DBG Notes

DGB Definition

Our basis functions are given by

$$\phi(x,\,\xi,\,\alpha) \;=\; N(\alpha)\; e^{-\alpha(x-\xi)^2}$$

where

$$N(\alpha) \;=\; \left(\frac{2\,\alpha}{\pi}\right)^{1/4}$$

The real saving grace of a DGB approach is that the product of two DGB functions is again a DGB function, just centered around the weighted average of the original DGB points

$$\phi(x,\,\xi_i,\,\alpha_i)\,\phi\big(x,\,\xi_j,\,\alpha_j\big) \;=\; W\!\left(\frac{\alpha_i\,\alpha_j}{\alpha_i+\alpha_j},\,\xi_i-\xi_j\right)\phi\!\left(x,\,\frac{\alpha_i\xi_i+\alpha_j\xi_j}{\alpha_i+\alpha_j},\,\alpha_i+\alpha_j\right)$$

where

$$W(A,\,\Delta x) \;=\; N(A)\; e^{-\mathrm{A}\Delta x^2}$$

which it should be noted is equivalent to $\phi\big(\xi_i,\,\xi_j,\,{}^{\alpha_i\,\alpha_j}\!/\!_{\alpha_i+\alpha_j}\big)$

Functional Form

Overlaps

As we have

$$\phi(x,\,\xi_i,\,\alpha_i)\,\phi\big(x,\,\xi_j,\,\alpha_j\big) \;=\; W\!\left(\frac{\alpha_i\,\alpha_j}{\alpha_i+\alpha_j},\,\xi_i-\xi_j\right)\phi\!\left(x,\,\frac{\alpha_i\xi_i+\alpha_j\xi_j}{\alpha_i+\alpha_j},\,\alpha_i+\alpha_j\right)$$

it is straightforward to note that

$$\begin{aligned}
\langle\varphi_i|\varphi_j\rangle \;&=\; \int P_{nm}^{(i,j)}(x)\,\phi^{(i)}(x)\,\phi^{(j)}(x)\\
&=\; W^{(i,j)}\int\phi\!\left(x,\,\frac{\alpha_i\xi_i+\alpha_j\xi_j}{\alpha_i+\alpha_j},\,\alpha_i+\alpha_j\right)\\
&=\; W^{(i,j)}\left(\frac{2\,\pi}{\alpha_i+\alpha_j}\right)^{1/4}
\end{aligned}$$

$$= \left(\frac{2 \frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j}}{\pi} \right)^{1/4} \left(\frac{2 \pi}{\alpha_i + \alpha_j} \right)^{1/4} \exp\left(-\frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j} \left(\xi_i - \xi_j\right)^2 \right)$$

$$= \left(\frac{4 \alpha_i \alpha_j}{\left(\alpha_i + \alpha_j\right)^2} \right)^{1/4} \exp\left(-\frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j} \left(\xi_i - \xi_j\right)^2 \right)$$

Using Mass-Weighted Coordinates

Integration of the Potential (Non-Rotated)

We start with our multivariate Gaussian basis function centered around a point $\xi^{(i)}$

$$\varphi_i(\boldsymbol{x}) = \prod_{j=1}^{3N} \phi\left(x_j, \xi_j^{(i)}, \alpha_i\right)$$

the integral we then want to evaluate is

$$\int_{\mathbb{R}^N} \varphi_i(\boldsymbol{x})\ V(\boldsymbol{x})\, \varphi_j(\boldsymbol{x})\, d\boldsymbol{x}$$

where then

$$\varphi_i(\boldsymbol{x})\, \varphi_j(\boldsymbol{x}) = \prod_{k=1}^{3N} \phi\left(x_k, \xi_k^{(i)}, \alpha_i\right) \phi\left(x_k, \xi_k^{(j)}, \alpha_j\right)$$

$$= \prod_{k=1}^{3N} W\left(\frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j}, \xi_k^{(i)} - \xi_k^{(j)} \right) \prod_{k=1}^{3N} \phi\left(x_k, \frac{\alpha_i \xi_k^{(i)} + \alpha_j \xi_k^{(j)}}{\alpha_i + \alpha_j}, \alpha_i + \alpha_j \right)$$

and so

$$\int_{\mathbb{R}^N} \varphi_i(\boldsymbol{x})\ V(\boldsymbol{x})\, \varphi_j(\boldsymbol{x})\, d\boldsymbol{x} = \prod_{k=1}^{3N} W\left(\frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j}, \xi_k^{(i)} - \xi_k^{(j)} \right) \int_{\mathbb{R}^N} V(\boldsymbol{x}) \prod_{k=1}^{3N} \phi\left(x_k, \frac{\alpha_i \xi_k^{(i)} + \alpha_j \xi_k^{(j)}}{\alpha_i + \alpha_j}, \alpha_i + \alpha_j \right) d\boldsymbol{x}$$

When evaluating this final integral, we then have a few approaches

Quadrature

- Straightforward
- The relevant Gauss-Hermite quadrature weights are built into `scipy`
- Scales poorly with dimension

Expansions

Taylor Series

ALTERNATE EXPRESSION

Final Expression

Local Expansions

The local expansion context is largely the same as the Taylor series context, except instead of picking one point to expand about, we expand locally around every integration point, i.e. we choose

$$\zeta_k = \frac{\alpha_i \, \xi_k^{(i)} + \alpha_j \, \xi_k^{(j)}}{\alpha_i + \alpha_j}$$

which means our final integrals end up as

$$\int_{\mathbb{R}^N} \prod_{k=1}^{3N} \phi\left(x_k, \frac{\alpha_i \, \xi_k^{(i)} + \alpha_j \, \xi_k^{(j)}}{\alpha_i + \alpha_j}, \alpha_i + \alpha_j \right) (x_k - \zeta_k)^{p_k} \, d\boldsymbol{x} = \prod_{k=1}^{3N} \int \phi\left(x_k, 0, \alpha_i + \alpha_j\right) x_k^{p_k} \, dx_k$$

which is easy to integrate

In[1695]:=

```
baseInt = Assuming[
  n ∈ Integers && n ≥ 0 && α > 0,
  Integrate[DGB[0, α][x] x^n, {x, -∞, ∞}]
 ]
```

Out[1695]=

$$\frac{\left(1 + (-1)^n\right) \alpha^{-\frac{1}{4} - \frac{n}{2}} \, \mathrm{Gamma}\left[\frac{1+n}{2}\right]}{2^{3/4} \, \pi^{1/4}}$$

And notably, this says the *odd-degree* contribution vanishes, giving us

$$\int \phi(x_k, 0, \alpha) \, x_k^{p_k} = \begin{cases} \left(\frac{2 \, \alpha^{-(2 \, p_k + 1)}}{\pi} \right)^{1/4} \Gamma\left(\frac{p_k + 1}{2} \right) & p_k \text{ even} \\ 0 & \text{else} \end{cases}$$

and then for even order terms we have

$$\Gamma\left(\frac{p_k+1}{2}\right) = \frac{\sqrt{\pi}}{2^{p_k/2}} \prod_{m=1}^{p_k/2}(2m-1)$$

giving us, for even p_k,

$$\begin{aligned}\int \phi(x_k, 0, \alpha)\, {x_k}^{p_k} &= \left(\frac{2\,\alpha^{-(2\,p_k+1)}}{\pi}\right)^{1/4} \frac{\sqrt{\pi}}{2^{p_k/2}} \prod_{m=1}^{p_k/2}(2m-1)\\ &= \frac{1}{\sqrt{2^{p_k/2}\,\alpha^{p_k/2}}} \left(\frac{2\,\pi}{\alpha}\right)^{1/4} \prod_{m=1}^{p_k/2}(2m-1)\end{aligned}$$

which we can also make proportional to contribution from the overlap, $S_{ij}^{(k)} = (2\,\pi/\alpha)^{1/4}$

$$\int \phi(x_k, 0, \alpha)\, {x_k}^{p_k} = \frac{S_{ij}^{(k)}}{\sqrt{2^{p_k}\,\alpha^{p_k}}} \prod_{m=1}^{p_k/2}(2m-1)$$

Then expanding back out we get (for entirely even p_k w/ $\sum_k p_k = m$)

$$\begin{aligned}\int_{\mathbb{R}^N} \prod_{k=1}^{3N} \phi(x_k, 0, \alpha_i+\alpha_j)\, {x_k}^{p_k} &= \prod_{k=1}^{3N} \frac{S_{ij}^{(k)}}{\sqrt{2^{p_k}\,{(\alpha_i+\alpha_j)_k}^{p_k}}} \prod_{l=1}^{p_k/2}(2l-1)\\ &= \frac{S_{ij}}{\sqrt{2^m}} \prod_{k=1}^{3N} \frac{1}{{(\alpha_i+\alpha_j)_k}^{p_k/2}} \prod_{l=1}^{p_k/2}(2l-1)\end{aligned}$$

so finally

$$\begin{aligned}&\int_{\mathbb{R}^N} V(\boldsymbol{x}) \prod_{k=1}^{3N} \phi\left(x_k, \frac{\alpha_i\,\xi_k^{(i)}+\alpha_j\,\xi_k^{(j)}}{\alpha_i+\alpha_j}, \alpha_i+\alpha_j\right) d\boldsymbol{x} =\\ &\quad S_{ij} \sum_{m=0}^{M} \sum_{p\in P_E(m)} \frac{1}{W_p\,\sqrt{2^m}} \frac{\partial V(\boldsymbol{\zeta})}{\partial x_1^{p_1} \ldots \partial x_{3N}^{p_{3N}}} \prod_{k=1}^{3N} \frac{1}{{(\alpha_i+\alpha_j)_k}^{p_k/2}} \prod_{l=1}^{p_k/2}(2l-1)\end{aligned}$$

where we pick $P_E(m)$ to be the *entirely even* partitions of m

For a quadratic expansion this becomes

$$\begin{aligned}\xi^{(ij)} &= \frac{\alpha^{(i)}\,\xi_k^{(i)}+\alpha^{(j)}\,\xi_k^{(j)}}{\alpha^{(i)}+\alpha^{(j)}}\\ \alpha^{(ij)} &= \alpha^{(i)}+\alpha^{(j)}\\ V_{ij} &= S_{ij}\left(V(\boldsymbol{\xi}^{(ij)}) + \frac{1}{4} \sum_{k=1}^{3N} \frac{1}{\alpha_k^{(ij)}} \frac{\partial^2}{\partial x_k^2} V(\boldsymbol{\zeta})\right)\end{aligned}$$

Equivalence to Taylor Series

Integration of the Kinetic Energy (Non-Rotated)

We start with our multivariate Gaussian basis function centered around a point $\xi^{(i)}$

$$\varphi_i(\boldsymbol{x}) = \prod_{j=1}^{3N} \phi\left(x_j, \xi_j^{(i)}, \alpha_i\right)$$

the integral we then want to evaluate is

$$\begin{aligned} T_{ij} &= -\int_{\mathbb{R}^N} \varphi_i(\boldsymbol{x}) \frac{\nabla^2}{2\boldsymbol{m}} \varphi_j(\boldsymbol{x})\, d\boldsymbol{x} \\ &= -\sum_k \frac{1}{2m_k} \int_{\mathbb{R}^N} \varphi_i(\boldsymbol{x}) \frac{\partial}{\partial x_k} \varphi_j(\boldsymbol{x})\, d\boldsymbol{x} \end{aligned}$$

where we note that

$$\frac{\partial}{\partial x_k} \varphi_j(\boldsymbol{x}) = 2\,\alpha_k^{(j)}\left(2\,\alpha_k^{(j)}\left(x_k - \xi_k^{(j)}\right)^2 - 1\right) \varphi_j(\boldsymbol{x})$$

so we have

$$\begin{aligned} \xi^{(ij)} &= \frac{\alpha^{(i)}\,\xi_k^{(i)} + \alpha^{(j)}\,\xi_k^{(j)}}{\alpha^{(i)} + \alpha^{(j)}} \\ \alpha^{(ij)} &= \alpha^{(i)} + \alpha^{(j)} \end{aligned}$$

$$\begin{aligned} T_{ij} &= -\int_{\mathbb{R}^N} \varphi_i(\boldsymbol{x}) \frac{\nabla^2}{2\boldsymbol{m}} \varphi_j(\boldsymbol{x})\, d\boldsymbol{x} \\ &= -\sum_k \frac{1}{2m_k} \int_{\mathbb{R}^N} 2\,\alpha_k^{(j)}\left(2\,\alpha_k^{(j)}\left(x_k - \xi_k^{(j)}\right)^2 - 1\right) \phi_i(\boldsymbol{x})\, \phi_j(\boldsymbol{x})\, d\boldsymbol{x} \\ &= \sum_k \frac{1}{2m_k}\; W^{(ij)} \int_{\mathbb{R}^N} 2\,\alpha_k^{(j)}\left(1 - 2\,\alpha_k^{(j)}\left(x_k - \xi_k^{(j)}\right)^2\right) \phi^{(ij)}(\boldsymbol{x})\, d\boldsymbol{x} \end{aligned}$$

Shifted Approach

We will now introduce the shift $\chi^{(ij)} = x - \xi^{(ij)}$, giving us

$$\alpha_k^{(j)}\left(1 - 2\,\alpha_k^{(j)}\left(x_k - \xi_k^{(j)}\right)^2\right) = \alpha_k^{(j)}\left(1 - 2\,\alpha_k^{(j)}\left(\chi^{(ij)} + \left(\xi_k^{(ij)} - \xi_k^{(j)}\right)\right)^2\right)$$

where

$$\begin{aligned} \xi^{(ij)} - \xi^{(j)} &= \frac{\alpha^{(i)}}{\alpha^{(i)} + \alpha^{(j)}} \left(\xi^{(i)} - \xi^{(j)}\right) \\ &= \frac{\alpha^{(i)}}{\alpha^{(ij)}}\; \Delta\xi^{(ij)} \end{aligned}$$

and so

$$\alpha^{(j)}\left(1-2\,\alpha^{(j)}\left(x-\xi^{(j)}\right)^2\right) = \alpha^{(j)} - 2\,\alpha^{(j)^2}\,\chi^{(ij)2} + 4\,\frac{\alpha^{(j)^2}\,\alpha^{(i)}}{\alpha^{(ij)}}\,\chi^{(ij)}\,\Delta\xi^{(ij)} - 2\left(\frac{\alpha^{(j)}\alpha^{(i)}}{\alpha^{(ij)}}\right)^2\,\Delta\xi^{(ij)^2}$$

