left( \left( 2 \text{Dab2} - \text{DabP9ab} + \frac{\text{Daa} \text{P999}}{3} + \frac{11 \text{P999}^2}{36} - \frac{\text{P9999}}{6} + \frac{5 \text{P99a2}}{8} - \frac{\text{P99aa}}{4} + \frac{\text{P9ab2}}{2} \right) \mathbf{w} + \right. \\
 &\quad \left. \left( \frac{11 \text{P999}^2}{72} - \frac{\text{P9999}}{12} + \frac{\text{P99a2}}{8} \right) \mathbf{w}^3 \right)
 \end{aligned}$$

### ■ double bootstrap

The z-value of the double bootstrap probability is  $\mathbf{zd}[\mathbf{v}] = -\Phi^{-1}[\text{Pr}\{\hat{Z}_0 \leq \hat{z}_0(\mathbf{v}); \mathbf{v0} = 0\}]$ .

$$\begin{aligned}
 \mathbf{zd}[\mathbf{v}_-] &= \text{Collect}[\text{geto2}[\mathbf{zfv0}[\mathbf{z0}[\mathbf{v}], 0]], \{\mathbf{o}, \mathbf{v}\}] \\
 &= \mathbf{v} + \mathbf{o} \left( -\text{Daa} - \frac{\text{P999}}{6} + \frac{\text{P999} \mathbf{v}^2}{6} \right) + \\
 &\quad \mathbf{o}^2 \left( \left( \text{Dab2} - \text{DabP9ab} + \frac{\text{Daa} \text{P999}}{6} + \frac{13 \text{P999}^2}{72} - \frac{\text{P9999}}{8} + \frac{\text{P99a2}}{2} - \frac{\text{P99aa}}{4} + \frac{\text{P9ab2}}{2} \right) \mathbf{v} + \right. \\
 &\quad \left. \left( -\frac{\text{P999}^2}{72} + \frac{\text{P9999}}{24} \right) \mathbf{v}^3 \right)
 \end{aligned}$$

This is equivalent to the pivot  $\mathbf{z8}[\mathbf{v}]$

$$\begin{aligned}
 \mathbf{z8}[\mathbf{v}] - \mathbf{zd}[\mathbf{v}] \\
 0
 \end{aligned}$$

### ■ two-level bootstrap

The ABC conversion formula of Efron (1987) and DiCiccio and Efron (1992) is

$$\mathbf{abcformula}[\mathbf{v}_-, \mathbf{ac}_-] = \frac{\mathbf{z0}[\mathbf{v}] - \mathbf{z0}[0]}{1 - \mathbf{ac} (\mathbf{z0}[\mathbf{v}] - \mathbf{z0}[0])} - \mathbf{z0}[0];$$

The acceleration constant "ac" is

$$\mathbf{ac} = -\frac{1}{6} \mathbf{o} \text{P999};$$

The z-value of the bootstrap probability around the projection is



$$z_0[0] \\ o \left( D_{aa} + \frac{P_{999}}{6} \right)$$

Thus the ABC formula, denoted  $z_a[v]$  here, becomes

$$z_a[v_] = \text{gets2}[\text{abcformula}[v, ac]] \\ v - \frac{1}{72} o^2 v \\ (72 D_{ab2} - 12 D_{aa} P_{999} + 5 P_{999}^2 - 3 P_{9999} + 9 P_{99a2} + 10 P_{999}^2 v^2 - 9 P_{9999} v^2 + 9 P_{99a2} v^2) + \\ \frac{1}{6} o (-6 D_{aa} + P_{999} (-1 + v^2))$$

The coefficients  $q_i$ 's are obtained by

$$qqza = \text{zq2qq}[z_a[v]] \\ \left\{ 0, -2 D_{ab2} + D_{ab} P_{9ab} - \frac{P_{999}^2}{4} + \frac{P_{9999}}{6} - \frac{5 P_{99a2}}{8} + \frac{P_{99aa}}{4} - \frac{P_{9ab2}}{2}, \right. \\ \left. 0, -\frac{P_{999}^2}{8} + \frac{P_{9999}}{12} - \frac{P_{99a2}}{8} \right\}$$

The distribution function of  $z_a[v]$  under  $\tau=1$  is  $\Pr\{z_a[V] \leq w; v_0, 1\} = \Phi[\text{zfq}[w, qqza, v_0, 1]]$

$$\text{Collect}[\text{zfq}[w, qqza, v_0, 1], \{o, w, v_0\}, \text{Expand}] \\ -v_0 + w + o \left( -\frac{P_{999} v_0^2}{3} + \frac{P_{999} v_0 w}{6} \right) + \\ o^2 \left( \left( D_{ab2} + \frac{7 P_{999}^2}{72} - \frac{P_{9999}}{24} + \frac{P_{99a2}}{8} \right) v_0 + \left( \frac{P_{999}^2}{18} - \frac{P_{9999}}{8} + \frac{P_{99a2}}{8} \right) v_0^3 + \right. \\ \left. \left( 2 D_{ab2} - D_{ab} P_{9ab} + \frac{P_{999}^2}{4} - \frac{P_{9999}}{6} + \frac{5 P_{99a2}}{8} - \frac{P_{99aa}}{4} + \frac{P_{9ab2}}{2} + \left( \frac{P_{9999}}{24} - \frac{P_{99a2}}{8} \right) v_0^2 \right) \right. \\ \left. w + \left( -\frac{5 P_{999}^2}{72} + \frac{P_{9999}}{24} \right) v_0 w^2 + \left( \frac{P_{999}^2}{8} - \frac{P_{9999}}{12} + \frac{P_{99a2}}{8} \right) w^3 \right)$$

Under  $v_0=0, \tau=1$ , it becomes

$$\text{Collect}[\text{zfq}[w, qqza, 0, 1], \{o, w\}, \text{Expand}] \\ w + o^2 \left( \left( 2 D_{ab2} - D_{ab} P_{9ab} + \frac{P_{999}^2}{4} - \frac{P_{9999}}{6} + \frac{5 P_{99a2}}{8} - \frac{P_{99aa}}{4} + \frac{P_{9ab2}}{2} \right) w + \right. \\ \left. \left( \frac{P_{999}^2}{8} - \frac{P_{9999}}{12} + \frac{P_{99a2}}{8} \right) w^3 \right)$$

### ■ multistep-multiscale bootstrap method

Here we calculate the asymptotic accuracy of the three-step multiscale bootstrap method.

The pivot  $z_8[v]$  is generalized to define  $\hat{z}_\infty(0, v, v_0, \tau) = z_8[v, v_0, \tau] = z_c[v, \{0, 0, 0, 0\}, v_0, \tau]$ , which reduces to  $z_8[v, 0, 1] = z_8[v]$ . We standardize  $z_8[v, v_0, \tau]$  by  $w_8[v, v_0, \tau] = z_8[v, v_0, \tau] \cdot \text{isz}_8 + v_0$ , where  $\text{isz}_8 = \tau - \frac{1}{6} P_{999} \tau v_0 + \frac{1}{36} P_{999}^2 \tau v_0^2$ , so that  $w_8[v, v_0, \tau] = v + O(n^{-1/2})$ . The distribution function is  $\Pr\{W_8 \leq w; v_0, \tau\} = \Phi\{\text{zfs}_8[w, v_0, \tau]\}$ . We show  $\Pr\{z_8[V, v_0, \tau] \leq w; v_0, \tau\} = \Pr\{W_8 \leq w \cdot \text{isz}_8 + v_0; v_0, \tau\} = \Phi\{\text{zfw}_8[w \cdot \text{isz}_8 + v_0]\} = \Phi(w)$ . We obtain the inverse function of  $z_8[v, v_0, \tau] = z$  in terms of  $v$  so that  $v_8[z, v_0, \tau] = v$  is defined.

Let  $\text{func}[z] = (az+b) + \text{rem}[z]$ , where  $\text{rem}[z] = \sum_{i=0}^m c[[i+1]] z^i$  is of order  $O(n^{-1/2})$ . We would like to calculate  $\text{intfz} = Q[\int_{-\infty}^{\infty} F[\text{func}[z]] f[z] dz]$ , where  $f, F$ , and  $Q$  are, respectively, the density, the distribution, and quantile functions of the standard normal distribution. Let us define  $\text{intxfg}[a, b, n] = \frac{\sqrt{1+a^2}}{f[\frac{b}{\sqrt{1+a^2}}]} \int_{-\infty}^{\infty} x^n f[a x + b] f[x] dx$ .

Then we will show that  $\text{intfz} = \text{ddint}[a, b, d, z] = \frac{b}{\sqrt{1+a^2}} + \sum_{i=0}^{2m+1} d[[i+1]] \frac{\text{intxfg}[a, b, i]}{\sqrt{1+a^2}} + \frac{1}{2} \frac{b}{\sqrt{1+a^2}} \left( \sum_{i=0}^{2m+1} d[[i+1]] \frac{\text{intxfg}[a, b, i]}{\sqrt{1+a^2}} \right)^2$ , where  $d = \text{func2dd}[a, b, \text{rem}, z]$  calculates the coefficients of the expansion  $\text{rem}[z] - \frac{1}{2} (az+b) \text{rem}[z]^2 = \sum_{i=0}^{2m+1} d[[i+1]] z^i$ .