Next we'll note that the linear term in $\chi^{(ij)}$ will vanish when integrating its product with $\phi^{(ij)}$, and so we are left with

$$\begin{aligned} T_{ij} &= \sum_k \frac{1}{m_k}\,W^{(ij)}\int_{\mathbb{R}^N}\left(\alpha_k^{(j)} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\,\Delta\xi_k^{(ij)^2}\right)\phi^{(ij)}(\boldsymbol{x}) \;\; - 2\,\alpha^{(j)^2}\,\chi_k^{(ij)2}\,d\boldsymbol{x} \\ &= \sum_k \frac{1}{m_k}\,S_{ij}\left(\alpha_k^{(j)} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\,\Delta\xi_k^{(ij)^2}\right) - 2\,\alpha_k^{(j)^2}\int_{\mathbb{R}^N}\chi_k^{(ij)2}\,\phi^{(ij)}(\boldsymbol{x})\,d\boldsymbol{x} \end{aligned}$$

where, as $\phi^{(ij)}(\boldsymbol{x})$ is really centered around $\chi_k^{(ij)}$ we get (from the portion on local expansions)

$$\int_{\mathbb{R}^N}\chi_k^{(ij)2}\,\phi^{(ij)}(\boldsymbol{x})\,d\boldsymbol{x} = \frac{S_{ij}}{2\,\alpha_k^{(ij)}}$$

giving us

$$\begin{aligned} T_{ij} &= S_{ij}\sum_k \frac{1}{m_k}\left(\alpha_k^{(j)} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\,\Delta\xi_k^{(ij)^2}\right) - \frac{\alpha_k^{(j)^2}}{\alpha_k^{(ij)}} \\ &= S_{ij}\sum_k \frac{1}{m_k}\left(\frac{\alpha_k^{(j)}\,\alpha_k^{(ij)} - \alpha_k^{(j)^2}}{\alpha_k^{(ij)}} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\,\Delta\xi_k^{(ij)^2}\right) \\ &= S_{ij}\sum_k \frac{1}{m_k}\left(\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(ij)}} - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)^2\,\Delta\xi_k^{(ij)^2}\right) \\ &= S_{ij}\sum_k \frac{1}{m_k}\,\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(ij)}}\left(1 - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)\Delta\xi_k^{(ij)^2}\right) \end{aligned}$$

Direct Strategy

Rotated Basis

By supplying a full covariance matrix we can use everything developed by the statistics community in arbitrary dimensions. Given a covariance matrix Σ, which will be by default the diagonal matrix with $1/2\alpha_i$ as its values, we have

$$\phi(x,\,\xi,\,\Sigma) = N(\Sigma)\,e^{-\frac{1}{2}\left(\Sigma^{-1}\odot(x-\xi)^2\right)}$$

where

$$N(\Sigma) = \left(\pi^{-d} \det\left(\Sigma^{-1}\right)\right)^{1/4}$$

we'll note that we are off from the standard Gaussian normalization by a factor of $2^{-d/2}\, N(\Sigma)$

Then we have (from the Matrix Cookbook)

$$\phi(x,\, \xi_i,\, \Sigma_i)\, \phi\left(x,\, \xi_j,\, \Sigma_j\right) = W\left(\Sigma_i+\Sigma_j,\, \xi_i-\xi_j\right) \phi(x,\, \xi_c,\, \Sigma_c)$$

where

$$\begin{aligned} \Sigma_c{}^{-1} &= \Sigma_i{}^{-1}+\Sigma_j{}^{-1} \\ \xi_c &= \Sigma_c\left(\Sigma_i{}^{-1}\xi_i + \Sigma_j{}^{-1}\xi_j\right) \end{aligned}$$

plus we'll add in the helpful identity that

$$\begin{aligned} \left(\Sigma_i+\Sigma_j\right)^{-1} &= \left(\left(\Sigma_i{}^{-1}\right)^{-1}+\left(\Sigma_j{}^{-1}\right)^{-1}\right)^{-1} \\ &= \Sigma_i{}^{-1}\left(\Sigma_i{}^{-1}+\Sigma_j{}^{-1}\right)^{-1}\Sigma_j{}^{-1} \\ &= \Sigma_i{}^{-1}\,\Sigma_c\,\Sigma_j{}^{-1} \end{aligned}$$

and to figure out exactly what W must be, we first note that for standard Gaussians we would have

$$W_N = \frac{1}{\sqrt{2^d\,\pi^d\left|\Sigma_i+\Sigma_j\right|}}\; e^{-\frac{1}{2}\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}$$

but letting $\varphi^{(i)}$ be a properly normalized Gaussian,

$$\phi^{(i)} = \frac{1}{2^{-d/2}\, N\left(\Sigma^{(i)}\right)}\, \varphi^{(i)}$$

so we have

$$\begin{aligned} \phi(x,\, \xi_i,\, \Sigma_i)\, \phi\left(x,\, \xi_j,\, \Sigma_j\right) &= \frac{1}{2^{-d/2}\, N\left(\Sigma^{(i)}\right)}\, \frac{1}{2^{-d/2}\, N\left(\Sigma^{(j)}\right)}\, \varphi^{(i)}\, \varphi^{(j)} \\ &= \frac{1}{2^{-d}\, N\left(\Sigma^{(i)}\right) N\left(\Sigma^{(j)}\right)}\, W_N\, \varphi^{(c)} \\ &= \frac{2^{-d/2}\, N\left(\Sigma^{(c)}\right)}{2^{-d}\, N\left(\Sigma^{(i)}\right) N\left(\Sigma^{(j)}\right)}\, W_N\, \phi^{(c)} \\ &= \frac{2^{-d/2}\left(\pi^{-d}\det\left(\Sigma^{(c)-1}\right)\right)^{1/4}}{2^{-d}\left(\pi^{-d}\det\left(\Sigma^{(i)-1}\right)\right)^{1/4}\left(\pi^{-d}\det\left(\Sigma^{(j)-1}\right)\right)^{1/4}}\, W_N\, \phi^{(c)} \\ &= \frac{1}{2^{-d/2}\left(\pi^{-d}\det\left(\Sigma^{(i)-1}\,\Sigma^{(c)}\,\Sigma^{(j)-1}\right)\right)^{1/4}}\, W_N\, \phi^{(c)} \end{aligned}$$

$$= \frac{2^{d/2}\left(\pi^d\left|\Sigma_i+\Sigma_j\right|\right)^{1/4}}{\sqrt{2^d\,\pi^d\left|\Sigma_i+\Sigma_j\right|}}\; e^{-\frac{1}{2}\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}\,\phi^{(c)}$$

$$= N\left(\Sigma_i+\Sigma_j\right) e^{-\frac{1}{2}\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}\,\phi^{(c)}$$

giving us

$$W\left(\Sigma_i+\Sigma_j,\, \xi_i-\xi_j\right) = N\left(\Sigma^{(i)}+\Sigma^{(j)}\right) e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}$$

and as a final note, this can be made more useful by considering that

$$\det\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right) = \det\left(\Sigma_i^{-1}\right)\det(\Sigma_c)\det\left(\Sigma_j^{-1}\right)$$

$$\Rightarrow \det(\Sigma_c) = \frac{\det\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)}{\det\left(\Sigma_i^{-1}\right)\det\left(\Sigma_j^{-1}\right)}$$

And to confirm we're on the right track, we can note that in the case that Σ_i is diagonal with diagonal entries $1/2\alpha_k^{(i)}$ and similarly with Σ_j we get

$$W\left(\Sigma_i+\Sigma_j,\, \xi_i-\xi_j\right) = \left(\frac{1}{\pi^d}\prod_k 2\left(\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\right)\right)^{1/4}\prod_k \exp\left(-\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\left(\xi_k^{(i)}-\xi_k^{(j)}\right)^2\right)$$

$$= \left(\frac{2}{\pi}\right)^{d/4}\prod_k\left(\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\right)^{1/4}\exp\left(-\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\left(\xi_k^{(i)}-\xi_k^{(j)}\right)^2\right)$$

which is of course our original expression.

Finally, by diagonalizing Σ_c^{-1} we can get a new set of normal effective modes and alphas, returning to a decoupled form, with $\alpha^{(c)} = \left(\Lambda^{(c)}\right)^{-1}/2$ for $\Lambda^{(c)}$ the vector of eigenvalues

Functional Form

Overlaps

Just for the heck of it,

$$N(\Sigma) = \left(\pi^{-d}\det\left(\Sigma^{-1}\right)\right)^{1/4}$$

$$\int_{\mathbb{R}^d}\phi(x,\,\xi_i,\,\Sigma_i)\,\phi\left(x,\,\xi_j,\,\Sigma_j\right)dx$$

$$= W\left(\Sigma_i+\Sigma_j,\, \xi_i-\xi_j\right)\int_{\mathbb{R}^d}\phi(x,\,\xi_c,\,\Sigma_c)\,dx$$

$$= \frac{N\left(\Sigma^{(i)}+\Sigma^{(i)}\right)}{2^{-d/2}\,N\left(\Sigma^{(c)}\right)}\; e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}$$

$$= 2^{d/2}\left(\frac{\left|\Sigma^{(c)}\right|}{\left|\Sigma^{(i)}+\Sigma^{(j)}\right|}\right)^{1/4} e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}$$

$$= 2^{d/2}\left(\frac{\left|\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\right|^2}{\left|\Sigma^{(i)}\right|\left|\Sigma^{(j)}\right|}\right)^{1/4} e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}$$

$$= 2^{d/2}\left(\frac{\left|\Sigma^{(i)-1}\right|\left|\Sigma^{(j)-1}\right|}{\left|\Sigma^{(c)-1}\right|^2}\right)^{1/4} e^{-\frac{1}{2}\left(\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)}$$

and then just to confirm that this makes sense, in the case that Σ_i and Σ_j are diagonal with $1/2\,\alpha_k^{(i)}$ we get

$$2^{d/2}\left(\frac{\left|\Sigma^{(i)-1}\right|\left|\Sigma^{(j)-1}\right|}{\left|\Sigma^{(c)-1}\right|^2}\right)^{1/4} e^{-\frac{1}{2}\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\odot\left(\xi_i-\xi_j\right)^2\right)} =$$

$$2^{d/2}\prod_k\left(\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\left(\alpha_k^{(i)}+\alpha_k^{(j)}\right)^2}\right)^{1/4} \exp\left(-\frac{\alpha_k^{(i)}\,\alpha_k^{(j)}}{\alpha_k^{(i)}+\alpha_k^{(j)}}\left(\xi_k^{(i)}-\xi_k^{(j)}\right)^2\right)$$

which ends up being the correct result

Tests

Kinetic Energy

Shifted Approach

As in the direct approach we note that

$$T_{ij}=-\frac{1}{2}\;W\left(\Sigma_i+\Sigma_j,\ \xi_i-\xi_j\right)\int_{\mathbb{R}^d}\phi(x,\ \xi_c,\ \Sigma_c)\ \mathrm{Tr}\left(M^{-1}\,\mathcal{T}_j\right)dx$$

where

$$\mathcal{T}_j = \left(\nabla_x\left(\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)\right)^2 - \nabla_{x^2}\left(\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)$$

then we'll note that

$$\Sigma_j^{-1} = \Sigma_c^{-1} - \Sigma_i^{-1}$$

and as before we'll write

$$x = x - \xi_c + \xi_c$$

which admittedly seems unhelpful, but we'll plow on, noting

$$\xi_c = \Sigma_c\left(\Sigma_i{}^{-1}\xi_i + \Sigma_j{}^{-1}\xi_j\right)$$

$$\begin{aligned}\xi_j &= \Sigma_c\left(\Sigma_c{}^{-1}\,\xi_j\right)\\ &= \Sigma_c\left(\Sigma_i{}^{-1}\xi_j + \Sigma_j{}^{-1}\xi_j\right)\\ \Rightarrow \xi_c-\xi_j &= \Sigma_c\,\Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\end{aligned}$$

So then when we have

$$\begin{aligned}\nabla_x\left(\frac{1}{2}\,\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right) &= \Sigma_j^{-1}\left(x-\xi_j\right)\\ \nabla_{x^2}\left(\frac{1}{2}\,\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right) &= \Sigma_j^{-1}\\ \nabla_x\left(\frac{1}{2}\,\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)^2 &= \left(\left[\Sigma_j^{-1}\left(x-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\left(x-\xi_j\right)\right]\right)\end{aligned}$$

we can replace $x-\xi_j$ with $x-\xi_c$

$$\Sigma_j^{-1}\left(x-\xi_c+\xi_c-\xi_j\right) = \Sigma_j^{-1}(x-\xi_c) + \Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)$$

and so

$$\begin{aligned}\left[\Sigma_j^{-1}\left(x-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\left(x-\xi_j\right)\right] &= \left[\Sigma_j^{-1}(x-\xi_c)\right]\otimes\left[\Sigma_j^{-1}(x-\xi_c)\right]\\ &\quad+\ \left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]\\ &\quad+\text{linear terms}\end{aligned}$$

Therefore we have

$$\begin{aligned}\mathcal{T}_j &= \left(\nabla_x\left(\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)\right)^2 - \nabla_{x^2}\left(\Sigma_j^{-1}\odot\left(x-\xi_j\right)^2\right)\\ &= \left[\Sigma_j^{-1}(x-\xi_c)\right]\otimes\left[\Sigma_j^{-1}(x-\xi_c)\right]\\ &\quad+\left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]-\Sigma_j^{-1}\\ &\quad+\text{linear terms}\\ &= \sum_n\left[\Sigma_j^{-1}(x-\xi_c)\right]_n^2\\ &\quad+\left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]\otimes\left[\Sigma_j^{-1}\,\Sigma_c\,\Sigma_i{}^{-1}\left(\xi_i-\xi_j\right)\right]-\Sigma_j^{-1}\\ &\quad+\text{linear terms}\end{aligned}$$

Next so we can actually integrate, we'll make the substitution

$$q = L(x-\xi_c)$$

where L diagonalizes Σ_c, i.e.

$$L\,\Sigma_c^{-1}\,L^T = A_c$$

and so

$$L\,\Sigma_i^{-1}\,L^T + L\,\Sigma_j^{-1}\,L^T = A_c$$

Putting this together,

$$\Sigma_j^{-1}(x{-}\xi_c) = \Sigma_j^{-1}\, L^T q$$

Giving us

$$\begin{aligned}
\mathcal{T}_j = {} & \sum_n \left[\Sigma_j^{-1}\, L^T q\right]_n^2 \\
& + \left[\Sigma_j^{-1}\, \Sigma_c\, \Sigma_i{}^{-1}\!\left(\xi_i{-}\xi_j\right)\right] \otimes \left[\Sigma_j^{-1}\, \Sigma_c\, \Sigma_i{}^{-1}\!\left(\xi_i{-}\xi_j\right)\right] - \Sigma_j^{-1} \\
& + \text{linear terms}
\end{aligned}$$

and when we evaluate the proper Laplacian we have

$$\mathrm{Tr}\!\left(M^{-1}\, \mathcal{T}_j\right) = \sum_n \frac{1}{m_n} \Big[\left[\Sigma_j^{-1}\, L^T q\right]_n^2 + \left[\Sigma_j^{-1}\, \Sigma_c\, \Sigma_i{}^{-1}\!\left(\xi_i{-}\xi_j\right)\right]_n^2 - \Sigma_j^{-1}{}_{nn} \Big]$$

This is again, not manifestly symmetric, but we'll consider the integration here where since the linear terms vanish we get

$$\int \left[\Sigma_j^{-1}\, L^T q\right]_n^2 \phi_c(q) = S^{(c)} \sum_k \frac{\left(\Sigma_j^{-1}\, L^T\right)_{nk}^2}{\alpha_k^{(c)}}$$

so in total we have

$$\int_{\mathbb{R}^d} \phi(x,\, \xi_c,\, \Sigma_c)\, \mathrm{Tr}\!\left(M^{-1}\, \mathcal{T}_j\right) dx = \sum_n \frac{1}{m_n} \Big[\sum_k \frac{\left(\Sigma_j^{-1}\, L^T\right)_{nk}^2}{\alpha_k^{(c)}} + \left[\Sigma_j^{-1}\, \Sigma_c\, \Sigma_i{}^{-1}\!\left(\xi_i{-}\xi_j\right)\right]_n^2 - \Sigma_j^{-1}{}_{nn} \Big]$$

and now I have to do some gymnastics to figure out how everything cancels, in particular I guess I have something like

$$\begin{aligned}
\sum_k \frac{\left(\Sigma_j^{-1}\, L^T\right)_{nk}^2}{\alpha_k^{(c)}} &= \left(\Sigma_j^{-1}\right)_{n:} \left(L^T\, A_c^{-1}\, L\right) \left(\Sigma_j^{-1}\right)_{:n} \\
&= \left(\Sigma_j^{-1}\right)_{n:} \Sigma_c \!\left(\Sigma_j^{-1}\right)_{:n} \\
&= \left(\Sigma_j^{-1}\right)_{n:} \left(\Sigma_i^{-1}{+}\Sigma_j^{-1}\right)^{-1} \left(\Sigma_j^{-1}\right)_{:n}
\end{aligned}$$

Next we'll use the Woodbury identity to write

$$\begin{aligned}
\left(\Sigma_i^{-1}{+}\Sigma_j^{-1}\right)^{-1} &= \left(L^{(i)}\, A_i\, L^{(i)\,T}{+}\Sigma_j^{-1}\right)^{-1} \\
&= \Sigma_j - \Sigma_j\, L^{(i)}\!\left(A_i^{-1} + L^{(i)\,T}\, \Sigma_j\, L^{(i)}\right)^{-1} L^{(i)\,T}\, \Sigma_j
\end{aligned}$$

which seems nasty, but we'll note that

$$\begin{aligned}
A_i^{-1} + L^{(i)}\, \Sigma_j\, L^{(i)\,T} &= L^{(i)\,T}\, \Sigma_i\, L^{(i)} + L^{(i)\,T}\, \Sigma_j\, L^{(i)} \\
&= L^{(i)\,T}\!\left(\Sigma_i{+}\Sigma_j\right) L^{(i)} \\
\left(L^{(i)\,T}\!\left(\Sigma_i{+}\Sigma_j\right) L^{(i)}\right)^{-1} &= L^{(i)\,T}\!\left(\Sigma_i{+}\Sigma_j\right)^{-1} L^{(i)}
\end{aligned}$$

and so

$$\Sigma_c = \left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1} = \Sigma_j - \Sigma_j\left(\Sigma_i+\Sigma_j\right)^{-1}\Sigma_j$$

Then,

$$\begin{aligned}\left(\Sigma_j^{-1}\right)_{n:}\left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1}\left(\Sigma_j^{-1}\right)_{:n} &= \left(\Sigma_j^{-1}\right)_{n:}\left(\Sigma_j - \Sigma_j\left(\Sigma_i+\Sigma_j\right)^{-1}\Sigma_j\right)\left(\Sigma_j^{-1}\right)_{:n} \\ &= \left(\Sigma_j^{-1}\right)_{n:}\delta_{:n} - \delta_{n:}\left(\Sigma_i+\Sigma_j\right)^{-1}\delta_{:n} \\ &= \left(\Sigma_j^{-1}\right)_{nn} - \left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{nn}\end{aligned}$$

so in total

$$T_{ij} = S_{ij}\sum_n \frac{1}{m_n}\left[\left[\Sigma_j^{-1}\Sigma_c\Sigma_i^{-1}\left(\xi_i-\xi_j\right)\right]_n^2 - \left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{nn}\right]$$

Finally, we'll consider

$$\begin{aligned}\Sigma_j^{-1}\Sigma_c\Sigma_i^{-1} &= \Sigma_j^{-1}\left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1}\Sigma_i^{-1} \\ &= \left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\end{aligned}$$

which is clearly symmetric

Therefore, we know that once and for all, T is symmetric with

$$T_{ij} = -\frac{1}{2}S_{ij}\sum_n \frac{1}{m_n}\left[\left[\Sigma_j^{-1}\Sigma_c\Sigma_i^{-1}\left(\xi_i-\xi_j\right)\right]_n^2 - \left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{nn}\right]$$

and to confirm for the diagonal case, we have

$$\begin{aligned}T_{ij} &= S_{ij}\sum_k \frac{1}{m_k}\frac{\alpha_k^{(i)}\alpha_k^{(j)}}{\alpha_k^{(ij)}}\left(1 - 2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)\Delta\xi_k^{(ij)^2}\right) \\ &= -\frac{1}{2}S_{ij}\sum_k \frac{1}{m_k}2\frac{\alpha_k^{(i)}\alpha_k^{(j)}}{\alpha_k^{(ij)}}\left(2\left(\frac{\alpha_k^{(j)}\alpha_k^{(i)}}{\alpha_k^{(ij)}}\right)\Delta\xi_k^{(ij)^2} - 1\right)\end{aligned}$$

where

$$\begin{aligned}\left(\Sigma_i+\Sigma_j\right)^{-1} &= 2\left(\frac{1}{\alpha^{(i)}}+\frac{1}{\alpha^{(j)}}\right)^{-1} \\ &= 2\frac{\alpha^{(i)}\alpha^{(j)}}{\alpha^{(i)}+\alpha^{(j)}} \\ &= \Sigma_j^{-1}\Sigma_c\Sigma_i^{-1}\end{aligned}$$

Tests

Misc Old Shit

Direct Approach

Alternate Formulation

Potential Energy

We're able to use everything from before, not even needing to rotate the derivatives. To confirm this, we'll consider our integral

$$V_{ij} = W\big(\Sigma_i{+}\Sigma_j,\ \xi_i{-}\xi_j\big) \int_{\mathbb{R}^N} V(\boldsymbol{x})\ \phi(x,\ \xi_c,\ \Sigma_c)\, d\boldsymbol{x}$$

where we'll expand $V(\boldsymbol{x})$ as

$$V(\boldsymbol{x}) = \sum_{m=0}^{M} \frac{1}{W}\ \nabla_{X^m} V(\boldsymbol{\zeta})\odot(x{-}\zeta)^m$$

so giving us

$$\int_{\mathbb{R}^N} V(\boldsymbol{x})\ \phi(x,\ \xi_c,\ \Sigma_c)\, d\boldsymbol{x} = \sum_{m=0}^{M}\ \int_{\mathbb{R}^N} \frac{1}{W}\ \nabla_{X^m} V(\boldsymbol{\zeta})\odot(x{-}\zeta)^m\ \phi(x,\ \xi_c,\ \Sigma_c)\, d\boldsymbol{x}$$

where for simplicity we'll first shift by ζ to give

$$\int_{\mathbb{R}^N} V(\boldsymbol{x})\ \phi(x,\ \xi_c,\ \Sigma_c)\, d\boldsymbol{x} = \sum_{m=0}^{M}\ \int_{\mathbb{R}^N} \frac{1}{W}\ \nabla_{X^m} V(\boldsymbol{\zeta})\odot(x)^m\ \phi(x,\ \xi_c{-}\zeta,\ \Sigma_c)\, d\boldsymbol{x}$$

then by applying L_c as our change of basis, we get up with

$$\int_{\mathbb{R}^N} \frac{1}{W}\ \nabla_{X^m} V(\zeta)\odot(x)^m\ \phi(x,\ \xi_c{-}\zeta,\ \Sigma_c)\, d\boldsymbol{x} =$$

$$= \int_{\mathbb{R}^N} \frac{1}{W}\ \nabla_{Q^m} V(\boldsymbol{\zeta})\odot(q)^m\ \phi(q,\ L_c\,(\xi_c{-}\zeta),\ \Lambda_c)\, d\boldsymbol{q}$$

which can be evaluated using what we did previously after recognizing that we have a linear transformation between $\boldsymbol{q}$ and $\boldsymbol{x}$ and so

$$\nabla_{Q^m} V(\boldsymbol{\zeta}) = L_c\,\langle 2,\ m\rangle\,(L_c\,\langle 2,\ m\rangle\,(\ldots\,(L_c\,\langle 2,\ m\rangle\,\nabla_{X^m} V(\boldsymbol{\zeta}))))$$

which is equivalent to just rotating the derivatives as claimed previously

---

Internal Coordinates

We likely will want to work in internals at some point, for which we have

$$H = pGp + V(r) + V'(r)$$

The integrals induced by G and V' now require some thought

Considering just one matrix element, we get

$$\left\langle \phi_i \right| T \left| \phi_j \right\rangle = \sum_{a,b} \left\langle \phi_i \right| p_a G_{ab} p_b \left| \phi_j \right\rangle$$

$$\left\langle \phi_i \right| p_a G_{ab} p_b \left| \phi_j \right\rangle = \int G_{ab}(r)\, \phi_i(r)\, p_a p_b\, \phi_j(r)$$

where we have assumed the internal coordinates live on the $[-\infty, \infty]$ range, ignoring the considerations given in Section IV of Frederick and Woywood

Such integrals are very difficult to handle generically, but we can approximate them by again doing local expansions of the G and V' terms

Rotations

It is straightforward to use the ideas developed previously for a rotated basis in this context, as these are all just polynomial and polynomial-product integrals.

Watson Coordinates

An alternative to proper internal coordinates is to use a rotated Cartesian-displacement normal mode coordinates. To start, we'll note that these coordinates can be expressed as

$$q_i = \sum_n L_{in}\, \Delta x_n$$

and their overlaps may be computed just like any Gaussian product basis

The difficulty arises in integrating the kinetic energy, where we have

$$T = P^2 + \frac{1}{2} \sum_\alpha I_\alpha^{-1}\, {p_\alpha}^2$$

for

$$p_\alpha = \sum_{r,s} \zeta_{rs}^{\alpha} (Q_r P_s - Q_s P_r)$$

where

$$\zeta_{rs}^{\alpha} = (-1)^{\beta} \sum_k L_{r\,(k,\beta)}\, L_{s\,(k,\gamma)} - L_{r\,(k,\gamma)}\, L_{s\,(k,\beta)}$$

for the cyclic permutations $\beta = \alpha{+}1 \bmod 3$, $\gamma = \alpha{+}2 \bmod 3$

This is clearly coming from the a cross-product like term (this is classically expressed with the Levi Cevita symbol), which is basically just a generator of rotation

Notably,

$$\zeta_{sr}^{\alpha} = -\zeta_{rs}^{\alpha}$$

$$\zeta_{rr}^{\alpha} = 0$$

This gives us

$$T = P^2 + \frac{1}{2} \sum_{i,j,k,l} \sum_{\alpha} I_{\alpha}^{-1} \zeta_{ij}^{\alpha} \zeta_{kl}^{\alpha} Q_i P_j Q_k P_l$$

We will note that under our approximation, L is *definitional*, which is to say our choice of L will not change no matter what value of Q we choose. Therefore

$$\left\langle \phi_n \right| I_{\alpha}^{-1} \zeta_{ij}^{\alpha} \zeta_{kl}^{\alpha} Q_i P_j Q_k P_l \left| \phi_m \right\rangle = \zeta_{ij}^{\alpha} \zeta_{kl}^{\alpha} \left\langle \phi_n \right| I_{\alpha}^{-1} Q_i P_j Q_k P_l \left| \phi_m \right\rangle$$

and then for simplicity, we will also assume I_{α}^{-1} is independent of Q, although this is simply an approximation (I think)

This gives us a 4D tensor described by

$$Q P Q P \left| \phi_j \right\rangle = K_j(q) \left| \phi_j \right\rangle$$

which we then element-wise multiply into

$$Z = \sum_{\alpha} I_{\alpha}^{-1} (\zeta^{\alpha} \otimes \zeta^{\alpha})$$

and then we can integrate the tensor expansion induced by $Z \circ K_j$

Tests

Symmetry Proof

But maybe we want to see that we truly get a symmetric form out of K_j after we integrate?