Using  $\text{ddint}$  function defined above, we will calculate  $z2[v0, \text{tau1}, \text{tau2}] = \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z1[v, \text{tau2}]) f[v, v0, \text{tau1}] dv] = \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z1[v8[z, v0, \text{tau1}], \text{tau2}]) f[z] dz]$ . This is the z-value of the twostep-multiscale bootstrap probability.

Similarly we will calculate the z-value of the threestep-multiscale bootstrap probability defined by  $z3[v0, \text{tau1}, \text{tau2}, \text{tau3}] = \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z2[v, \text{tau2}, \text{tau3}]) f[v, v0, \text{tau1}] dv] = \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z2[v8[z, v0, \text{tau1}], \text{tau2}, \text{tau3}]) f[z] dz]$ .

The six geometric quantities  $\gamma_1, \dots, \gamma_6$  are denoted by  $G1, \dots, G6$  here. The scaling parameter  $s_1, \dots, s_4$  are denoted by  $S1, \dots, S4$  here. We define  $Z3G$  and  $Z8G$  in terms of  $G1, \dots, G6, S1, \dots, S4$ , and will show that  $Z3G = z3[v, \text{tau1}, \text{tau2}, \text{tau3}]$  and  $Z8G = z8[v]$ .

■ a generalization of the pivot

We define a generalization of the pivot by  $\hat{z}_{\infty}(0, v, v0, \text{tau}) = z8[v, v0, \text{tau}] = zc[v, \{0, 0, 0, 0\}, v0, \text{tau}]$ . We use  $z8$  in the analysis of the multistep bootstrap.

$$\begin{aligned} z8[v_, v0_, tau_] &= \text{Collect}[zc[v, \{0, 0, 0, 0\}, v0, tau], \{tau, v, v0\}] \\ &= \tau \left( -\frac{Daa}{6} - \frac{P999}{6} \right) + \\ &\quad \tau^2 \left( Dab2 - DabP9ab + \frac{Daa P999}{6} + \frac{13 P999^2}{72} - \frac{P9999}{8} + \frac{P99a2}{2} - \frac{P99aa}{4} + \frac{P9ab2}{2} \right) v + \\ &\quad \tau^2 \left( Dab2 - \frac{Daa P999}{6} + \frac{5 P999^2}{72} - \frac{P9999}{24} + \frac{P99a2}{8} \right) v0 + \\ &\quad \frac{1}{\tau} \left( \tau^2 \left( -\frac{P999^2}{72} + \frac{P9999}{24} \right) v^3 - v0 - \frac{1}{3} \tau P999 v0^2 + \tau^2 \left( \frac{P999^2}{18} - \frac{P9999}{8} + \frac{P99a2}{8} \right) v0^3 + \right. \\ &\quad \left. v^2 \left( \frac{\tau P999}{6} + \tau^2 \left( -\frac{P999^2}{24} + \frac{P9999}{24} \right) v0 \right) + v \left( 1 + \frac{\tau P999 v0}{6} + \tau^2 \left( \frac{P9999}{24} - \frac{P99a2}{8} \right) v0^2 \right) \right) \end{aligned}$$

This reduces to the pivot when  $v0=0, \text{tau}=1$ .

$$\begin{aligned} &\text{Simplify}[z8[v, 0, 1] - z8[v]] \\ &= 0 \end{aligned}$$

We standardize  $z8[v, v0, \text{tau}]$  so that it can be regarded as  $w$  with proper coefficients. First, we find the rescaling factor.

$$\begin{aligned} scz8 &= \frac{1}{\tau} \left( 1 + \frac{\tau P999}{6} v0 \right) \\ &= \frac{1 + \frac{\tau P999 v0}{6}}{\tau} \end{aligned}$$

**isz8 = gets2[1 / scz8]**

$$\tau - \frac{1}{6} o P999 \tau v_0 + \frac{1}{36} o^2 P999^2 \tau v_0^2$$

The standardization of  $z8[v, v_0, \tau]$  up to  $O(n^{-1/2})$  term is denoted  $w8[v, v_0, \tau] = z8[v, v_0, \tau] * isz8 + v_0$ .

**w8[v\_, v0\_, tau\_] = Collect[geto2[z8[v, v0, tau] isz8 + v0], {o, v, tau, v0}]**

$$v + o \left( \left( -Daa - \frac{P999}{6} \right) \tau^2 + \frac{P999 v^2}{6} - \frac{P999 v_0^2}{6} \right) +$$

$$o^2 \left( \left( -\frac{P999^2}{72} + \frac{P9999}{24} \right) v^3 + \left( Dab2 + \frac{7 P999^2}{72} - \frac{P9999}{24} + \frac{P99a2}{8} \right) \tau^2 v_0 + \right.$$

$$\left. \left( -\frac{5 P999^2}{72} + \frac{P9999}{24} \right) v^2 v_0 + \left( \frac{P999^2}{12} - \frac{P9999}{8} + \frac{P99a2}{8} \right) v_0^3 + \right.$$

$$v \left( \left( Dab2 - DabP9ab + \frac{Daa P999}{6} + \frac{13 P999^2}{72} - \frac{P9999}{8} + \frac{P99a2}{2} - \frac{P99aa}{4} + \frac{P9ab2}{2} \right) \tau^2 + \right.$$

$$\left. \left( \frac{P9999}{24} - \frac{P99a2}{8} \right) v_0^2 \right)$$

**qqw8 = Collect[zq2qq[w8[v, v0, tau]], o, Simplify]**

$$\left\{ \frac{1}{6} (-6 Daa (-1 + \tau^2) - P999 (-1 + \tau^2 + v_0^2)) + \right.$$

$$\frac{1}{72} o v_0 (72 Dab2 \tau^2 - 3 P9999 \tau^2 + 9 P99a2 \tau^2 -$$

$$9 P9999 v_0^2 + 9 P99a2 v_0^2 + P999^2 (7 \tau^2 + 6 v_0^2)),$$

$$\frac{1}{72} (-12 Daa P999 - 13 P999^2 + 9 P9999 - 36 P99a2 + 18 P99aa - 36 P9ab2 + 12 Daa P999 \tau^2 +$$

$$13 P999^2 \tau^2 - 9 P9999 \tau^2 + 36 P99a2 \tau^2 - 18 P99aa \tau^2 + 36 P9ab2 \tau^2 +$$

$$72 Dab2 (-1 + \tau^2) - 72 DabP9ab (-1 + \tau^2) + 3 P9999 v_0^2 - 9 P99a2 v_0^2),$$

$$\left. \frac{1}{72} o (-5 P999^2 v_0 + 3 P9999 v_0), 0 \right\}$$

Then the distribution function of  $W8 = w8[V, v_0, \tau]$  is  $\Pr\{W8 \leq w; v_0, \tau\} = \Phi\{zfw8[w, v_0, \tau]\}$ .

**zfw8[w\_, v0\_, tau\_] = Simplify[geto2[zfzq[w, qqw8, v0, tau]]]**

$$-\frac{(6 + o P999 v_0) (v_0 - w)}{6 \tau}$$

Then,  $\Pr\{z8[V, v_0, \tau] \leq w; v_0, \tau\} = \Pr\{W8 \leq w isz8 + v_0; v_0, \tau\} = \Phi\{zfw8[w isz8 + v_0]\}$ . The following equation implies that  $\Pr\{z8[V, v_0, \tau] \leq w; v_0, \tau\} = \Phi(w)$ .

**geto2[zfw8[w isz8 + v0, v0, tau]]**

w

We obtain the inverse function of  $z8[v, v_0, \tau] = z$  in terms of  $v$  so that  $v8[z, v_0, \tau] = v$  by applying the inversion formula of the modified signed distance to  $w8$ . We use  $v8$ -function in the following section.

**ccw8 = Collect[zq2cc[w8[v, v0, tau]], o, Simplify];**

**ccw8o = ccw8 \* {o, o^2, o, o^2};**

$$\begin{aligned}
 v8[z_, v0_, tau_] &= \text{geto2}[(w - \text{geto2}[\text{Sum}[\text{ccw8o}[[i]] w^{i-1}, \{i, 4\}]])] /. w \to z \text{isz8} + v0] \\
 v0 + tau z - \frac{1}{72} o^2 tau & \\
 (36 \text{Daa} \text{P999} tau v0 + 24 \text{P999}^2 tau v0 - 12 \text{P9999} tau v0 + 45 \text{P99a2} tau v0 - 18 \text{P99aa} tau v0 + & \\
 36 \text{P9ab2} tau v0 + 36 \text{Daa} \text{P999} tau^2 z + 17 \text{P999}^2 tau^2 z - 9 \text{P9999} tau^2 z + 36 \text{P99a2} tau^2 z - & \\
 18 \text{P99aa} tau^2 z + 36 \text{P9ab2} tau^2 z - 27 \text{P999}^2 v0^2 z + 18 \text{P9999} v0^2 z - & \\
 9 \text{P99a2} v0^2 z - 24 \text{P999}^2 tau v0 z^2 + 12 \text{P9999} tau v0 z^2 - 5 \text{P999}^2 tau^2 z^3 + & \\
 3 \text{P9999} tau^2 z^3 - 72 \text{DabP9ab} tau (v0 + tau z) + 72 \text{Dab2} tau (2 v0 + tau z)) + & \\
 \frac{1}{6} o tau (6 \text{Daa} tau + \text{P999} (tau - 3 v0 z - tau z^2)) &
 \end{aligned}$$

Check if  $z8[v8[z]] = z$  and  $v8[z8[v]] = v$

$$\begin{aligned}
 &\text{geto2}[z8[v8[z, v0, tau], v0, tau]] \\
 &z \\
 &\text{geto2}[v8[z8[v, v0, tau], v0, tau]] \\
 &v
 \end{aligned}$$

■ some useful formula for normal integration

The normal distribution function  $\Phi[x]$ , the quantile function  $\Phi^{-1}[p]$ , and the normal density function  $\phi[x]$ .

$$\{F[x], Q[p], f[x]\}$$

$$\left\{ \frac{1}{2} \left( 1 + \text{Erf} \left[ \frac{x}{\sqrt{2}} \right] \right), \sqrt{2} \text{InverseErf}[0, -1 + 2 p], \frac{e^{-\frac{x^2}{2}}}{\sqrt{2} \pi} \right\}$$

First, we will calculate the following  $\text{intxfp}[a,b]$

$$\begin{aligned}
 \text{intxfp}[a_, b_] &= \text{FullSimplify} \left[ \int_{-\infty}^{\infty} F[ax + b] f[x] dx, a \in \text{Reals} \wedge b \in \text{Reals} \right] \\
 &= \frac{\int_{-\infty}^{\infty} e^{-\frac{x^2}{2}} \left( 1 + \text{Erf} \left[ \frac{b+ax}{\sqrt{2}} \right] \right) dx}{2 \sqrt{2} \pi}
 \end{aligned}$$

Mathematica does not calculate  $\text{intxfp}$ , so we consider change of variables. First rewrite  $\text{intxfp}$  as follows.

$$\begin{aligned}
 &\text{FullSimplify} \left[ \int_{-\infty}^{\infty} \int_{-\infty}^{ax1+b} f[x1] f[x2] dx2 dx1, a \in \text{Reals} \wedge b \in \text{Reals} \right] \\
 &= \frac{\int_{-\infty}^{\infty} e^{-\frac{x1^2}{2}} \left( 1 + \text{Erf} \left[ \frac{b+ax1}{\sqrt{2}} \right] \right) dx1}{2 \sqrt{2} \pi}
 \end{aligned}$$

Then,  $\{x1,x2\}$  is transformed to  $\{y1,y2\}$ .

$$\text{foo1} = \left\{ x1 \rightarrow -\frac{-y1 + ay2}{\sqrt{1+a^2}}, x2 \rightarrow -\frac{-ay1 - y2}{\sqrt{1+a^2}} \right\};$$

The range of the integration is now expressed as

$$\begin{aligned}
 \text{foo2} &= \text{FullSimplify}[x2 \leq ax1 + b /. \text{foo1}, a \in \text{Reals} \wedge b \in \text{Reals}] \\
 &= \sqrt{1+a^2} y2 \leq b
 \end{aligned}$$

Now we get the integration  $\text{intxfp}[a, b] = \int_{-\infty}^{\infty} F[a x + b] f[x] dx$

$$\text{intxfp}[a_, b_] = F\left[\frac{b}{\sqrt{1+a^2}}\right];$$

The following  $\text{intx2f}[n] = \int_{-\infty}^{\infty} x^{2n} f[x] dx$  gives  $\frac{(2n)!}{(2^n n!)}$ .

$$\text{intx2f}[n_] = \text{FullSimplify}\left[\int_{-\infty}^{\infty} x^{2n} f[x] dx, n \geq 0 \wedge n \in \text{Integers}\right]$$

$$\frac{2^n \text{Gamma}\left[\frac{1}{2} + n\right]}{\sqrt{\pi}}$$

**Table**[intxf[n], {n, 10}]

{intxf[1], intxf[2], intxf[3], intxf[4],  
intxf[5], intxf[6], intxf[7], intxf[8], intxf[9], intxf[10]}

The following  $\text{intxfg}[a, b, n] =$

$$\frac{\sqrt{1+a^2}}{f\left[\frac{b}{\sqrt{1+a^2}}\right]} \int_{-\infty}^{\infty} x^n f[a x + b] f[x] dx$$

will be used repeatedly. This may be obtained by using the integration by parts and  $\text{intx2f}[n]$ , but *Mathematica* does it automatically.

$$\text{foo5} = \frac{\sqrt{1+a^2}}{f\left[\frac{b}{\sqrt{1+a^2}}\right]} \int_{-\infty}^{\infty} x^n f[a x + b] f[x] dx;$$

**intxfg**[a\_, b\_, n\_] = **Simplify**[foo5, n ≥ 0 ∧ n ∈ Integers ∧ a ∈ Reals ∧ b ∈ Reals]

$$\frac{1}{\sqrt{\pi}} \left( 2^{\frac{1}{2}(-3+n)} (1+a^2)^{\frac{1}{2}(-1-n)} \left( 2(-1+(-1)^n) a b \text{Gamma}\left[1+\frac{n}{2}\right] \text{Hypergeometric1F1}\left[\frac{1}{2}-\frac{n}{2}, \frac{3}{2}, \frac{a^2 b^2}{-2-2a^2}\right] + \sqrt{2}(1+(-1)^n) \sqrt{1+a^2} \text{Gamma}\left[\frac{1+n}{2}\right] \text{Hypergeometric1F1}\left[-\frac{n}{2}, \frac{1}{2}, \frac{a^2 b^2}{-2-2a^2}\right] \right) \right)$$

$$\begin{aligned} & \text{Simplify}[\text{Table}[\text{intxf}[a, b, n], \{n, 0, 10\}]] \\ & \left\{ 1, -\frac{a b}{1+a^2}, \frac{1+a^2(1+b^2)}{(1+a^2)^2}, -\frac{a b(3+a^2(3+b^2))}{(1+a^2)^3}, \right. \\ & \frac{3+6a^2(1+b^2)+a^4(3+6b^2+b^4)}{(1+a^2)^4}, -\frac{a b(15+10a^2(3+b^2)+a^4(15+10b^2+b^4))}{(1+a^2)^5}, \\ & \frac{15+45a^2(1+b^2)+15a^4(3+6b^2+b^4)+a^6(15+45b^2+15b^4+b^6)}{(1+a^2)^6}, \\ & -\frac{1}{(1+a^2)^7} (a b(105+105a^2(3+b^2)+21a^4(15+10b^2+b^4)+a^6(105+105b^2+21b^4+b^6))), \\ & \frac{1}{(1+a^2)^8} (105+420a^2(1+b^2)+210a^4(3+6b^2+b^4)+ \\ & 28a^6(15+45b^2+15b^4+b^6)+a^8(105+420b^2+210b^4+28b^6+b^8)), \\ & -\frac{1}{(1+a^2)^9} (a b(945+1260a^2(3+b^2)+378a^4(15+10b^2+b^4)+ \\ & 36a^6(105+105b^2+21b^4+b^6)+a^8(945+1260b^2+378b^4+36b^6+b^8))), \\ & \left. \frac{1}{(1+a^2)^{10}} (945(1+a^2)^5+4725a^2(1+a^2)^4b^2+3150a^4(1+a^2)^3b^4+ \right. \\ & \left. 630a^6(1+a^2)^2b^6+45a^8(1+a^2)b^8+a^{10}b^{10}) \right\} \end{aligned}$$

Finally we consider some asymptotic expansions.

$$\begin{aligned} \text{foo7} &= \text{gets2}\left[\frac{F[x+o y]-F[x]}{f[x]}\right] \\ o y &= \frac{1}{2} o^2 x y^2 \end{aligned}$$

Thus,  $F[x+o y] = F[x] + f[x](o y - \frac{1}{2} o^2 x y^2) = F[x] + f[x] * \text{expandF}[x+o y, x]$ , where  $x = \text{Coefficient}[x+o y, o, 0]$ .

$$\text{expandF}[\text{exp}_-, \text{x}_-] := \text{gets2}\left[(\text{exp} - \text{x}) - \frac{1}{2} (\text{exp} - \text{x})^2 \text{x}\right]$$

Next, note that

$$\begin{aligned} & \text{Simplify}[\text{gets2}[F[x+o y + \frac{1}{2} o^2 x y^2]] - (F[x] + f[x] o y)] \\ & 0 \end{aligned}$$

Thus,  $Q[F[x]+f[x] o y] = x + o y + \frac{1}{2} o^2 x y^2 = \text{expandQ}[x, y]$ .

$$\text{expandQ}[\text{x}_-, \text{y}_-] := \text{gets2}\left[x + y + \frac{1}{2} x y^2\right]$$

Combining these asymptotic expansions, we obtain the following integration. Let  $\text{func}[z] = (az+b) + \text{rem}[z]$ , where  $\text{rem}[z] = \sum_{i=0}^m c[[i+1]] z^i$  is of order  $O(n^{-1/2})$ . We would like to calculate  $\text{intfz} = Q[\int_{-\infty}^{\infty} F[\text{func}[z]] f[z] dz]$ .