Computer Assisted Expressions

Hand Simplification: Case 0

In[4409]:=

```
niceExpr // pruneLinear[#, Q[ξ[c]]] & // watFmt /@ #[0] & // Column
```

Out[4409]=

$$-(\xi^{(c)} \otimes \mathrm{TQ}\left[(\xi^{(c)} \otimes {\Sigma^{(j)}}^{-1}),\ 2 \to 1\right])$$
$$\xi^{(c)} \otimes \mathbb{I} \otimes \Sigma^{(d)} \Delta$$
$$\xi^{(c)} \otimes \Sigma^{(d)} \Delta \otimes \xi^{(c)} \otimes \Sigma^{(d)} \Delta$$

Annoyingly, all of these terms survive, although we *can* write

$${\Sigma^{(j)}}^{-1} = \sum_{s} 2\, \alpha_s^{(j)}\, L_s^{(j)} \otimes L_s^{(j)}$$

to get the first term to become

$$\sum_s 2\,\alpha_s^{(j)}\,\xi^{(c)}\otimes L_s^{(j)}\otimes\xi^{(c)}\otimes L_s^{(j)}$$

we can do the same trick with the second one if we want, too giving us

$$\sum_s \xi^{(c)}\otimes e_s\otimes e_s\otimes\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)$$

Term Expressions

Old Pretranspose Note ;____;

Old Tests

Hand Simplification: Case 2

Base Expressions

Integration

Term 1:

$$\begin{aligned}
-\sum_s 2\,\alpha_s^{(j)}\,Q^{(c)}\otimes L_s^{(j)}\otimes Q^{(c)}\otimes L_s^{(j)} &= -\sum_{numv}\zeta_{nu}^{\alpha}\,\zeta_{mv}^{\alpha}\sum_s 2\,\alpha_s^{(j)}\left(L_s^{(j)}{}_u\,L_s^{(j)}{}_v\right)\left(\Sigma^{(c)}\right)_{nm}\\
&= -\sum_{numv}\zeta_{nu}^{\alpha}\,\zeta_{mv}^{\alpha}\left(\Sigma^{(c)}\right)_{nm}\sum_s 2\,\alpha_s^{(j)}\left(L_s^{(j)}{}_u\,L_s^{(j)}{}_v\right)\\
&= -\sum_{numv}\zeta_{nu}^{\alpha}\,\zeta_{mv}^{\alpha}\left(\Sigma^{(c)}\right)_{nm}\left(\Sigma^{(j)^{-1}}\right)_{uv}
\end{aligned}$$

Term 2:

$$\begin{aligned}
-\sum_s Q^{(c)}\otimes e_s\otimes e_s\otimes\left(\Sigma^{(j)^{-1}}\,Q^{(c)}\right) &= -\sum_{numv}\zeta_{nu}^{\alpha}\,\zeta_{mv}^{\alpha}\sum_s (e_s)_u\,(e_s)_m\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\\
&= -\sum_{nmv}\zeta_{nm}^{\alpha}\,\zeta_{mv}^{\alpha}\,\delta_{um}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}
\end{aligned}$$

Term 3:

$$Q^{(c)}\otimes\Sigma^{(d)}\,\Delta^{(i,j)}\otimes Q^{(c)}\otimes\Sigma^{(d)}\,\Delta^{(i,j)} = \sum_{numv}\zeta_{nu}^{\alpha}\,\zeta_{mv}^{\alpha}\left(\Sigma^{(c)}\right)_{nm}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_u\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_v$$

Term(s) 4:

$$-2\left((Q-\xi^{(c)})\otimes\Sigma^{(d)}\Delta\otimes\xi^{(c)}\otimes\Sigma^{(j)^{-1}}(Q-\xi^{(c)})\right)$$

$$Q^{(c)}\otimes\Sigma^{(d)}\,\Delta^{(i,j)}\otimes\xi^{(c)}\otimes\Sigma^{(j)^{-1}}\,Q^{(c)} = -2\sum_{numv}\zeta_{nu}^{\alpha}\,\zeta_{mv}^{\alpha}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\xi^{(c)}\right)_u\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m$$

$$Q^{(c)}\otimes\Sigma^{(j)^{-1}}\,Q^{(c)}\otimes\xi^{(c)}\otimes\Sigma^{(d)}\,\Delta^{(i,j)} = -2\sum_{numv}\zeta_{nv}^{\alpha}\,\zeta_{mu}^{\alpha}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\xi^{(c)}\right)_v\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m$$

Term 5:

$$\xi^{(c)} \otimes \Sigma^{(j)^{-1}} (Q - \xi^{(c)}) \otimes \xi^{(c)} \otimes \Sigma^{(j)^{-1}} (Q - \xi^{(c)})$$

$$\xi^{(c)} \otimes \Sigma^{(j)^{-1}} Q^{(c)} \otimes \xi^{(c)} \otimes \Sigma^{(j)^{-1}} Q^{(c)} = \sum_{numv} \zeta^{\alpha}_{nu} \zeta^{\alpha}_{mv} \left(\Sigma^{(j)^{-1}} \Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{uv} (\xi^{c})_n (\xi^{c})_m$$
$$= \sum_{numv} \zeta^{\alpha}_{nu} \zeta^{\alpha}_{mv} \left(\Sigma^{(j)^{-1}} \Sigma^{(c)} \Sigma^{(j)^{-1}}\right)_{nm} (\xi^{c})_u (\xi^{c})_v$$

Integral Test

Sad Tests

Old Pretranspose Note ;_____;

Old Tests

Hand Simplification: Case 4

In[4269]:=

```
niceExpr // pruneLinear[#, Q[ξ[c]]] & // watFmt /@ #[4] & // Column
```

Out[4269]=

$$(\mathrm{Q} - \xi^{(\mathrm{c})}) \otimes \Sigma^{(\mathrm{j})^{-1}} (\mathrm{Q} - \xi^{(\mathrm{c})}) \otimes (\mathrm{Q} - \xi^{(\mathrm{c})}) \otimes \Sigma^{(\mathrm{j})^{-1}} (\mathrm{Q} - \xi^{(\mathrm{c})})$$

Integration

In[3475]:=

$$\left(\frac{\left(1 + (-1)^{n}\right) \alpha^{-\frac{1}{4}-\frac{n}{2}} \mathrm{Gamma}\left[\frac{1+n}{2}\right]}{2^{3/4} \pi^{1/4}} \text{ /. } n \to 4\right) \Big/ \left(\frac{\left(1 + (-1)^{n}\right) \alpha^{-\frac{1}{4}-\frac{n}{2}} \mathrm{Gamma}\left[\frac{1+n}{2}\right]}{2^{3/4} \pi^{1/4}} \text{ /. } n \to 0\right)$$

Out[3475]=

$$\frac{3}{4\,\alpha^2}$$

This will be somewhat tedious, but we have

$$L^{(1)} L^T R \otimes L^{(2)} L^T R \otimes L^{(3)} L^T R \otimes L^{(4)} L^T R$$

and since only the even order terms contribute we can consider that writing

$$\int \left(L^{(1)} L^T R\right)_i \left(L^{(2)} L^T R\right)_j \left(L^{(3)} L^T R\right)_k \left(L^{(4)} L^T R\right)_l$$
$$= \int \left(\left(L^{(1)} L^T\right)_i \otimes \left(L^{(2)} L^T\right)_j \otimes \left(L^{(3)} L^T\right)_k \otimes \left(L^{(4)} L^T\right)_l\right) \odot R^4$$
$$= S^{(c)}\, 3 \sum_s \frac{\left(\left(L^{(1)} L^T\right)_i \otimes \left(L^{(2)} L^T\right)_j \otimes \left(L^{(3)} L^T\right)_k \otimes \left(L^{(4)} L^T\right)_l\right)_{ssss}}{4\,\alpha^{(c)}_s} + \text{quadratics}$$

and now

$$\sum_s \frac{([\text{see above}])_{ss}}{4\,\alpha_s^{(c)}} = \sum_s \left(L^{(1)}\,L^T\right)_{is}\left(A^{(c)}\right)_{ss}\left(L^{(2)}\,L^T\right)_{js}\left(L^{(3)}\,L^T\right)_{ks}\left(A^{(c)}\right)_{ss}\left(L^{(4)}\,L^T\right)_{ls}$$

$$= \sum_s \left(L^{(1)}\,L^T\right)_{is}\left(A^{(c)}\right)_{ss}\left(L^{(2)}\,L^T\right)^T{}_{sj}\left(L^{(3)}\,L^T\right)_{ks}\left(A^{(c)}\right)_{ss}\left(L^{(4)}\,L^T\right)^T{}_{sl}$$

$$= \left(L^{(1)}\,\Sigma^{(c)}\,L^{(2)}\right)_{ij}\left(L^{(3)}\,\Sigma^{(c)}\,L^{(4)}\right)_{kl}$$

and accounting for the quadratic products we have have to take all the different possible permutations of $(s,\ s,\ t,\ t)$ to get terms like

$$\left(L^{(1)}\,L^T R\right)_{is}\left(L^{(2)} L^T R\right)_{js}\left(L^{(3)}\,L^T R\right)_{kt}\left(L^{(4)} L^T R\right)_{lt}$$

which means we will get

$$\sum_s \sum_{t\neq s} \frac{\left(L^{(1)}\,L^T R\right)_{is}\left(L^{(2)} L^T R\right)_{js}\left(L^{(3)}\,L^T R\right)_{kt}\left(L^{(4)} L^T R\right)_{lt}}{2\,\alpha_s^{(c)}\,2\,\alpha_t^{(c)}} + \frac{\left(L^{(1)}\,L^T R\right)_{is}\left(L^{(2)} L^T R\right)_{jt}\left(L^{(3)}\,L^T R\right)_{ks}\left(L^{(4)} L^T R\right)_{lt}}{2\,\alpha_s^{(c)}\,2\,\alpha_t^{(c)}} + \frac{\left(L^{(1)}\,L^T R\right)_{is}\left(L^{(2)} L^T R\right)_{jt}\left(L^{(3)}\,L^T R\right)_{kt}\left(L^{(4)} L^T R\right)_{ls}}{2\,\alpha_s^{(c)}\,2\,\alpha_t^{(c)}}$$

which is unfortunate because we need the $t{=}s$ term to simplify, but then we can realize that we can actually add it in since *from above* the quartic term just pops in a 3!

and each of these will reduce to give us a form like and so in total we have

$$\int \left(L^{(1)}\,L^T R\right)_i\left(L^{(2)} L^T R\right)_j\left(L^{(3)}\,L^T R\right)_k\left(L^{(4)} L^T R\right)_l = \left(L^{(1)}\Sigma^{(c)}\,L^{(2)}\right)_{ij}\left(L^{(3)}\,\Sigma^{(c)}\,L^{(4)}\right)_{kl} + \left(L^{(1)}\Sigma^{(c)}\,L^{(3)}\right)_{ik}\left(L^{(2)}\,\Sigma^{(c)}\,L^{(4)}\right)_{jl} + \left(L^{(1)}\Sigma^{(c)}\,L^{(4)}\right)_{il}\left(L^{(2)}\,\Sigma^{(c)}\,L^{(3)}\right)_{jk}$$

Test

Term

giving us

$$Q^{(c)} \otimes \Sigma^{(j)^{-1}}\,Q^{(c)} \otimes Q^{(c)} \otimes \Sigma^{(j)^{-1}}\,Q^{(c)} \;\to= \sum_{numv} \zeta^{\alpha}_{nu}\,\zeta^{\alpha}_{mv}(\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv} + \left(\Sigma^{(c)}\right)_{nm}\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{uv} + \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\right)_{um})$$

which we can contract further by noting that (by symmetry)

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\right)_{um} = \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mu}$$

giving us

$$\begin{aligned} Q^{(c)}\otimes\Sigma^{(j)^{-1}}\,Q^{(c)}\otimes Q^{(c)}\otimes\Sigma^{(j)^{-1}}\,Q^{(c)} \to= \sum_{numv}\zeta^{\alpha}_{nu}\,\zeta^{\alpha}_{mv}(\\ &\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv} \\ &+\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mu} \\ &+\left(\Sigma^{(c)}\right)_{nm}\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{uv} \\ &) \end{aligned}$$

Sad Tests

Old Pretranspose Note ;_____;

Adding all terms

Setup

Our total term list is

$$\begin{aligned} &.{=}-\left(\xi^{(c)}\right)_{n}\left(\xi^{(c)}\right)_{m}\left(\Sigma^{(j)^{-1}}\right)_{uv} \\ &.{=}\ \delta_{um}\left(\xi^{(c)}\right)_{n}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{v} \\ &.{=}\ \left(\xi^{(c)}\right)_{n}\left(\xi^{(c)}\right)_{m}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{u}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{v} \\ &.{=}\ -\left(\Sigma^{(c)}\right)_{nm}\left(\Sigma^{(j)^{-1}}\right)_{uv} \\ &.{=}\ -\delta_{um}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} \\ &.{=}\ \left(\Sigma^{(c)}\right)_{nm}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{u}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{v} \\ &.{=}\ \left(\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nm}\left(\xi^{c}\right)_{u}\left(\xi^{c}\right)_{v} \\ &.{=}\ -2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\xi^{(c)}\right)_{u}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m} \\ &.{=}\ -2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\xi^{(c)}\right)_{v}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{m} \\ &.{=}\ \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv}+\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mu}+\left(\Sigma^{(c)}\right)_{nm}\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{uv} \end{aligned}$$

Test

Simplification

Now we'll collect everything with two ξ terms,

$$\begin{aligned} &.{=}\ -\left(\xi^{(c)}\right)_{n}\left(\xi^{(c)}\right)_{m}\left(\Sigma^{(j)^{-1}}\right)_{uv} \\ &.{=}\ \left(\xi^{(c)}\right)_{n}\left(\xi^{(c)}\right)_{m}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{u}\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_{v} \\ &.{=}\ \left(\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nm}\left(\xi^{c}\right)_{u}\left(\xi^{c}\right)_{v} \end{aligned}$$

and we'll swap $u{\to}m$ and $n{\to}v$ (two flips $\Rightarrow$ no sign change) to get

$$
\begin{aligned}
&.= -\left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(j)^{-1}}\right)_{uv}\\
&.= \left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_v\\
&.= \left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{uv}
\end{aligned}
$$