The integrand  $F[\text{func}[z]] f[z]$  is  $\text{expandF}[\text{func}[z], az+b] f[z] = F[az+b] f[z] + f[az+b] f[z] (\text{rem}[z] - \frac{1}{2} (az+b) \text{rem}[z]^2)$ . We denote  $\text{rem}[z] - \frac{1}{2} (az+b) \text{rem}[z]^2 = \sum_{i=0}^{2m+1} d[[i+1]] z^i$ . The coefficients d's are obtained from a, b, and c's.

$$\begin{aligned} & \text{func2dd}[\text{a}_-, \text{b}_-, \text{rem}_-, \text{z}_-] := \\ & \text{Collect}[\text{CoefficientList}[\text{gets2}[\text{rem} - \frac{1}{2} (a z + b) \text{rem}^2], z], o, \text{Simplify}] \end{aligned}$$

Now the integration is  $\text{intfz} = Q[\int_{-\infty}^{\infty} (F[az+b] + f[az+b] \sum_{i=0}^{2m+1} d[[i+1]] z^i) f[z] dz]$ . Since  $\int_{-\infty}^{\infty} F[az+b] f[z] dz = F[\frac{b}{\sqrt{1+a^2}}]$ , and  $\int_{-\infty}^{\infty} z^n f[az+b] f[z] dz = f[\frac{b}{\sqrt{1+a^2}}] \frac{\text{intxfg}[a,b,n]}{\sqrt{1+a^2}}$ , we obtain

$$\text{intfz} = Q[F[\frac{b}{\sqrt{1+a^2}}] + f[\frac{b}{\sqrt{1+a^2}}] \sum_{i=0}^{2m+1} d[[i+1]] \frac{\text{intxfg}[a,b,i]}{\sqrt{1+a^2}}].$$

Using `expandQ`, this becomes

$$\text{intfz} = \frac{b}{\sqrt{1+a^2}} + \sum_{i=0}^{2m+1} d[[i+1]] \frac{\text{intxfg}[a,b,i]}{\sqrt{1+a^2}} + \frac{1}{2} \frac{b}{\sqrt{1+a^2}} \left( \sum_{i=0}^{2m+1} d[[i+1]] \frac{\text{intxfg}[a,b,i]}{\sqrt{1+a^2}} \right)^2.$$

```
dd2int[a_, b_, dd_, z_] := Module[{intg},
  intg = Sum[dd[[i]]  $\frac{\text{intxfg}[a, b, i - 1]}{\sqrt{1 + a^2}}$ ; gets2[ $\frac{b}{\sqrt{1 + a^2}}$  (1 +  $\frac{1}{2}$  intg2) + intg]]
  , {i, 1, Length[dd]}]
```

Now, the integration function may be written as `intfz=dd2int[a,b,func2dd[a,b,rem,z],z]`;

■ **two-step multiscale bootstrap**

In the below, we will calculate  $z2[v0, \text{tau1}, \text{tau2}] = \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z1[v, \text{tau2}]) f[v, v0, \text{tau1}] dv]$   
 $= \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z1[v8[z, v0, \text{tau1}], \text{tau2}]) f[z] dz]$ .

`z1v8=z1[v8[z,v0,tau1],tau2]`. This is regarded as a polynomial of `z`, and then `intfz` will be applied to `z1v8`.

```
z1v8 = geto2[z1[v8[z, v0, tau1], tau2]]
 $\frac{v0 + \text{tau1} z}{\text{tau2}} + \frac{o(6 \text{Daa} (\text{tau1}^2 + \text{tau2}^2) + \text{P999} (\text{tau2}^2 + 2 v0^2 + \text{tau1} v0 z + \text{tau1}^2 (1 + z^2)))}{6 \text{tau2}}$ 
 $o^2 \left( -\frac{1}{72} (72 \text{Dab2} - 12 \text{Daa} \text{P999} + 5 \text{P999}^2 - 3 \text{P9999} + 9 \text{P99a2}) \text{tau2} (v0 + \text{tau1} z) - \right.$ 
 $\frac{1}{72 \text{tau2}} ((4 \text{P999}^2 - 9 \text{P9999} + 9 \text{P99a2}) (v0 + \text{tau1} z)^3 +$ 
 $\text{tau1} (36 \text{Daa} \text{P999} \text{tau1} v0 + 24 \text{P999}^2 \text{tau1} v0 - 12 \text{P9999} \text{tau1} v0 +$ 
 $45 \text{P99a2} \text{tau1} v0 - 18 \text{P99aa} \text{tau1} v0 + 36 \text{P9ab2} \text{tau1} v0 + 36 \text{Daa} \text{P999} \text{tau1}^2 z +$ 
 $17 \text{P999}^2 \text{tau1}^2 z - 9 \text{P9999} \text{tau1}^2 z + 36 \text{P99a2} \text{tau1}^2 z - 18 \text{P99aa} \text{tau1}^2 z +$ 
 $36 \text{P9ab2} \text{tau1}^2 z - 27 \text{P999}^2 v0^2 z + 18 \text{P9999} v0^2 z - 9 \text{P99a2} v0^2 z -$ 
 $24 \text{P999}^2 \text{tau1} v0 z^2 + 12 \text{P9999} \text{tau1} v0 z^2 - 5 \text{P999}^2 \text{tau1}^2 z^3 + 3 \text{P9999} \text{tau1}^2 z^3 -$ 
 $72 \text{DabP9ab} \text{tau1} (v0 + \text{tau1} z) + 72 \text{Dab2} \text{tau1} (2 v0 + \text{tau1} z)) +$ 
 $\left. 8 \text{P999} \text{tau1} (v0 + \text{tau1} z) (-6 \text{Daa} \text{tau1} + \text{P999} (3 v0 z + \text{tau1} (-1 + z^2))) \right)$ 
```

`fool1` is the  $O(1)$  term

```
z1v8o0 = Coefficient[z1v8, o, 0]
 $\frac{v0 + \text{tau1} z}{\text{tau2}}$ 
z1v8ab = CoefficientList[z1v8o0, z]
{  $\frac{v0}{\text{tau2}}$ ,  $\frac{\text{tau1}}{\text{tau2}}$  }
```

We may make replacements `b→z1v8ab[[1]]`, `a→z1v8ab[[2]]` later for the normal integration with `intxfg[a,b,n]`, i.e., `z1v8o0=az+b`.

Get the `dd` coefficients and store them in `z1v8dd`

```
z1v8dd = Collect[func2dd[z1v8ab[[2]], z1v8ab[[1]], z1v8 - z1v8o0, z],
o, Simplify[#, tau1 > 0 & tau2 > 0] &]
```

$$\left\{ \frac{o(6 \text{Daa}(\tau_1^2 + \tau_2^2) + \text{P999}(\tau_1^2 + \tau_2^2 + 2v_0^2))}{6\tau_2} - \frac{1}{72\tau_2^3} \right. \\ \left( o^2 v_0 (36 \text{Daa}^2(\tau_1^2 + \tau_2^2)^2 + 12 \text{Daa} \text{P999}(\tau_1^2 + \tau_2^2)(\tau_1^2 + 2v_0^2) + 3\tau_2^2 \right. \\ \left. (-24 \text{DabP9ab}\tau_1^2 - 4 \text{P9999}\tau_1^2 + 15 \text{P99a2}\tau_1^2 - 6 \text{P99aa}\tau_1^2 + 12 \text{P9ab2}\tau_1^2 - \right. \\ \left. \text{P9999}\tau_2^2 + 3 \text{P99a2}\tau_2^2 + 24 \text{Dab2}(2\tau_1^2 + \tau_2^2) - 3 \text{P9999}v_0^2 + 3 \text{P99a2}v_0^2) + \right. \\ \left. \text{P999}^2(\tau_1^4 + 6\tau_2^4 + 8\tau_2^2 v_0^2 + 4v_0^4 + 2\tau_1^2(9\tau_2^2 + 2v_0^2)) \right), \\ \frac{o \text{P999}\tau_1 v_0}{6\tau_2} - \frac{1}{72\tau_2^3} \left( o^2 \tau_1 (36 \text{Daa}^2(\tau_1^2 + \tau_2^2)^2 + \right. \\ \left. 12 \text{Daa} \text{P999}(\tau_1^2 + \tau_2^2)(\tau_1^2 + 3v_0^2) + 3\tau_2^2 \right. \\ \left. (-24 \text{DabP9ab}\tau_1^2 - 3 \text{P9999}\tau_1^2 + 12 \text{P99a2}\tau_1^2 - 6 \text{P99aa}\tau_1^2 + 12 \text{P9ab2}\tau_1^2 - \right. \\ \left. \text{P9999}\tau_2^2 + 3 \text{P99a2}\tau_2^2 + 24 \text{Dab2}(\tau_1^2 + \tau_2^2) - 3 \text{P9999}v_0^2 + 6 \text{P99a2}v_0^2) + \right. \\ \left. \text{P999}^2(\tau_1^4 + 6\tau_2^4 + 15\tau_2^2 v_0^2 + 8v_0^4 + \tau_1^2(11\tau_2^2 + 6v_0^2)) \right), \\ \frac{o \text{P999}\tau_1^2}{6\tau_2} - \frac{1}{72\tau_2^3} \left( o^2 \tau_1^2 v_0 (3(-5 \text{P9999} + 9 \text{P99a2})\tau_2^2 + \right. \\ \left. 24 \text{Daa} \text{P999}(\tau_1^2 + \tau_2^2) + \text{P999}^2(4\tau_1^2 + 24\tau_2^2 + 9v_0^2)) \right), \\ \left. - \frac{1}{72\tau_2^3} \left( o^2 \tau_1^3 (3(-2 \text{P9999} + 3 \text{P99a2})\tau_2^2 + 12 \text{Daa} \text{P999}(\tau_1^2 + \tau_2^2) + \right. \right. \\ \left. \left. \text{P999}^2(2\tau_1^2 + 9\tau_2^2 + 7v_0^2)) \right), - \frac{o^2 \text{P999}^2 \tau_1^4 v_0}{24\tau_2^3}, - \frac{o^2 \text{P999}^2 \tau_1^5}{72\tau_2^3} \right\}$$

```
Length[z1v8dd]
```

6

Now the integration is  $z2[v_0, \tau_1, \tau_2] = \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z1v8) f[z] dz] \dots$

```
z2[v0_, tau1_, tau2_] = Collect[
dd2int[z1v8ab[[2]], z1v8ab[[1]], z1v8dd, z], o, FullSimplify[#, tau1 > 0 & tau2 > 0] &]
```

$$\frac{v_0}{\sqrt{\tau_1^2 + \tau_2^2}} + \frac{1}{72(\tau_1^2 + \tau_2^2)^{9/2}} \left( o^2 \right. \\ \left( -72 \text{Dab2}(\tau_1^2 + \tau_2^2)^5 v_0 + (\tau_1^2 + \tau_2^2) \left( (12 \text{Daa} \text{P999} - 5 \text{P999}^2 + 3 \text{P9999} - 9 \text{P99a2}) \right. \right. \\ \left. \tau_1^8 + 3(24 \text{DabP9ab} + 8 \text{Daa} \text{P999} - 7 \text{P999}^2 + 5 \text{P9999} - 21 \text{P99a2} + 6 \text{P99aa} - 12 \text{P9ab2}) \right. \\ \left. \tau_1^6 \tau_2^2 + (144 \text{DabP9ab} + 24 \text{Daa} \text{P999} - 73 \text{P999}^2 + \right. \\ \left. 42 \text{P9999} - 135 \text{P99a2} + 36 \text{P99aa} - 72 \text{P9ab2}) \tau_1^4 \tau_2^4 + \right. \\ \left. 3(24 \text{DabP9ab} + 8(\text{Daa} - 2 \text{P999}) \text{P999} + 11 \text{P9999} + 6(-5 \text{P99a2} + \text{P99aa} - 2 \text{P9ab2})) \right. \\ \left. \tau_1^2 \tau_2^6 + (12 \text{Daa} \text{P999} - 5 \text{P999}^2 + 3 \text{P9999} - 9 \text{P99a2}) \tau_2^8 \right) v_0 - \\ \left( (4 \text{P999}^2 - 9 \text{P9999} + 9 \text{P99a2}) \tau_1^8 + 3(7 \text{P999}^2 - 11 \text{P9999} + 9 \text{P99a2}) \tau_1^6 \tau_2^2 + \right. \\ \left. (17 \text{P999}^2 - 42 \text{P9999} + 27 \text{P99a2}) \tau_1^4 \tau_2^4 + 3(4 \text{P999}^2 - 9 \text{P9999} + 6 \text{P99a2}) \right. \\ \left. \tau_1^2 \tau_2^6 + (4 \text{P999}^2 - 9 \text{P9999} + 9 \text{P99a2}) \tau_2^8 \right) v_0^3 \left. \right) + \\ \frac{1}{6(\tau_1^2 + \tau_2^2)^{5/2}} \left( o(6 \text{Daa}(\tau_1^2 + \tau_2^2)^3 + \text{P999} \right. \\ \left. (\tau_1^6 + 4\tau_1^4 \tau_2^2 + 4\tau_1^2 \tau_2^4 + \tau_2^6 + (2\tau_1^4 + 3\tau_1^2 \tau_2^2 + 2\tau_2^4) v_0^2) \right)$$

Check if z2 reduces to z1 when one of the scales is zero

```
Simplify[Limit[z2[v, tau1, tau2], tau2 -> 0] - z1[v, tau1], tau1 > 0]
```

0

```
Simplify[Limit[z2[v, tau1, tau2], tau1 -> 0] - z1[v, tau2], tau2 > 0]
```

0



■ three-step multiscale bootstrap

In the below, we will calculate  $z3[v0, \tau1, \tau2, \tau3] = \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z2[v, \tau2, \tau3]) f[v, v0, \tau1] dv]$   
 $= \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z2[v8[z, v0, \tau1], \tau2, \tau3]) f[z] dz]$ .

$z2v8 = z2[v8[z, v0, \tau1], \tau2, \tau3]$ . This is regarded as a polynomial of  $z$ , and then `intfz` will be applied to  $z2v8$ .

`z2v8 = geto2[z2[v8[z, v0, tau1], tau2, tau3]]`

$$\frac{v0 + \tau1 z}{\sqrt{\tau2^2 + \tau3^2}} + \frac{1}{6 (\tau2^2 + \tau3^2)^{5/2}} \left( o \left( 6 \text{Daa} (\tau2^2 + \tau3^2)^3 + \text{P999} (\tau2^6 + 4 \tau2^4 \tau3^2 + 4 \tau2^2 \tau3^4 + \tau3^6 + (2 \tau2^4 + 3 \tau2^2 \tau3^2 + 2 \tau3^4) (v0 + \tau1 z)^2) + \tau1 (\tau2^2 + \tau3^2)^2 (6 \text{Daa} \tau1 + \text{P999} (\tau1 - 3 v0 z - \tau1 z^2)) \right) \right) + \frac{1}{72 (\tau2^2 + \tau3^2)^{9/2}} \left( o^2 \left( -72 \text{Dab2} (\tau2^2 + \tau3^2)^5 (v0 + \tau1 z) + (\tau2^2 + \tau3^2) (12 \text{Daa} \text{P999} (\tau2^2 + \tau3^2)^2 (\tau2^4 + \tau3^4) - \text{P999}^2 (5 \tau2^8 + 21 \tau2^6 \tau3^2 + 73 \tau2^4 \tau3^4 + 48 \tau2^2 \tau3^6 + 5 \tau3^8) + 3 (\tau2^2 + \tau3^2) (\text{P9999} (\tau2^6 + 4 \tau2^4 \tau3^2 + 10 \tau2^2 \tau3^4 + \tau3^6) - 3 (-2 (4 \text{DabP9ab} + \text{P99aa} - 2 \text{P9ab2}) \tau2^2 \tau3^2 (\tau2^2 + \tau3^2) + \text{P99a2} (\tau2^6 + 6 \tau2^4 \tau3^2 + 9 \tau2^2 \tau3^4 + \tau3^6))) \right) (v0 + \tau1 z) - ((4 \text{P999}^2 - 9 \text{P9999} + 9 \text{P99a2}) \tau2^8 + 3 (7 \text{P999}^2 - 11 \text{P9999} + 9 \text{P99a2}) \tau2^6 \tau3^2 + (17 \text{P999}^2 - 42 \text{P9999} + 27 \text{P99a2}) \tau2^4 \tau3^4 + 3 (4 \text{P999}^2 - 9 \text{P9999} + 6 \text{P99a2}) \tau2^2 \tau3^6 + (4 \text{P999}^2 - 9 \text{P9999} + 9 \text{P99a2}) \tau3^8) (v0 + \tau1 z)^3 - \tau1 (\tau2^2 + \tau3^2)^4 (36 \text{Daa} \text{P999} \tau1 v0 + 24 \text{P999}^2 \tau1 v0 - 12 \text{P9999} \tau1 v0 + 45 \text{P99a2} \tau1 v0 - 18 \text{P99aa} \tau1 v0 + 36 \text{P9ab2} \tau1 v0 + 36 \text{Daa} \text{P999} \tau1^2 z + 17 \text{P999}^2 \tau1^2 z - 9 \text{P9999} \tau1^2 z + 36 \text{P99a2} \tau1^2 z - 18 \text{P99aa} \tau1^2 z + 36 \text{P9ab2} \tau1^2 z - 27 \text{P999}^2 v0^2 z + 18 \text{P9999} v0^2 z - 9 \text{P99a2} v0^2 z - 24 \text{P999}^2 \tau1 v0 z^2 + 12 \text{P9999} \tau1 v0 z^2 - 5 \text{P999}^2 \tau1^2 z^3 + 3 \text{P9999} \tau1^2 z^3 - 72 \text{DabP9ab} \tau1 (v0 + \tau1 z) + 72 \text{Dab2} \tau1 (2 v0 + \tau1 z)) + 4 \text{P999} \tau1 (\tau2^2 + \tau3^2)^2 (2 \tau2^4 + 3 \tau2^2 \tau3^2 + 2 \tau3^4) (v0 + \tau1 z) (6 \text{Daa} \tau1 + \text{P999} (\tau1 - 3 v0 z - \tau1 z^2)) \right) \right)$$

`foo11` is the  $O(1)$  term

`z2v8o0 = Coefficient[z2v8, o, 0]`

$$\frac{v0 + \tau1 z}{\sqrt{\tau2^2 + \tau3^2}}$$

`z2v8ab = CoefficientList[z2v8o0, z]`

$$\left\{ \frac{v0}{\sqrt{\tau2^2 + \tau3^2}}, \frac{\tau1}{\sqrt{\tau2^2 + \tau3^2}} \right\}$$

We may make replacements `b→z2v8ab[[1]]`, `a→z2v8ab[[2]]` later for the normal integration with `intfxg[a,b,n]`, i.e.,  $z2v8o0 = az + b$ .