Now we note that by the Woodbury identity

$$\Sigma_c = \left(\Sigma_i^{-1}+\Sigma_j^{-1}\right)^{-1} = \Sigma_j - \Sigma_j\left(\Sigma_i+\Sigma_j\right)^{-1}\Sigma_j$$

so

$$\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}} = \Sigma_j - \left(\Sigma_i+\Sigma_j\right)^{-1}$$

and so we get

$$\left(\Sigma^{(j)^{-1}}\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-\Sigma^{(j)^{-1}}\right)_{uv} = -\left(\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{uv}$$

and in total we have

$$\left(\xi^{(c)}\right)_n \left(\xi^{(c)}\right)_m \left(\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)\otimes\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)-\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{uv}$$

which is clearly symmetric with respect to index interchange

We get to do the same simplification with the terms

$$
\begin{aligned}
&.= -\left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}}\right)_{uv}\\
&.= \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_v\\
&.= \left(\Sigma^{(c)}\right)_{nm} \left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{uv}
\end{aligned}
$$

giving us

$$\left(\Sigma^{(c)}\right)_{nm} \left(\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)\otimes\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)-\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{uv}$$

and so this whole block becomes

$$\left(\Sigma^{(c)} + \xi^{(c)}\otimes\xi^{(c)}\right)_{nm} \left(\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)\otimes\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)-\left(\Sigma_i+\Sigma_j\right)^{-1}\right)_{uv} \tag{1}$$

Through experimentation we also find the following are symmetric when added up

$$
\begin{aligned}
&.= -\delta_{um}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\\
&.= \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu} \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv}\\
&.= \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mu}
\end{aligned}
$$

It is initially strange that this works, but perhaps we try an initial condensation

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mu}-\delta_{um}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} = \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-I\right)_{mu}$$

and we'll recall that we can write

$$\Sigma^{(c)-1} = \Sigma^{(i)-1} + \Sigma^{(j)^{-1}}$$

$$\alpha^{(c)} = \alpha^{(i)} + \alpha^{(j)}$$

$$\Sigma^{(c)}\,\Sigma^{(j)^{-1}} = \Sigma^{(c)}\left(\Sigma^{(c)-1}-\Sigma^{(i)-1}\right)$$

so we get

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-I\right)_{mu} = -\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mu}$$

which is clearly symmetric once we add up every term

And similarly

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv} = \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(I-\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mv}$$

which isn't an issue for the very, very subtle reason that $m = v \Rightarrow \zeta^{(\alpha)}_{mv} = 0$ and so the asymmetric term disappears, which *also* means that we get away with just writing

$$\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{mv} = -\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mv}$$

And these two can be condensed into

$$-\left(\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mu} + \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{mv}\right) \tag{2}$$

Finally, we have

$$\begin{aligned}
&.= \delta_{um}\left(\xi^{(c)}\right)_n\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_v \\
&.= -2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\left(\xi^{(c)}\right)_u\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \\
&.= -2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\xi^{(c)}\right)_v\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m
\end{aligned}$$

which will cancel for a very similar reason to what we had above, first off we have

$$-2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\xi^{(c)}\right)_v\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m = -\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{nu}\left(\xi^{(c)}\right)_v\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m$$

by the exact same argument as before, *and then* we note that $\Delta^{(i,j)} = -\Delta^{(j,i)}$ and so

$$-2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu}\left(\xi^{(c)}\right)_v\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m = -2\left(\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{nu}\left(\xi^{(c)}\right)_v\left(\Sigma^{(d)}\,\Delta^{(j,i)}\right)_m$$

which gives us the symmetry we need

We'll handle the other term by first swapping $n{\to}u$ and $m{\to}v$ which doesn't change the sign, this means we have

$$\left(\xi^{(c)}\right)_u\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m\left(\delta_{nv} - 2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv}\right) = \left(\xi^{(c)}\right)_u\left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m\left(I-2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)\right)_{nv}$$

which isn't exactly the pattern we had before, but here's a mind-blowing fact

$$2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right) = \Sigma^{(c)}\,\Sigma^{(j)^{-1}} + \Sigma^{(c)}\,\Sigma^{(j)^{-1}}$$

and so we can use the first copy to perform the previous trick

$$I - \Sigma^{(c)}\,\Sigma^{(j)^{-1}} = \Sigma^{(c)}\,\Sigma^{(i)^{-1}}$$

and so we get to do the same double negative as before, giving us

$$\left(\xi^{(c)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \left(\Sigma^{(c)}\,\Sigma^{(i)^{-1}}-\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nv} = -\left(\xi^{(c)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-\Sigma^{(c)}\,\Sigma^{(i)^{-1}}\right)_{nv}$$
$$= \left(\xi^{(c)}\right)_u \left(\Sigma^{(d)}\,\Delta^{(j,i)}\right)_m \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-\Sigma^{(c)}\,\Sigma^{(i)^{-1}}\right)_{nv}$$

And we can combine some of this to make for less typing, first using the same mind blowing $2\,x = x + x$ trick to write

$$-2\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}\right)_{nu} \left(\xi^{(c)}\right)_v \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m = -\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{nu} \left(\xi^{(c)}\right)_v \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m$$

and so we get

$$\begin{aligned}\left(\left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-\Sigma^{(c)}\,\Sigma^{(i)^{-1}}\right)_{nv} \left(\xi^{(c)}\right)_u - \left(\Sigma^{(c)}\,\Sigma^{(j)^{-1}}-\Sigma^{(c)}\,\Sigma^{(i)-1}\right)_{nu} \left(\xi^{(c)}\right)_v\right) \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \\ = \left(\Sigma^{(c)}\right)_n \left(\left(\Sigma^{(j)^{-1}}-\Sigma^{(i)-1}\right)_v \left(\xi^{(c)}\right)_u - \left(\Sigma^{(j)^{-1}}-\Sigma^{(i)-1}\right)_u \left(\xi^{(c)}\right)_v\right) \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m \\ = \left(\Sigma^{(c)}\right)_n \left(\Delta\Sigma_v\left(\xi^{(c)}\right)_u - \Delta\Sigma_u\left(\xi^{(c)}\right)_v\right) \left(\Sigma^{(d)}\,\Delta^{(i,j)}\right)_m\end{aligned} \tag{3}$$

Full Expression

From above we get three classes of terms (I dropped a negative on part of the third expression initially and a 1/2 on the second...)

$$\left(\Sigma^{(c)}+\xi^{(c)}\otimes\xi^{(c)}\right)_{nm} \left(\Delta\xi\otimes\Delta\xi-\Sigma^{+}\right)_{uv} \tag{4}$$

$$-\frac{1}{2}\left(\Gamma^{(j)}_{nv}\Gamma^{(i)}_{mu} + \Gamma^{(j)}_{nu}\Gamma^{(i)}_{mv}\right) \tag{5}$$

$$-\Sigma^{(c)}_n\left(\Delta\Sigma_v\,\xi^{(c)}_u+\Delta\Sigma_u\,\xi^{(c)}_v\right)\Delta\xi_m \tag{6}$$

where

$$\begin{aligned}\Sigma^{+} &= \left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1} \\ \Delta\xi &= \Sigma^{+}\left(\xi^{(i)}-\xi^{(j)}\right) \\ \Gamma^{(i)} &= \Sigma^{(c)}\,\Sigma^{(i)^{-1}} \\ \Delta\Sigma &= \Sigma^{(i)^{-1}}-\Sigma^{(j)^{-1}}\end{aligned}$$

Test 2

Full Integration (old)

Bad Symmetry, Good Math

Value Test

Momentum Inclusion

To account for the momentum we change our Gaussian definition to include a momentum dependent phase as

$$\varphi^{(i)} = \exp\left(-\frac{1}{2}\left(q-\xi^{(i)}\right)\Sigma^{(i)-1}\left(q-\xi^{(i)}\right) + \mathbb{i}\, J^{(i)}\, q\right)$$

where $J = Q_\Sigma\, p_0$ are chosen to be the momenta along the rotated Gaussian axes

Rephasing

Function

Generic Shifted Integral

In[1023]:=

```
baseShiftedIntegral =
 Assuming[a > 0 && p > 0 && k > 0 && k ∈ Integers && c ∈ Reals,
  Integrate[q^k Exp[-a q^2 + I p (q - c)], {q, -∞, ∞}]
 ]
```

Out[1023]=

$$\frac{1}{2} a^{-1-\frac{k}{2}} e^{-i c p} \left(-i \left(-1+(-1)^k\right) p \,\text{Gamma}\left[1+\frac{k}{2}\right] \text{Hypergeometric1F1}\left[1+\frac{k}{2}, \frac{3}{2}, -\frac{p^2}{4 a}\right] + \left(1+(-1)^k\right) \sqrt{a}\, \text{Gamma}\left[\frac{1+k}{2}\right] \text{Hypergeometric1F1}\left[\frac{1+k}{2}, \frac{1}{2}, -\frac{p^2}{4 a}\right]\right)$$

Not quite right...

Solving for Hypergeometric Expressions

We start out by noting that the even term is just built off a Hermite polynomial, so we'll ignore it. The second term

$$\text{Gamma}\left[1+\frac{k}{2}\right] \text{Hypergeometric1F1}\left[\frac{2+k}{2}, \frac{3}{2}, -x\right]$$

is rather more annoying, so we return to the definition of the HGF

$${}_1F_1(a;\; b;\; x) = \sum_{m=0}^{\infty} \frac{(a)_m}{(b)_m} \frac{x^m}{m!}$$

where $(a)_m$ is the rising factorial starting at a and going to $a+m-1$

Noting that

$$(a)_m = \frac{\Gamma(a+m)}{\Gamma(a)}$$

and that in our case, $a = b + k$, we have

$$\frac{(a)_m}{(b)_m} = \frac{\Gamma(b+k+m)}{\Gamma(b+k)} \frac{\Gamma(b)}{\Gamma(b+m)} = \frac{(b+m)_k}{(b)_k}$$

and the $(b)_k$ can be factored and $(b+m)_k$ can be expressed as a polynomial with

$$(b+m)_k = \sum_{j=1}^{k} |S_1(k,\ j)|\, (b+m)^j$$

and then we can express this in terms of m alone by writing

$$(b+m)_k = \sum_{j=1}^{k} \sum_{l=0}^{j} |S_1(k,\ j)| \binom{j}{j-l} b^{(j-l)}\, m^l$$

and then we flip the sum to get

$$(b+m)_k = \sum_{l=0}^{k} \sum_{j=l}^{k} |S_1(k,\ j)| \binom{j}{j-l} b^{(j-l)}\, m^l$$

where we've explicitly taken advantage of the fact that $S_1(k,\ 0) = 0$, so now we have

$${}_1F_1(b+k;\ b;\ x) = \frac{1}{(b)_k} \sum_{l=0}^{k} \sum_{j=l}^{k} |S_1(k,\ j)| \binom{j}{j-l} b^{(j-l)} \sum_{m=0}^{\infty} m^l \frac{x^m}{m!}$$

and then that final sum actually has a simple form as

$$\sum_{m=0}^{\infty} m^l \frac{x^m}{m!} = e^x \sum_{n=1}^{l} S_2(l,\ n)\ x^n$$

which means in total we get

$${}_1F_1(b+k;\ b;\ x) = \frac{1}{(b)_k}\ e^x \sum_{l=0}^{k} \sum_{j=l}^{k} \sum_{n=1}^{l} |S_1(k,\ j)| \binom{j}{j-l} b^{(j-l)}\, S_2(l,\ n)\ x^n$$

and then flipping the sum once more we have

$${}_1F_1(b+k;\ b;\ x) = \frac{1}{(b)_k}\ e^x \sum_{n=1}^{k} \sum_{l=n}^{k} \sum_{j=l}^{k} |S_1(k,\ j)| \binom{j}{j-l} b^{(j-l)}\, S_2(l,\ n)\ x^n$$

finally, flipping that rising factorial back around we have (I dropped a power but otherwise everything is fine)

$$\begin{aligned} {}_1F_1(b+k;\ b;\ x) &= \frac{(b-1)!}{(k+b-1)!}\ e^x \sum_{n=0}^{k} \sum_{l=n}^{k} \sum_{j=l}^{k} |S_1(k,\ j)| \binom{j}{l} b^{(j-l)}\, S_2(l,\ n)\ x^n \\ &= \frac{(b-1)!}{(k+b-1)!}\ e^x \sum_{n=0}^{k} \sum_{l=n}^{k} \sum_{j=l}^{k} S_1(k,\ j) \binom{j}{l} b^{(j-l)}\, S_2(l,\ n)\ (-x)^n \end{aligned}$$

and we can view this as a type of matrix transform in the basis of rising/falling factorials, which leads us to

$$
\begin{aligned}
{}_1F_1(b+k;\ b;\ x) &= \frac{1}{(b)_k}\ e^x \sum_{n=0}^{k} \binom{k+b-1}{n} [k]_{k-n}\, x^n \\
&= e^x \sum_{n=0}^{k} \binom{k+b-1}{n} \frac{[k]_{(k-n)}}{(b)_k}\ x^n
\end{aligned}
$$

Finally, we have the prefactor, so

$$
\begin{aligned}
\Gamma(b+k)\,{}_1F_1(b+k;\ b;\ x) &= \Gamma(b+k)\,\frac{\Gamma(b)}{\Gamma(b+k)}\ e^x \sum_{n=0}^{k} \binom{k+b-1}{k-n} [k]_{(k-n)}\, x^n \\
&= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k+b)}{\Gamma(k-n+1)\,\Gamma(n+b)}\,[k]_{(k-n)}\, x^n \\
&= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k+b)}{\Gamma(n+b)}\,\frac{\Gamma(k+1)}{\Gamma(k-n+1)\,\Gamma(n+1)}\ x^n \\
&= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k+b)}{\Gamma(n+b)} \binom{k}{n} x^n
\end{aligned}
$$