Get the `dd` coefficients and store them in `z2v8dd`

`z2v8dd = Collect[func2dd[z2v8ab[[2]], z2v8ab[[1]], z2v8 - z2v8o0, z], o, FullSimplify[#, tau1 > 0 & tau2 > 0 & tau3 > 0] &]`

$$\left\{ \frac{1}{6 (\tau_2^2 + \tau_3^2)^{5/2}} \left( o \left( 6 \text{Daa} (\tau_2^2 + \tau_3^2)^2 (\tau_1^2 + \tau_2^2 + \tau_3^2) + \right. \right. \right.$$

$$\begin{aligned}
 & \text{P999} (\tau_2^2 + \tau_3^2) (\tau_2^4 + 3 \tau_2^2 \tau_3^2 + \tau_3^4 + \tau_1^2 (\tau_2^2 + \tau_3^2)) + \\
 & \left. \left. \text{P999} (2 \tau_2^4 + 3 \tau_2^2 \tau_3^2 + 2 \tau_3^4) v_0^2 \right) \right) - \\
 & \left( o^2 v_0 \left( 36 \text{Daa}^2 (\tau_2^2 + \tau_3^2)^4 (\tau_1^2 + \tau_2^2 + \tau_3^2)^2 + 3 (\tau_2^2 + \tau_3^2)^2 \right. \right. \\
 & \quad \left( 24 \text{Dab2} (\tau_2^2 + \tau_3^2)^3 (2 \tau_1^2 + \tau_2^2 + \tau_3^2) - (\tau_2^2 + \tau_3^2) \left( (24 \text{DabP9ab} + \right. \right. \\
 & \quad \quad \left. \left. 4 \text{P9999} - 15 \text{P99a2} + 6 \text{P99aa} - 12 \text{P9ab2}) \tau_1^2 \tau_2^4 + (\text{P9999} - 3 \text{P99a2}) \right. \right. \\
 & \quad \quad \left. \tau_2^6 + 2 \tau_2^2 \left( (24 \text{DabP9ab} + 4 \text{P9999} - 15 \text{P99a2} + 6 \text{P99aa} - 12 \text{P9ab2}) \tau_1^2 + \right. \right. \\
 & \quad \quad \left. \left. (12 \text{DabP9ab} + 2 \text{P9999} - 9 \text{P99a2} + 3 \text{P99aa} - 6 \text{P9ab2}) \tau_2^2 \right) \tau_3^2 + \right. \\
 & \quad \quad \left. \left( (24 \text{DabP9ab} + 4 \text{P9999} - 15 \text{P99a2} + 6 \text{P99aa} - 12 \text{P9ab2}) \tau_1^2 + \right. \right. \\
 & \quad \quad \left. \left. (24 \text{DabP9ab} + 10 \text{P9999} - 27 \text{P99a2} + 6 \text{P99aa} - 12 \text{P9ab2}) \tau_2^2 \right) \tau_3^4 + \right. \\
 & \quad \quad \left. (\text{P9999} - 3 \text{P99a2}) \tau_3^6 \right) - (3 (\text{P9999} - \text{P99a2}) \tau_2^6 + 2 (4 \text{P9999} - 3 \text{P99a2}) \\
 & \quad \quad \tau_2^4 \tau_3^2 + 3 (2 \text{P9999} - \text{P99a2}) \tau_2^2 \tau_3^4 + 3 (\text{P9999} - \text{P99a2}) \tau_3^6) v_0^2 \Big) + \\
 & \text{P999}^2 \left( (\tau_2^2 + \tau_3^2)^2 \left( 6 \tau_2^8 + 27 \tau_2^6 \tau_3^2 + 84 \tau_2^4 \tau_3^4 + \right. \right. \\
 & \quad \left. \left. 54 \tau_2^2 \tau_3^6 + 6 \tau_3^8 + \tau_1^4 (\tau_2^2 + \tau_3^2)^2 + \right. \right. \\
 & \quad \left. \left. 6 \tau_1^2 (\tau_2^2 + \tau_3^2) (3 \tau_2^4 + 7 \tau_2^2 \tau_3^2 + 3 \tau_3^4) \right) + \right. \\
 & \quad \left. (\tau_2^2 + \tau_3^2) (8 \tau_2^8 + 39 \tau_2^6 \tau_3^2 + 43 \tau_2^4 \tau_3^4 + 30 \tau_2^2 \tau_3^6 + \right. \\
 & \quad \left. 8 \tau_3^8 + 2 \tau_1^2 (\tau_2^2 + \tau_3^2) (2 \tau_2^4 + 3 \tau_2^2 \tau_3^2 + 2 \tau_3^4)) v_0^2 + \right. \\
 & \quad \left. (2 \tau_2^4 + 3 \tau_2^2 \tau_3^2 + 2 \tau_3^4)^2 v_0^4 \right) + 12 \text{Daa} \text{P999} (\tau_2^2 + \tau_3^2)^2 \\
 & \quad \left( \tau_1^2 + \tau_2^2 + \tau_3^2 \right) \left( \tau_1^2 (\tau_2^2 + \tau_3^2)^2 + 2 \tau_3^4 v_0^2 + \right. \\
 & \quad \left. 3 \tau_2^2 \tau_3^2 (\tau_3^2 + v_0^2) + \tau_2^4 (3 \tau_3^2 + 2 v_0^2) \right) \Big) \Big) / \\
 & \left( 72 (\tau_2^2 + \tau_3^2)^{11/2} \right), \frac{o \text{P999} \tau_1 (\tau_2^4 + \tau_3^4) v_0}{6 (\tau_2^2 + \tau_3^2)^{5/2}} - \\
 & \left( o^2 \right. \\
 & \quad \tau_1 \\
 & \quad \left( 36 \text{Daa}^2 (\tau_2^2 + \tau_3^2)^4 (\tau_1^2 + \tau_2^2 + \tau_3^2)^2 + \right. \\
 & \quad \left. 12 \text{Daa} \text{P999} (\tau_2^2 + \tau_3^2)^2 (\tau_1^2 + \tau_2^2 + \tau_3^2) (3 \tau_2^2 \tau_3^2 (\tau_2^2 + \tau_3^2) + \right. \\
 & \quad \left. \tau_1^2 (\tau_2^2 + \tau_3^2)^2 + 3 (\tau_2^4 + \tau_2^2 \tau_3^2 + \tau_3^4) v_0^2 \right) + \\
 & \quad \left. 3 (\tau_2^2 + \tau_3^2)^2 \left( 24 \text{Dab2} (\tau_2^2 + \tau_3^2)^3 (\tau_1^2 + \tau_2^2 + \tau_3^2) - (\tau_2^2 + \tau_3^2) \right. \right. \\
 & \quad \left. \left( 3 (8 \text{DabP9ab} + \text{P9999} - 4 \text{P99a2} + 2 \text{P99aa} - 4 \text{P9ab2}) \tau_1^2 \tau_2^4 + (\text{P9999} - 3 \text{P99a2}) \right. \right. \\
 & \quad \left. \left. \tau_2^6 + 2 \tau_2^2 (3 (8 \text{DabP9ab} + \text{P9999} - 4 \text{P99a2} + 2 \text{P99aa} - 4 \text{P9ab2}) \tau_1^2 + \right. \right. \\
 & \quad \left. \left. (12 \text{DabP9ab} + 2 \text{P9999} - 9 \text{P99a2} + 3 \text{P99aa} - 6 \text{P9ab2}) \tau_2^2 \right) \tau_3^2 + \right. \\
 & \quad \left. (3 (8 \text{DabP9ab} + \text{P9999} - 4 \text{P99a2} + 2 \text{P99aa} - 4 \text{P9ab2}) \tau_1^2 + \right. \\
 & \quad \left. (24 \text{DabP9ab} + 10 \text{P9999} - 27 \text{P99a2} + 6 \text{P99aa} - 12 \text{P9ab2}) \tau_2^2 \right) \tau_3^4 + \right. \\
 & \quad \left. (\text{P9999} - 3 \text{P99a2}) \tau_3^6 \right) - 3 ((\text{P9999} - 2 \text{P99a2}) \tau_2^6 + \\
 & \quad \left. (2 \text{P9999} - 3 \text{P99a2}) \tau_2^4 \tau_3^2 + (\text{P9999} - 2 \text{P99a2}) \tau_3^6) v_0^2 \right) + \\
 & \text{P999}^2 \left( (\tau_2^2 + \tau_3^2)^2 \left( 6 \tau_2^8 + 27 \tau_2^6 \tau_3^2 + 84 \tau_2^4 \tau_3^4 + \right. \right. \\
 & \quad \left. \left. 54 \tau_2^2 \tau_3^6 + 6 \tau_3^8 + \tau_1^4 (\tau_2^2 + \tau_3^2)^2 + \right. \right. \\
 & \quad \left. \left. \tau_1^2 (\tau_2^2 + \tau_3^2) (11 \tau_2^4 + 28 \tau_2^2 \tau_3^2 + 11 \tau_3^4) \right) + \right. \\
 & \quad \left. 3 (\tau_2^2 + \tau_3^2) (5 \tau_2^8 + 21 \tau_2^6 \tau_3^2 + 13 \tau_2^4 \tau_3^4 + 12 \tau_2^2 \tau_3^6 + \right. \\
 & \quad \left. 5 \tau_3^8 + 2 \tau_1^2 (\tau_2^6 + 2 \tau_2^4 \tau_3^2 + 2 \tau_2^2 \tau_3^4 + \tau_3^6)) v_0^2 + \right. \\
 & \quad \left. (8 \tau_2^8 + 18 \tau_2^6 \tau_3^2 + 25 \tau_2^4 \tau_3^4 + 18 \tau_2^2 \tau_3^6 + 8 \tau_3^8) v_0^4 \right) \Big) \Big) / \\
 & \left( 72 (\tau_2^2 + \tau_3^2)^{11/2} \right), \frac{o \text{P999} \tau_1^2 (\tau_2^4 + \tau_2^2 \tau_3^2 + \tau_3^4)}{6 (\tau_2^2 + \tau_3^2)^{5/2}} + \\
 & \left( o^2 \right. \\
 & \quad \tau_1^2 \\
 & \quad v_0 \\
 & \quad \left( - (\tau_2^2 + \tau_3^2) (4 \text{P999} (6 \text{Daa} + \text{P999}) \tau_1^2 \tau_2^6 + \right. \\
 & \quad \quad \left. 3 (8 \text{P999} (\text{Daa} + \text{P999}) - 5 \text{P9999} + 9 \text{P99a2}) \tau_2^8 + 3 \tau_2^4 \right. \\
 & \quad \quad \left. (2 \text{P999} (6 \text{Daa} + \text{P999}) \tau_1^2 + (20 \text{Daa} \text{P999} + 31 \text{P999}^2 - 17 \text{P9999} + 27 \text{P99a2}) \tau_2^2) \right)
 \end{aligned}$$