And then to clean up the $\Gamma(b)$ terms we get

$$
\begin{aligned}
\Gamma(b+k)\,{}_1F_1(b+k;\ b;\ x) &= \Gamma(b+k)\,\frac{\Gamma(b)}{\Gamma(b+k)}\ e^x \sum_{n=0}^{k} \binom{k+b-1}{k-n} [k]_{(k-n)}\, x^n \\
&= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k+b)}{\Gamma(k-n+1)\,\Gamma(n+b)}\,[k]_{(k-n)}\, x^n \\
&= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(k+b)}{\Gamma(n+b)}\,\frac{\Gamma(k+1)}{\Gamma(k-n+1)\,\Gamma(n+1)}\ x^n \\
&= e^x \sum_{n=0}^{k} \frac{\Gamma(b)\,\Gamma(b+k)}{\Gamma(n+b)} \binom{k}{n} x^n
\end{aligned}
$$

which actually just shows that

$$
{}_1F_1(b+k;\ b;\ x) = e^x \sum_{n=0}^{k} \frac{1}{(b)_{(n)}} \binom{k}{n} x^n
$$

then adding on that pre-factor we get

$$
\Gamma(b+k)\,{}_1F_1(b+k;\ b;\ x) = e^x \sum_{n=0}^{k} \frac{\Gamma(b+k)}{(b)_{(n)}} \binom{k}{n} x^n
$$

where letting $b = c + 1/2$

$$\frac{\Gamma(b+k)}{(b)_{(n)}} = \frac{\sqrt{\pi}}{2^{c+k-n}} \frac{(2\,(c+k)-1)!!\,(2c-1)!!}{(2(n+c)-1)!!}$$

Derivation Work

Generic Integral Form

We get in total

$$\int_{-\infty}^{\infty} (q-c)^k \exp\left(-\alpha(q-c)^2 + ipq\right) = e^{-icp} \begin{cases} \alpha^{-(1+k/2)}\; ip\, \Gamma\left(\frac{2+k}{2}\right) F_1\left(\frac{2+k}{2};\, \frac{3}{2};\, -\frac{p^2}{4\alpha}\right) & k \text{ odd} \\ \alpha^{-(1/2+k/2)}\; \Gamma\left(\frac{1+k}{2}\right) F_1\left(\frac{1+k}{2};\, \frac{1}{2};\, -\frac{p^2}{4\alpha}\right) & k \text{ even} \end{cases}$$

where both of these branches use the symbolic form from above, as

$$\frac{2+k}{2} - \frac{3}{2} = \frac{3}{2} + \frac{(k-1)}{2}$$
$$\frac{1+k}{2} - \frac{1}{2} = \frac{1}{2} + \frac{k}{2}$$

and therefore, letting $m = \lfloor k/2 \rfloor$ we have both integrals having the form of powers in p

$$\Gamma(b+m)\, F_1\left(b+m;\; b+m;\; -\frac{p^2}{4\alpha}\right) = \exp\left(-\frac{p^2}{4\alpha}\right) \sum_{n=0}^{m} (-1)^n \frac{\Gamma(b+m)}{(b)_{(n)}} \binom{m}{n} \left(\frac{p}{2\sqrt{\alpha}}\right)^{2\,n}$$

and in the case that $p = 0$, letting $0^0 = 1$ we recover the original form

$$\Gamma(b+m)\, F_1\left(b+m;\; b+m;\; -\frac{p^2}{4\;a}\right) = \Gamma(b+m)$$

for convenience, we will write

$$G_b^k(\alpha,\; p) = \Gamma(b+\lfloor k/2 \rfloor)\, F_1\left(b+\lfloor k/2 \rfloor;\; b+\lfloor k/2 \rfloor;\; -\frac{p^2}{4\alpha}\right)$$

and so our total integral is

$$\int_{-\infty}^{\infty} (q-c)^k \exp\left(-\alpha(q-c)^2 + \mathbb{i}pq\right) = e^{-\mathbb{i}cp} \begin{cases} \alpha^{-(1+k/2)}\; \mathbb{i}p\; G_{3/2}^k(\alpha,\; p) & k \text{ odd} \\ \alpha^{-(1/2+k/2)}\; G_{1/2}^k(\alpha,\; p) & k \text{ even} \end{cases}$$

Rephasing

Generic form for M

To make the derivations simpler, we will introduce the notation

$$M_b^k(\alpha,\ p) = \frac{2^{\lceil k/2 \rceil}}{\sqrt{\pi}} \sum_{n=0}^{\lfloor k/2 \rfloor} \left(-\frac{1}{2}\right)^n \frac{\Gamma(b+\lfloor k/2 \rfloor)}{(b)_{(n)}} \binom{\lfloor k/2 \rfloor}{n} \left(\frac{p^2}{2\,\alpha}\right)^n$$

and more specifically,

$$M_k^{(i,j)} = \begin{cases} M_{3/2}^k\left(\alpha_s^{(i,j)},\ p_s^{(i,j)}\right) & k \text{ odd} \\ M_{1/2}^k\left(\alpha_s^{(i,j)},\ p_s^{(i,j)}\right) & k \text{ even} \end{cases}$$

we'll also take this chance to figure out what the two relevant values of M_k evaluate to

First we have

$$\frac{\Gamma(3/2+k)}{(3/2)_{(n)}} = \frac{\sqrt{\pi}}{2^{k+1-n}} \frac{2k!!}{2n!!}$$

$$\frac{\Gamma(1/2+k)}{(1/2)_{(n)}} = \frac{\sqrt{\pi}}{2^{k-n}} \frac{(2\,k-1)!!}{(2n-1)!!}$$

then we get

$$\begin{aligned} M_{1/2}^k(\alpha,\ p) &= \frac{2^{k/2}}{\sqrt{\pi}} \sum_{n=0}^{k/2} \left(-\frac{1}{2}\right)^n \frac{\sqrt{\pi}}{2^{k/2-n}} \frac{(k-1)!!}{(2n-1)!!} \binom{k/2}{n} \left(\frac{p^2}{2\,\alpha}\right)^n \\ &= \sum_{n=0}^{k/2} (-1)^n \frac{(k-1)!!}{(2n-1)!!} \binom{k/2}{n} \left(\frac{p^2}{2\,\alpha}\right) \\ &= \sum_{n=0}^{k/2} (-1)^n \left(\prod_{j=n+1}^{k/2} 2j-1\right) \binom{k/2}{n} \left(\frac{p^2}{2\,\alpha}\right) \\ M_{3/2}^k(\alpha,\ p) &= \sum_{n=0}^{(k-1)/2} (-1)^n \frac{(k-1)!!}{2n!!} \binom{(k-1)/2}{n} \left(\frac{p^2}{2\,\alpha}\right)^n \\ &= \sum_{n=0}^{(k-1)/2} (-1)^n \left(\prod_{j=n}^{(k-1)/2} 2j+1\right) \binom{(k-1)/2}{n} \left(\frac{p^2}{2\,\alpha}\right)^n \end{aligned}$$

this then provides a recurrence relation in k on the coefficients as we have the generic form

$$\mu_n^k = (-1)^n \left(\prod_{j=n+1}^{\lfloor k/2 \rfloor} 2j + (-1)^{k+1}\right) \binom{\lfloor k/2 \rfloor}{n}$$

and

$$\binom{\lfloor k/2 \rfloor}{n} = \binom{\lfloor (k-2)/2 \rfloor}{n} + \binom{\lfloor (k-2)/2 \rfloor}{n-1}$$

$$\left(\prod_{j=n+1}^{\lfloor k/2 \rfloor} 2j + (-1)^{k+1}\right) = \left(2\,\lfloor k/2 \rfloor - (-1)^k\right) \left(\prod_{j=n+1}^{\lfloor (k-2)/2 \rfloor} 2j + (-1)^{k+1}\right)$$

therefore

$$
\begin{aligned}
\mu_n^k &= (-1)^n\left(\prod_{j=n+1}^{\lfloor k/2\rfloor} 2j + (-1)^{k+1}\right)\binom{\lfloor k/2\rfloor}{n} \\
&= (-1)^n\left(2\lfloor k/2\rfloor + (-1)^{k+1}\right)\left(\prod_{j=n+1}^{\lfloor (k-2)/2\rfloor} 2j - (-1)^k\right)\left(\binom{\lfloor (k-2)/2\rfloor}{n} + \binom{\lfloor (k-2)/2\rfloor}{n-1}\right) \\
&= \left(2\lfloor k/2\rfloor + (-1)^{k+1}\right)\left(\mu_n^{k-2} - \left(\prod_{j=n+1}^{\lfloor (k-2)/2\rfloor} 2j - (-1)^k\right)\binom{\lfloor (k-2)/2\rfloor}{n-1}\right) \\
&= \left(2\lfloor k/2\rfloor + (-1)^{k+1}\right)\left(\mu_n^{k-2} - \frac{1}{2n - (-1)^k}\,\mu_{n-1}^{k-2}\right)
\end{aligned}
$$

and finally

$$
\begin{aligned}
\left(2\lfloor k/2\rfloor + (-1)^{k+1}\right) &= 2\left(k - \left(1 - (-1)^k\right)/2\right)/2 - (-1)^k \\
&= k - \left(1 - (-1)^k\right)/2 - (-1)^k \\
&= \lceil k/2\rceil
\end{aligned}
$$

so we get

$$
\mu_n^k = \lceil k/2\rceil\left(\mu_n^{k-2} - \frac{1}{2n - (-1)^k}\,\mu_{n-1}^{k-2}\right)
$$

where it should be noted that $\lceil k/2\rceil$ is always odd and so the first term will always just be the product of odd integers

Tests

Notation

Final Integrals

$$
\int_{-\infty}^{\infty}\left(q_s - \xi_s^{(i,j)}\right)^k \varphi^{(i)}\,\varphi^{*(j)} = \frac{X_0^{(i,j)}}{\left(2\,\alpha_s^{(i,j)}\right)^{\lceil k/2\rceil}}\begin{cases} \mathbb{i}\,p^{(i,j)} M_{3/2}^k\left(\alpha_s^{(i,j)},\ p_s^{(i,j)}\right) & k \text{ odd} \\ M_{1/2}^k\left(\alpha_s^{(i,j)},\ p_s^{(i,j)}\right) & k \text{ even} \end{cases}
$$

where

$$
\begin{aligned}
X_0^{(i,j)} &= \sqrt{\pi^d\left|\Sigma^{(i,j)}\right|}\exp\left(-\frac{1}{2}\,p^{(i,j)\top}\,\Lambda^{(i,j)}\,p^{(i,j)}\right)\exp\left(-\mathbb{i}\xi^{(i,j)}\cdot p^{(i,j)}\right) \\
p^{(i,j)} &= \left(J^{(i)} - J^{(j)}\right)L^{(i,j)\top} = J^{(i,j)}\,L^{(i,j)\top}
\end{aligned}
$$

and for convenience we will enumerate the relevant values of M

$$
M_1^{(i,j)} = 1
$$

$$
\begin{aligned}
M_2^{(i,j)} &= 1-\frac{p_s^{(i,j)2}}{2\alpha_s^{(i,j)}} \\
M_3^{(i,j)} &= 3-\frac{p_s^{(i,j)2}}{2\alpha_s^{(i,j)}} \\
M_4^{(i,j)} &= 3-\frac{6\ p_s^{(i,j)2}}{2\ \alpha_s^{(i,j)}}+\frac{p_s^{(i,j)4}}{4\alpha_s^{(i,j)}}
\end{aligned}
$$

where generically

$$
M_k = \sum_{n=0}^{\lfloor k/2 \rfloor} \mu_n^{(k)} \left(\frac{p_m^2}{2\ \alpha_m} \right)^n
$$

with

$$
\begin{aligned}
\mu_n^{(k)} &= \lceil k/2 \rceil \left(\mu_n^{(k-2)} - \frac{1}{2n - (-1)^k} \mu_{n-1}^{(k-2)} \right) \\
&= (-1)^n \left(\prod_{j=n+1}^{\lfloor k/2 \rfloor} 2j - (-1)^k \right) \binom{\lfloor k/2 \rfloor}{n}
\end{aligned}
$$

which is just a binomial coefficient times the appropriate falling factorial in odd numbers

This means the generic integral form is

$$
\int_{-\infty}^{\infty} \left(q_s - \xi_s^{(i,j)} \right)^k \varphi^{(i)}\ \varphi^{*(j)} = \frac{X_0^{(i,j)}}{\left(2\ \alpha_s^{(i,j)} \right)^{\lceil k/2 \rceil}} \left(\sum_{n=0}^{\lfloor k/2 \rfloor} \mu_n^{(k)} \left(\frac{p_s^{(i,j)^2}}{2\ \alpha_s^{(i,j)}} \right)^n \right) \begin{cases} \mathbb{i}\,p^{(i,j)} & k \text{ odd} \\ 1 & k \text{ even} \end{cases}
$$

Rephased

Old

Tests

Dephased

Examples

Rotated Integrations

We can integrate along the rotated coordinates, but it is perhaps more useful to have expressions in terms of the covariance matrices

The basic form of the integrals will be, e.g.,

$$
\int A\left(Q - \xi^{(i,j)} \right) \varphi^{(i)}\ \varphi^{*(j)}
$$

and the $\phi^{(i)}\,\phi^{(j)}$ component will provide the Gaussian axes and all the usual data such that

$$\left(Q-\xi^{(i,j)}\right) = L^T R$$

at the phase factors will combine to give

$$\exp\left(\mathbb{i}\left(J^{(i)}-J^{(j)}\right)Q\right)$$

To that end, we'll consider the different forms of expressions we have. In the k=0 case, we'll have terms like

Constants

$$\int_{-\infty}^{\infty} V^{(0)}\,\varphi^{(i)}\,\varphi^{*(j)} = V^{(0)}\,X_0^{(i,j)}$$

Linear Terms

We'll have things like

$$\begin{aligned}\int_{-\infty}^{\infty} V_n^{(1)}\left(Q-\xi^{(i,j)}\right)\varphi^{(i)}\,\varphi^{*(j)} &= \mathbb{i}\,X_0^{(i,j)}\sum_s \frac{\left(V^{(1)}L^{\mathrm{T}}\right)_{ns}}{2\,\alpha_s^{(i,j)}}\;p_s^{(i,j)} \\ &= \mathbb{i}\,X_0^{(i,j)}\sum_s \left(V^{(1)}L^{\mathrm{T}}\right)_{ns}\Lambda_{ss}^{(i,j)}\left(J^{(i,j)}\,L^{\mathrm{T}}\right)_s \\ &= \mathbb{i}\,X_0^{(i,j)}\sum_s V_n^{(1)}(L^{\mathrm{T}})_{:s}\,\Lambda_{ss}^{(i,j)}(L)_{s:}\;J^{(i,j)\mathrm{T}} \\ &= \mathbb{i}\,X_0^{(i,j)}\;V_n^{(1)}\,\Sigma^{(i,j)}\;J^{(i,j)\mathrm{T}}\end{aligned}$$

and we'll shorthand momentum correlation vector as

$$\rho^{(i,j)} = \Sigma^{(i,j)}\;J^{(i,j)\mathrm{T}}$$

so we get

$$\int_{-\infty}^{\infty} V^{(1)}\left(Q-\xi^{(i,j)}\right)\varphi^{(i)}\,\varphi^{*(j)} = \mathbb{i}\,X_0^{(i,j)}\;V_n^{(1)}\,\rho^{(i,j)}$$

Quadratic Terms

We have

$$\frac{\int V_n^{(1)}\left(Q-\xi^{(i,j)}\right)\,V_m^{(2)}\left(Q-\xi^{(i,j)}\right)\varphi^{(i)}\,\varphi^{(j)}}{X_0^{(i,j)}} = \sum_s\sum_t \frac{\left(V^{(1)}L^{(i,j)\mathrm{T}}\right)_{ns}\left(V^{(2)}L^{(i,j)\mathrm{T}}\right)_s}{2\,\alpha_s^{(i,j)}}\begin{cases} M_2^{(i,j)} & s=t \\ -\dfrac{p_s^{(i,j)}\,p_t^{(i,j)}}{2\,\alpha_t^{(i,j)}}\,M_1^{(i,j)} & s\neq t\end{cases}$$

but then we note that

$$M_2^{(i,j)} = 1 - \frac{p_s^{(i,j)2}}{2\alpha_s^{(i,j)}}$$

and the momentum contributions add, giving us

$$\begin{aligned}\frac{\int \cdots}{X_0^{(i,j)}} &= \sum_s \frac{V_n^{(1)} L_s^{(i,j)\mathrm{T}} \otimes V_m^{(2)} L_t^{(i,j)\mathrm{T}}}{2\,\alpha_s^{(i,j)}} - \sum_s \frac{V_n^{(1)} L_s^{(i,j)\mathrm{T}}\, p_s^{(i,j)}}{2\,\alpha_s^{(i,j)}} \sum_t \frac{V_m^{(2)} L_t^{(i,j)\mathrm{T}}\, p_t^{(i,j)}}{2\,\alpha_t^{(i,j)}} \\ &= \left(V^{(1)} \Sigma^{(i,j)} V^{(2)}\right)_{nm} - \left(V^{(1)} \rho^{(i,j)}\right)_n \left(V^{(2)} \rho^{(i,j)}\right)_m\end{aligned}$$

General Term

$$\frac{\int_{-\infty}^{\infty} \left[\prod_{n=1}^{d} V_{b_n}^{(a_n)}\left(Q - \xi^{(i,j)}\right)\right] \varphi^{(i)}\, \varphi^{(j)}}{X_0^{(i,j)}} =$$

$$\sum_{k\in\mathcal{P}(d)} \left(\sum_{s=\mathcal{D}(k)} \left(\prod_{n=1}^{d} V_{b_n}^{(a_n)} L_{s_n}^{(i,j)\mathrm{T}} \right) \right) \prod_{m=1}^{d} \frac{X_0^{(i,j)}}{\left(2\,\alpha_m^{(i,j)}\right)^{\lceil k/2 \rceil}} \begin{cases} \mathbb{i}\, p_m^{(i,j)} M_m^{k_m} & k_m \text{ odd} \\ M_m^{k_m} & k_m \text{ even} \end{cases}$$

which is just the classic way of saying we sum over $\mathcal{P}(d)$, the set of partitions of permutations of the total order of the polynomial, to figure out what order polynomial we have in each dimension. Then for each order we sum over the ways to distribute these across the $V^{(a_n)}$ boxes. Finally, each order partition permutation gets the appropriate prefactor.

We'll probably want to show how to construct this whole deal via induction, but first we should look at the function

$$\begin{aligned} Z(k) &= \prod_{m=1}^{d} \frac{X_0^{(i,j)}}{\left(2\,\alpha_m^{(i,j)}\right)^{\lceil k/2 \rceil}} \begin{cases} \mathbb{i}\, p_m^{(i,j)} M_m^{k_m} & k_m \text{ odd} \\ M_m^{k_m} & k_m \text{ even} \end{cases} \\ &= \mathbb{i}^d (-1)^{z(k)-1}\, X_0^{(i,j)} \prod_{m=1}^{d} \frac{1}{\left(2\,\alpha_m^{(i,j)}\right)^{\lceil k_m/2 \rceil}} \sum_{n=0}^{\lfloor k_m/2 \rfloor} \mu_n^{k_m} \left(\frac{p_m^2}{2\,\alpha_m} \right)^n \end{aligned}$$

where $z(k)$ is the number of odd partitions in k and μ_n^k is given by

$$\begin{aligned} \mu_n^{(k)} &= \lceil k/2 \rceil \left(\mu_n^{(k-2)} - \frac{1}{2n - (-1)^k}\, \mu_{n-1}^{(k-2)} \right) \\ &= (-1)^n \left(\prod_{j=n+1}^{\lfloor k/2 \rfloor} 2j - (-1)^k \right) \binom{\lfloor k/2 \rfloor}{n} \end{aligned}$$

therefore we get a product of expansions in $p_m^2/2\,\alpha_m$ for each dimension

Next we'll note that for any $s\in\mathcal{D}(k)$, we can isolate the product of the form

$$\prod_{n=1}^{k_m} V_{b_n}^{(a_n)} L_m^{(i,j)\mathrm{T}}$$

where we WLOG chose n to start at 1

And so we have $\lfloor k_m/2 \rfloor$ terms like

$$\frac{\left(V_{b_{n_1}}^{(a_{n_1})} L_m^{(i,j)\mathrm{T}}\right)\left(V_{b_{n_2}}^{(a_{n_2})} L_m^{(i,j)\mathrm{T}}\right)}{2\,\alpha_m^{(i,j)}}$$

and if k_m is odd, one additional term of the form

$$\frac{\left(V_{b_{n_3}}^{a_{n_3}} L_m^{(i,j)\mathrm{T}}\right) p_m^{(i,j)}}{2\,\alpha_m^{(i,j)}}$$

and generically if we add up over all the appropriate m, the first of these turns into things of the form

$$\left(V^{(a_{n_1})}\,\Sigma^{(i,j)}\;V^{(a_{n_2})}\right)_{b_{n_1}\;b_{n_2}}$$

and the latter becomes

$$\left(V^{(a_{n_3})}\,\rho^{(i,j)}\right)_{b_{n_3}}$$

We might worry that we aren't adding over the correct set of m, but this fear is alleviated by considering that the μ_n weight the permutations appropriately once we consider the sum over s

This is tedious to show, but it becomes clear at least for the no momentum case when looking back at that 4th order integration from the Watson term

The other way to see this is to note that μ_0 always provides the number of partitions of the k_m elements into pairs

General Integral Form

Finally, the sign of the contribution will clearly depend on how many momentum terms we have, e.g. in the d=2 case we had

$$\left(V^{(1)}\Sigma^{(i,j)}\,V^{(2)}\right)_{nm} - \left(V^{(1)}\rho^{(i,j)}\right)_n\left(V^{(2)}\rho^{(i,j)}\right)_m$$

and similarly in the d=3 case by this argument we get

$$\begin{aligned}&\left(V^{(1)}\Sigma^{(i,j)}\,V^{(2)}\right)_{nm}\left(V^{(3)}\rho^{(i,j)}\right)_l\\ &\quad+\left(V^{(1)}\Sigma^{(i,j)}\,V^{(3)}\right)_{nl}\left(V^{(2)}\rho^{(i,j)}\right)_m\\ &\quad+\left(V^{(2)}\Sigma^{(i,j)}\,V^{(3)}\right)_{ml}\left(V^{(3)}\rho^{(i,j)}\right)_n\\ &\quad-\left(V^{(1)}\rho\right)_n\left(V^{(2)}\,\rho\right)_m\left(V^{(3)}\rho^{(i,j)}\right)_l\end{aligned}$$

which matches up with the form

In[337]:=

```
testMk[3]
```

Out[337]=

```
{3, -1}
```

and in the 4th order case we'll expect

In[338]:=

```
testMk[4]
```

Out[338]=

```
{3, -6, 1}
```

and when we enumerate this we get

$$
\begin{aligned}
&\left(V^{(1)}\Sigma^{(i,j)}V^{(2)}\right)_{nm}\left(V^{(3)}\Sigma^{(i,j)}V^{(4)}\right)_{uv}\\
&\quad+\left(V^{(1)}\Sigma^{(i,j)}V^{(3)}\right)_{nu}\left(V^{(2)}\Sigma^{(i,j)}V^{(4)}\right)_{mv}\\
&\quad+\left(V^{(1)}\Sigma^{(i,j)}V^{(4)}\right)_{nv}\left(V^{(2)}\Sigma^{(i,j)}V^{(3)}\right)_{mu}\\
&\quad-\left(V^{(1)}\Sigma^{(i,j)}V^{(2)}\right)_{nm}\left(V^{(3)}\rho^{(i,j)}\right)_{u}\left(V^{(4)}\rho^{(i,j)}\right)_{v}\\
&\quad-\left(V^{(1)}\Sigma^{(i,j)}V^{(3)}\right)_{nu}\left(V^{(2)}\rho^{(i,j)}\right)_{m}\left(V^{(4)}\rho^{(i,j)}\right)_{v}\\
&\quad-\left(V^{(1)}\Sigma^{(i,j)}V^{(4)}\right)_{nv}\left(V^{(2)}\rho^{(i,j)}\right)_{m}\left(V^{(3)}\rho^{(i,j)}\right)_{u}\\
&\quad-\left(V^{(2)}\Sigma^{(i,j)}V^{(3)}\right)_{mu}\left(V^{(1)}\rho^{(i,j)}\right)_{n}\left(V^{(4)}\rho^{(i,j)}\right)_{v}\\
&\quad-\left(V^{(2)}\Sigma^{(i,j)}V^{(4)}\right)_{mv}\left(V^{(1)}\rho^{(i,j)}\right)_{n}\left(V^{(3)}\rho^{(i,j)}\right)_{u}\\
&\quad-\left(V^{(3)}\Sigma^{(i,j)}V^{(4)}\right)_{uv}\left(V^{(1)}\rho^{(i,j)}\right)_{n}\left(V^{(2)}\rho^{(i,j)}\right)_{m}\\
&\quad+\left(V^{(1)}\rho\right)_{n}\left(V^{(2)}\rho\right)_{m}\left(V^{(3)}\rho^{(i,j)}\right)_{u}\left(V^{(4)}\rho^{(i,j)}\right)_{v}
\end{aligned}
$$

Generic Algorithm

Take all integer partitions of d with maximum element at most 2

In[339]:=

```
Select[IntegerPartitions[4], Max[#] ≤ 2 &]
```

Out[339]=

```
{{2, 2}, {2, 1, 1}, {1, 1, 1, 1}}
```

The sign of the contribution will depend on the length of the partition

These will be our "bucket sizes", we'll split the indices we have into these buckets

Finally, we'll do successive swaps between the buckets to get unique permutations. This final step is a bit tricky, but for $d \leq 6$ we can do it quickly as there are only $6! = 720$ possible permutations to filter over.

Implementation

Cubic Terms

Tests

General Term

For any term of the form

$$\int_{-\infty}^{\infty} \prod_n V_n^{(1)}\left(Q - \xi^{(i,j)}\right)$$

Old

Tensor Expression Generator

We need the ability to build expressions involving φ and γ, including Watson-term expressions

Setup

Differentiate

Evaluate

Tests

Matrix Elements

Overlaps

Dealt with above

Kinetic Terms

In[3036]:=

```
dQ[dQ[φ[j]]] // watSymm // Expand // ReplaceAll[{
     φ[j] → 1
    }] // watSimp // Expand // watFmt
```

Out[3036]=

$$(\Sigma^{(d)}\Delta\otimes\Sigma^{(d)}\Delta) - (\Sigma^{(d)}\Delta\otimes{\Sigma^{(j)}}^{-1}(Q - \xi^{(c)})) - i\, (\Sigma^{(d)}\Delta\otimes J^{(j)}) - ({\Sigma^{(j)}}^{-1}(Q - \xi^{(c)})\otimes\Sigma^{(d)}\Delta) + ({\Sigma^{(j)}}^{-1}(Q - \xi^{(c)})\otimes{\Sigma^{(j)}}^{-1}(Q - \xi^{(c)})) + i\, ({\Sigma^{(j)}}^{-1}(Q - \xi^{(c)})\otimes J^{(j)}) - i\, (J^{(j)}\otimes\Sigma^{(d)}\Delta) + i\, (J^{(j)}\otimes{\Sigma^{(j)}}^{-1}(Q - \xi^{(c)})) - (J^{(j)}\otimes J^{(j)}) - {\Sigma^{(j)}}^{-1}$$

In[3037]:=

```
evaledKTerms = dQ[dQ[φ[j]]] // watSymm // Expand // ReplaceAll[{
        φ[j] → 1
       }] // watSimp // Expand // groupOrders[#, Q[ξ[c]]] & // Map[
    Total@*Flatten@*Map[evaluateTerm[#, Q[ξ[c]], {m, m}] &]
   ] // Values // Total // Apply[List] // Total;
evaledKTerms // intFmt
```

Out[3038]=

$$[\Sigma^{(j)^{-1}}\Sigma^{(c)}\Sigma^{(j)^{-1}}]_{mm} - [\Sigma^{(j)^{-1}}\rho^{(c)}]_m[\Sigma^{(j)^{-1}}\rho^{(c)}]_m - 2\,\mathbb{i}\,[\Sigma^{(j)^{-1}}\rho^{(c)}]_m\,[\Sigma^{(d)}\Delta]_m - 2\,[\Sigma^{(j)^{-1}}\rho^{(c)}]_m\,[J^{(j)}]_m - [\Sigma^{(j)^{-1}}]_{mm} + [\Sigma^{(d)}\Delta\otimes\Sigma^{(d)}\Delta]_{mm} - \mathbb{i}\,[\Sigma^{(d)}\Delta\otimes J^{(j)}]_{mm} - \mathbb{i}\,[J^{(j)}\otimes\Sigma^{(d)}\Delta]_{mm} - [J^{(j)}\otimes J^{(j)}]_{mm}$$