$$\begin{aligned}
 & \tau_3^2 + 3 \tau_2^2 (2 P999 (6 Daa + P999) \tau_1^2 + \\
 & \quad 3 (8 Daa P999 + 9 P999^2 - 6 P9999 + 9 P99a2) \tau_2^2) \tau_3^4 + \\
 & (4 P999 (6 Daa + P999) \tau_1^2 + 3 (20 Daa P999 + 22 P999^2 - 11 P9999 + 18 P99a2) \tau_2^2) \\
 & \quad \tau_3^6 + 3 (8 P999 (Daa + P999) - 5 P9999 + 9 P99a2) \tau_3^8) - \\
 & P999^2 (9 \tau_2^8 + 16 \tau_2^6 \tau_3^2 + 24 \tau_2^4 \tau_3^4 + 16 \tau_2^2 \tau_3^6 + 9 \tau_3^8) v0^2) / \\
 & (72 (\tau_2^2 + \tau_3^2)^{11/2}), (o^2 \\
 & \tau_1^3 \\
 & (- (\tau_2^2 + \tau_3^2) \\
 & \quad (12 Daa P999 (\tau_2^2 + \tau_3^2) (\tau_1^2 + \tau_2^2 + \tau_3^2) \\
 & \quad (\tau_2^2 - \tau_2 \tau_3 + \tau_3^2) (\tau_2^2 + \tau_2 \tau_3 + \tau_3^2) - \\
 & \quad 3 (\tau_2^2 + \tau_3^2) (P9999 (\tau_2^2 + 2 \tau_3^2) (2 \tau_2^4 + \tau_2^2 \tau_3^2 + \tau_3^4) - \\
 & \quad 3 P99a2 (\tau_2^6 + 2 \tau_2^4 \tau_3^2 + \tau_2^2 \tau_3^4 + \tau_3^6)) + \\
 & \quad P999^2 (9 \tau_2^8 + 37 \tau_2^6 \tau_3^2 + 37 \tau_2^4 \tau_3^4 + 28 \tau_2^2 \tau_3^6 + \\
 & \quad 9 \tau_3^8 + 2 \tau_1^2 (\tau_2^6 + 2 \tau_2^4 \tau_3^2 + 2 \tau_2^2 \tau_3^4 + \tau_3^6))) - \\
 & \quad P999^2 (7 \tau_2^8 + 12 \tau_2^6 \tau_3^2 + 20 \tau_2^4 \tau_3^4 + 12 \tau_2^2 \tau_3^6 + 7 \tau_3^8) v0^2) / \\
 & (72 (\tau_2^2 + \tau_3^2)^{11/2}), -(o^2 \\
 & P999^2 \\
 & \tau_1^4 \\
 & (3 \tau_2^8 + 4 \tau_2^6 \tau_3^2 + 7 \tau_2^4 \tau_3^4 + \\
 & \quad 4 \tau_2^2 \tau_3^6 + 3 \tau_3^8) v0) / (72 (\tau_2^2 + \tau_3^2)^{11/2}), \\
 & - \frac{o^2 P999^2 \tau_1^5 (\tau_2^4 + \tau_2^2 \tau_3^2 + \tau_3^4)^2}{72 (\tau_2^2 + \tau_3^2)^{11/2}} \}
 \end{aligned}$$

**Length[z2v8dd]**

6

Now the integration is  $z3[v0, \tau_1, \tau_2, \tau_3] = \Phi^{-1}[\int_{-\infty}^{\infty} \Phi(z2v8) f[z] dz] . .$

```
z3[v0_, tau1_, tau2_, tau3_] = Collect[dd2int[z2v8ab[[2]], z2v8ab[[1]], z2v8dd, z],
o, FullSimplify[#, tau1 > 0 & tau2 > 0 & tau3 > 0] &]
```

$$\frac{v_0}{\sqrt{\tau_1^2 + \tau_2^2 + \tau_3^2}} + \left( o \left( (\tau_1^2 + \tau_2^2 + \tau_3^2) \left( 6 \text{Daa} (\tau_1^2 + \tau_2^2 + \tau_3^2)^2 + \text{P999} (\tau_1^4 + \tau_2^4 + 3 \tau_2^2 \tau_3^2 + \tau_3^4 + 3 \tau_1^2 (\tau_2^2 + \tau_3^2)) \right) + \text{P999} (2 \tau_1^4 + 2 \tau_2^4 + 3 \tau_2^2 \tau_3^2 + 2 \tau_3^4 + 3 \tau_1^2 (\tau_2^2 + \tau_3^2)) v_0^2 \right) \right) / \left( 6 (\tau_1^2 + \tau_2^2 + \tau_3^2)^{5/2} \right) + \left( o^2 \left( -72 \text{Dab2} (\tau_1^2 + \tau_2^2 + \tau_3^2)^5 v_0 + (\tau_1^2 + \tau_2^2 + \tau_3^2) \left( 12 \text{Daa} \text{P999} (\tau_1^2 + \tau_2^2 + \tau_3^2)^2 (\tau_1^4 + \tau_2^4 + \tau_3^4) + \text{P999}^2 (-5 \tau_1^8 - 21 \tau_1^6 \tau_2^2 - 73 \tau_1^4 \tau_2^4 - 48 \tau_1^2 \tau_2^6 - 5 \tau_2^8 - 3 (7 \tau_1^6 + 40 \tau_1^4 \tau_2^2 + 49 \tau_1^2 \tau_2^4 + 7 \tau_2^6) \tau_3^2 - (73 \tau_1^4 + 174 \tau_1^2 \tau_2^2 + 73 \tau_2^4) \tau_3^4 - 48 (\tau_1^2 + \tau_2^2) \tau_3^6 - 5 \tau_3^8) + 3 (\tau_1^2 + \tau_2^2 + \tau_3^2) (-3 \text{P99a2} (\tau_1^6 + 6 \tau_1^4 \tau_2^2 + 9 \tau_1^2 \tau_2^4 + \tau_2^6) - 18 \text{P99a2} (\tau_1^4 + 3 \tau_1^2 \tau_2^2 + \tau_2^4) \tau_3^2 - 27 \text{P99a2} (\tau_1^2 + \tau_2^2) \tau_3^4 - 3 \text{P99a2} \tau_3^6 + 6 (4 \text{DabP9ab} + \text{P99aa} - 2 \text{P9ab2}) (\tau_1^2 + \tau_2^2 + \tau_3^2) (\tau_1^2 \tau_2^2 + (\tau_1^2 + \tau_2^2) \tau_3^2) + \text{P9999} (\tau_1^6 + \tau_2^6 + 4 \tau_2^4 \tau_3^2 + 10 \tau_2^2 \tau_3^4 + \tau_3^6 + 4 \tau_1^4 (\tau_2^2 + \tau_3^2) + 2 \tau_1^2 (5 \tau_2^4 + 9 \tau_2^2 \tau_3^2 + 5 \tau_3^4)) \right) \right) v_0 - (\text{P999}^2 (4 \tau_1^8 + 4 \tau_2^8 + 21 \tau_2^6 \tau_3^2 + 17 \tau_2^4 \tau_3^4 + 12 \tau_2^2 \tau_3^6 + 4 \tau_3^8 + 21 \tau_1^6 (\tau_2^2 + \tau_3^2) + \tau_1^4 (17 \tau_2^4 + 48 \tau_2^2 \tau_3^2 + 17 \tau_3^4) + 3 \tau_1^2 (4 \tau_2^6 + 13 \tau_2^4 \tau_3^2 + 10 \tau_2^2 \tau_3^4 + 4 \tau_3^6)) - 3 (\tau_1^2 + \tau_2^2 + \tau_3^2) (-3 \text{P99a2} (\tau_1^6 + 2 \tau_1^4 \tau_2^2 + \tau_1^2 \tau_2^4 + \tau_2^6) - 6 \text{P99a2} (\tau_1^4 + \tau_1^2 \tau_2^2 + \tau_2^4) \tau_3^2 - 3 \text{P99a2} (\tau_1^2 + \tau_2^2) \tau_3^4 - 3 \text{P99a2} \tau_3^6 + \text{P9999} (3 \tau_1^6 + 3 \tau_2^6 + 8 \tau_2^4 \tau_3^2 + 6 \tau_2^2 \tau_3^4 + 3 \tau_3^6 + 8 \tau_1^4 (\tau_2^2 + \tau_3^2) + 6 \tau_1^2 (\tau_2^2 + \tau_3^2))) v_0^3 \right) \right) / (72 (\tau_1^2 + \tau_2^2 + \tau_3^2)^{9/2})$$

Check if z3 reduces to z2 when one of the scales is zero

```
Simplify[Limit[z3[v, tau1, tau2, tau3], tau3 -> 0] - z2[v, tau1, tau2], tau1 > 0 & tau2 > 0]
```

0

```
Simplify[Limit[z3[v, tau1, tau2, tau3], tau2 -> 0] - z2[v, tau1, tau3], tau1 > 0 & tau3 > 0]
```

0

```
Simplify[Limit[z3[v, tau1, tau2, tau3], tau1 -> 0] - z2[v, tau2, tau3], tau2 > 0 & tau3 > 0]
```

0

```

z3[v, tau1, tau2, tau3] // InputForm
v/Sqrt[tau1^2 + tau2^2 + tau3^2] +
(o*((tau1^2 + tau2^2 + tau3^2)*(6*Daa*(tau1^2 + tau2^2 + tau3^2)^2 +
P999*(tau1^4 + tau2^4 + 3*tau2^2*tau3^2 + tau3^4 +
3*tau1^2*(tau2^2 + tau3^2))) +
P999*(2*tau1^4 + 2*tau2^4 + 3*tau2^2*tau3^2 + 2*tau3^4 +
3*tau1^2*(tau2^2 + tau3^2))*v^2))/
(6*(tau1^2 + tau2^2 + tau3^2)^(5/2)) +
(o^2*(-72*Dab2*(tau1^2 + tau2^2 + tau3^2)^5*v +
(tau1^2 + tau2^2 + tau3^2)*(12*Daa*P999*(tau1^2 + tau2^2 + tau3^2)^2*
(tau1^4 + tau2^4 + tau3^4) + P999^2*(-5*tau1^8 -
21*tau1^6*tau2^2 - 73*tau1^4*tau2^4 - 48*tau1^2*tau2^6 -
5*tau2^8 - 3*(7*tau1^6 + 40*tau1^4*tau2^2 + 49*tau1^2*tau2^4 +
7*tau2^6)*tau3^2 - (73*tau1^4 + 174*tau1^2*tau2^2 + 73*tau2^4)*
tau3^4 - 48*(tau1^2 + tau2^2)*tau3^6 - 5*tau3^8) +
3*(tau1^2 + tau2^2 + tau3^2)*(-3*P99a2*(tau1^6 + 6*tau1^4*tau2^2 +
9*tau1^2*tau2^4 + tau2^6) - 18*P99a2*(tau1^4 +
3*tau1^2*tau2^2 + tau2^4)*tau3^2 - 27*P99a2*(tau1^2 + tau2^2)*
tau3^4 - 3*P99a2*tau3^6 + 6*(4*DabP9ab + P99aa - 2*P9ab2)*
(tau1^2 + tau2^2 + tau3^2)*(tau1^2*tau2^2 + (tau1^2 + tau2^2)*
tau3^2) + P9999*(tau1^6 + tau2^6 + 4*tau2^4*tau3^2 +
10*tau2^2*tau3^4 + tau3^6 + 4*tau1^4*(tau2^2 + tau3^2) +
2*tau1^2*(5*tau2^4 + 9*tau2^2*tau3^2 + 5*tau3^4))))*v -
(P999^2*(4*tau1^8 + 4*tau2^8 + 21*tau2^6*tau3^2 + 17*tau2^4*tau3^4 +
12*tau2^2*tau3^6 + 4*tau3^8 + 21*tau1^6*(tau2^2 + tau3^2) +
tau1^4*(17*tau2^4 + 48*tau2^2*tau3^2 + 17*tau3^4) +
3*tau1^2*(4*tau2^6 + 13*tau2^4*tau3^2 + 10*tau2^2*tau3^4 +
4*tau3^6)) - 3*(tau1^2 + tau2^2 + tau3^2)*
(-3*P99a2*(tau1^6 + 2*tau1^4*tau2^2 + tau1^2*tau2^4 + tau2^6) -
6*P99a2*(tau1^4 + tau1^2*tau2^2 + tau2^4)*tau3^2 -
3*P99a2*(tau1^2 + tau2^2)*tau3^4 - 3*P99a2*tau3^6 +
P9999*(3*tau1^6 + 3*tau2^6 + 8*tau2^4*tau3^2 + 6*tau2^2*tau3^4 +
3*tau3^6 + 8*tau1^4*(tau2^2 + tau3^2) +
6*tau1^2*(tau2^2 + tau3^2)^2))*v^3))/
(72*(tau1^2 + tau2^2 + tau3^2)^(9/2))

```

■ simplifying z3 and z8

We define six geometric quantities;

$$\begin{aligned}
 GG &= \left\{ G1 \rightarrow v0 + \frac{1}{3} o P999 v0^2 + o^2 \left( -\frac{P999^2}{18} + \frac{P9999}{8} - \frac{P99a2}{8} \right) v0^3, \right. \\
 G2 &\rightarrow o \left( -Daa - \frac{P999}{6} \right) v0 + o^2 \left( Dab2 - \frac{Daa P999}{2} + \frac{P999^2}{72} - \frac{P9999}{24} + \frac{P99a2}{8} \right) v0^2, \\
 G3 &\rightarrow -\frac{1}{6} o P999 v0 + o^2 \left( \frac{P999^2}{9} - \frac{P9999}{8} + \frac{P99a2}{4} \right) v0^2, \\
 G4 &\rightarrow o^2 \left( -DabP9ab + \frac{Daa P999}{3} + \frac{2 P999^2}{9} - \frac{P9999}{6} + \frac{P99a2}{2} - \frac{P99aa}{4} + \frac{P9ab2}{2} \right) v0^2, \\
 G5 &\rightarrow o^2 \left( -\frac{P999^2}{8} + \frac{P9999}{12} - \frac{P99a2}{8} \right) v0^2, \quad G6 \rightarrow o^2 \left( -\frac{P999^2}{8} + \frac{P9999}{24} - \frac{P99a2}{8} \right) v0^2 \};
 \end{aligned}$$

We also define four scale parameters (but there are only three degrees of freedom among them).

$$SS = \left\{ S1 \rightarrow \frac{1}{\sqrt{\tau_1^2 + \tau_2^2 + \tau_3^2}}, S2 \rightarrow \frac{\tau_1^2 \tau_2^2 + \tau_1^2 \tau_3^2 + \tau_2^2 \tau_3^2}{(\tau_1^2 + \tau_2^2 + \tau_3^2)^2}, S3 \rightarrow \frac{\tau_1^2 \tau_2^2 \tau_3^2 + \tau_2^4 \tau_3^2 + \tau_1^4 (\tau_2^2 + \tau_3^2)}{(\tau_1^2 + \tau_2^2 + \tau_3^2)^3}, S4 \rightarrow \frac{\tau_1^2 \tau_2^2 \tau_3^2}{(\tau_1^2 + \tau_2^2 + \tau_3^2)^3} \right\};$$

The pivot  $z8[v0,1]$  is denoted by  $Z8G$

$$z8G = \frac{G2 + \frac{G3^2}{2} + G4 + G5}{G1} + G1 (1 + G3 + 4 G3^2 + G6);$$

`Simplify[gets2[z8G /. GG] - z8[v0]]`

0

The three-step multiscale z-value  $z3[v0,\tau_1,\tau_2,\tau_3]$  is denoted by  $Z3G$

$$Z3G = G1 S1 (1 + G3 S2 + 4 G3^2 S2^2 + G5 S3 + G6 S4) - \frac{G2 + G3 S2 + G4 S2 + 7 G3^2 S2^2 + 3 G5 S3 + 3 G6 S4}{G1 S1};$$

`Simplify[gets2[Z3G /. Join[GG, SS]] - z3[v0, tau1, tau2, tau3]]`

0