Test

Simplification

The first simplification is a classic

$$\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,\Sigma^{(j)^{-1}} - \Sigma^{(j)^{-1}}\right) = -\left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1} \tag{7}$$

For the real component of the moment terms, we start with

$$\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)}\right)_m^2 + 2\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)}\right)J_m^{(j)} + \left(J_m^{(j)}\right)^2 = \left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)} + J_m^{(j)}\right)^2$$

then we can get the symmetry from this by noting that

$$\begin{aligned}\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)} + J^{(j)} &= J^{(i,j)} - \Sigma^{(i)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)} + J^{(j)}\\ &= \Sigma^{(i)^{-1}}\,\Sigma^{(c)}\,J^{(j,i)} + J^{(i)}\end{aligned}$$

and so to put this in an explicitly symmetric form we'll write this as

$$\frac{1}{2}\left(J^{(i)}+J^{(j)} + \left(\Sigma^{(j)^{-1}}-\Sigma^{(i)^{-1}}\right)\Sigma^{(c)}\,J^{(i,j)}\right)$$

The complex portion is given by

$$\Delta_m^{(i,j)}\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)}\right)_m + \Delta_m^{(i,j)}\left(J^{(j)}\right)_m = \Delta_m^{(i,j)}\left(\Sigma^{(j)^{-1}}\,\Sigma^{(c)}\,J^{(i,j)} + J^{(j)}\right)_m$$

and for exactly the same reason as above this will be anti-symmetric, since Δ is

So in total, letting

$$\begin{aligned}J^{+} &= J^{(i)}+J^{(j)}+\left(\Sigma^{(j)^{-1}} - \Sigma^{(i)^{-1}}\right)\Sigma^{(c)}\,J^{(i,j)}\\ \Sigma^{+} &= \left(\Sigma^{(i)}+\Sigma^{(j)}\right)^{-1}\end{aligned}$$

we get

$$T = \sum_k \frac{1}{m_k}\left((\Sigma^{+}\Delta\xi)_k^2 - \Sigma^{+}{}_{kk} - J_k^{+2} - \mathbb{i}(\Sigma^{+}\Delta\xi)_k\,J_k^{+}\right)$$

Old and Bad

Ugh

Coriolis

Computer Assisted Expressions

Simplification

Real Terms

We'll reduce this bit by bit, here's our set of terms to reduce over

```
GroupBy[jPTerms,
    Cases[#, _giMomEl, Infinity] &, Simplify@*Total] // Values //
  ReplaceAll[d → "+"] // Scan[intPrint]
```

$$-\left(\left[\xi^{(c)}\right]_m \left[\xi^{(c)}\right]_n+\left[\Sigma^{(c)}\right]_{n\,m}\right) \left[J^{(+)}\right]_u \left[J^{(+)}\right]_v$$

$$\left(\left(\left[\Sigma^{(+)}\,\Delta\right]_v \left[\xi^{(c)}\right]_n-\left[\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right]_{v\,n}\right) \left[J^{(+)}\right]_u+\left(\left[\Sigma^{(+)}\,\Delta\right]_u \left[\xi^{(c)}\right]_n+\left[\Sigma^{(c)}\,\Sigma^{(j)\,-1}\right]_{n\,u}\right) \left[J^{(+)}\right]_v\right) \left[\rho^{(c)}\right]_m$$

$$\left(\left(\left[\Sigma^{(+)}\,\Delta\right]_v \left[\xi^{(c)}\right]_m-\left[\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right]_{v\,m}\right) \left[J^{(+)}\right]_u+ \left(\left[\Sigma^{(+)}\,\Delta\right]_u \left[\xi^{(c)}\right]_m-\left[\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right]_{u\,m}\right) \left[J^{(+)}\right]_v+[\mathrm{I}]_{u\,m} \left[J^{(+)}\right]_v\right) \left[\rho^{(c)}\right]_n$$

$$\left(-\left[\Sigma^{(+)}\,\Delta\right]_u \left[\Sigma^{(+)}\,\Delta\right]_v+\left[J^{(+)}\right]_u \left[J^{(+)}\right]_v+\left[\Sigma^{(+)}\right]_{u\,v}\right) \left[\rho^{(c)}\right]_m \left[\rho^{(c)}\right]_n$$

Simps

We have two easy terms we can just read off

$$-\left(\Sigma^{(i,j)}+\xi\otimes\xi\right)_{nm} J^{(+)}_u J^{(+)}_v \tag{9}$$

$$\left(\Sigma^{(+)}-\Delta\otimes\Delta+J^{(+)}\otimes J^{(+)}\right)_{nm} \rho_u\,\rho_v \tag{10}$$

We also have all the permutations of terms of the form

$$\Delta_a\,\xi_b J^{(+)}_c\,\rho_d = \Delta_v\,\xi_n J^{(+)}_u\,\rho_m+\Delta_u\,\xi_n J^{(+)}_v\,\rho_m+\Delta_v\,\xi_m J^{(+)}_u\,\rho_n+\Delta_u\,\xi_m J^{(+)}_v\,\rho_n \tag{11}$$

all of which are symmetric due to the two flips from the Δ and ρ terms

Then we have a subtle one where we have

$$\left(\left(-\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{vn} J^{(+)}_u + \left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{nu} J^{(+)}_v\right)\rho_m$$

and we can write

$$\begin{aligned}\left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{nu} &= \left(I-\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{nu}\\ &\sim= -\left(\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{nu}\end{aligned}$$

since we have $n{=}u \Rightarrow \zeta_{nu}{=}0$

$$\left(-\left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{vn}\,J_u^{(+)}\,-\,\left(\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{nu}\,J_v^{(+)}\right)\rho_m$$

and then since ρ_m is anti-symmetric with respect to exchange of i and j, we need the interior term to be anti-symmetric too, but since we're summing over every possible n and u, we can swap them on just the right term, giving us

$$\left(\left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{un}\,J_v^{(+)}\,-\,\left(\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{vn}\,J_u^{(+)}\right)\rho_m \tag{12}$$

which respects the total symmetry of the system

Finally, we have

$$\left(-\left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{v\,m}\,J_u^{(+)}-\left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{u\,m}\,J_v^{(+)}+\mathrm{I}_{u\,m}\,\,{J^{(+)}}_v\right)\rho_n$$

and we will do basically the same trick as before, but now with

$$\begin{aligned}\left(I-\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{um} &= \left(\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{nu}\\ &\sim= \left(\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{nu}\end{aligned}$$

giving us

$$\left(\left(\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{um}J_v^{(+)}-\left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{vm}\,J_u^{(+)}\right)\rho_n \tag{13}$$

Giving us the total expression

$$\begin{aligned}&-\left(\Sigma^{(i,j)}+\xi\otimes\xi\right)_{nm}\,J_u^{(+)}\,J_v^{(+)}\\ &\quad+\,\left(\Sigma^{(+)}-\Delta\otimes\Delta+J^{(+)}\otimes J^{(+)}\right)_{nm}\rho_u\,\rho_v\\ &\quad+\,\left(\left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{un}J_v^{(+)}\,-\,\left(\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{vn}J_u^{(+)}\right)\rho_m\\ &\quad+\,\left(\left(\Sigma^{(i)-1}\,\Sigma^{(c)}\right)_{um}J_v^{(+)}\,-\,\left(\Sigma^{(j)\,-1}\,\Sigma^{(c)}\right)_{vm}J_u^{(+)}\right)\rho_n\\ &\quad+\,\Delta_v\,\xi_nJ_u^{(+)}\,\rho_m+\Delta_u\,\xi_nJ_v^{(+)}\,\rho_m+\Delta_v\,\xi_mJ_u^{(+)}\,\rho_n+\Delta_u\,\xi_mJ_v^{(+)}\,\rho_n\end{aligned} \tag{14}$$

Complex Terms

We'll automate two of the simplifications from before

In[3699]:=

```
imagJPTerms /. {
    giMatEl[{I̤ | I, Σ[j]}, {n, u}] :→ giMatEl[{Σ[i], I̤}, {u, n}],
    giMatEl[{Σ[j], I̤ | I}, {n, u}] → -giMatEl[{Σ[i], I̤}, {n, u}],

    giMatEl[{I̤ | I, Σ[j]}, {m, v}] :→ giMatEl[{Σ[i], I̤}, {v, m}],
    giMatEl[{I̤ | I, Σ[j]}, {v, m}] :→ -giMatEl[{Σ[i], I̤}, {v, m}],
    giMatEl[{Σ[j], I̤ | I}, {m, v}] → giMatEl[{Σ[i], I̤}, {v, m}],
    giMatEl[{Σ[j], I̤ | I}, {v, m}] → -giMatEl[{Σ[i], I̤}, {v, m}]
  } // GroupBy[#, Cases[#, _giMomEl, Infinity] &, Simplify@*Total] & //
 Scan[Scan[simpIntPrint]@*Apply[List]@*Distribute]
```

Term List

$i\,(\rho_m\,\rho_n - \xi_m\,\xi_n + \Sigma_{n\,m})\left(\Delta_u\,J^{(+)}_v + \Delta_v\,J^{(+)}_u\right)$

$i\left(\xi_n\left[\Sigma^{(j)\,-1}\,\Sigma\right]_{u\,m} - \xi_m\left[\Sigma^{(i)\,-1}\,\Sigma\right]_{u\,n}\right)J^{(+)}_v$

$i\left(\xi_m\left[\Sigma^{(j)\,-1}\,\Sigma\right]_{v\,n} - \xi_n\left[\Sigma^{(i)\,-1}\,\Sigma\right]_{v\,m}\right)J^{(+)}_u$

$i\,(\xi_n\,\rho_m + \xi_m\,\rho_n)\left(\Delta_u\,\Delta_v - J^{(+)}_u\,J^{(+)}_v - \Sigma^{(+)}_{u\,v}\right)$

$i\,\mathrm{I}_{u\,m}\left(\Delta_v\,\rho_n - J^{(+)}_v\,\xi_n\right)$

$i\left(\rho_m\left[\Sigma^{(i)-1}\,\Sigma\right]_{u\,n} - \rho_n\left[\Sigma^{(j)\,-1}\,\Sigma\right]_{u\,m}\right)\Delta_v$

$i\left(\rho_n\left[\Sigma^{(i)-1}\,\Sigma\right]_{v\,m} - \rho_m\left[\Sigma^{(j)\,-1}\,\Sigma\right]_{v\,n}\right)\Delta_u$

Terms

Test

A Note on Polynomial Evaluation

A Note on Alpha Choice

On a point-by-point basis for local quadratic expansions, assuming a diagonal Σ^{-1} matrix with diagonal elements $2\,\alpha_i$

$$H(\phi_i) = V\left(\xi^{(i)}\right) + \sum_k \frac{\alpha_k^{(i)}}{2\,m_k} + \frac{1}{4\,\alpha_k^{(i)}}\,\frac{\partial^2}{\partial {x_k}^2}\,V\left(\xi^{(i)}\right)$$

and if we want Virial to hold, letting $V\left(\xi^{(i)}\right) = 0 + V''\left(\xi^{(i)}\right)x^2$

$$\frac{\alpha_k^{(i)}}{2\, m_k} = \frac{1}{8\, \alpha_k^{(i)}} \frac{\partial^2}{\partial {x_k}^2} V\!\left(\xi^{(i)}\right)$$

and so

$$\begin{aligned} \alpha_k^{(i)} &= \frac{1}{4} \sqrt{m_k \frac{\partial^2}{\partial {x_k}^2} V\!\left(\xi^{(i)}\right)} \\ &= \frac{m_k\, \omega_k}{4} \end{aligned}$$

or expressed in local modes

$$\begin{aligned} \alpha_k^{(i)} &= \frac{1}{4} \sqrt{\frac{1}{g_{kk}} \frac{\partial^2}{\partial {x_k}^2} V\!\left(\xi^{(i)}\right)} \\ &= \frac{m_k\, \omega_k}{4} \end{aligned}$$

Evaluation of Properties

Our final wavefunctions are expressed as a linear combination of the DGB functions

$$\psi_n(\boldsymbol{x}) = \sum_i c_i^{(n)} \varphi_i(\boldsymbol{x})$$

Meaning we can apply the same ideas to evaluating properties that we used for integrating the potential.

Projections

Normal Mode Gaussians

Subindices in A Rotated Basis

Initializing Runs

Multi-Harmonic Basis

Polynomial Augmentation

Mass-Weighted Transformation

Morse Fits

Reduced Integrations

Multivariate Gaussian Quadrature

We start from the idea that we want to reduce an integral of the form

$$\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\, \Sigma^{-1}\, \boldsymbol{x}\right)}\, d\boldsymbol{x}$$

and want to express it as

$$\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\, \Sigma^{-1}\, \boldsymbol{x}\right)}\, d\boldsymbol{x} = N \int V(r)\, e^{-(\ldots)}\, d?$$

For this, we will note that we can write

$$r = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}$$

and therefore letting $\delta_c = c_1 - c_2$, we get what we want with

$$\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\, \Sigma^{-1}\, \boldsymbol{x}\right)}\, d\boldsymbol{x} = N \int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{\delta}^T\, \Sigma_\delta^{-1}\, \boldsymbol{\delta}\right)}\, d\boldsymbol{\delta}$$

and to do this, we just need to let

$$A = \begin{pmatrix} A_\delta \\ A_P \end{pmatrix}$$

where, e.g. in 3D

$$\begin{aligned} (A_\delta)_1 &= (1\ \ 0\ \ 0\ \ -1\ \ 0\ \ 0) \\ (A_P)_1 &= (1\ \ 0\ \ 0\ \ 1\ \ 0\ \ 0) \end{aligned}$$

Using this transformation we have

$$A^T\, \Sigma A = \begin{pmatrix} \Sigma_\delta & C \\ C^T & \Sigma_P \end{pmatrix}$$

Then we can integrate out the dependence on $\boldsymbol{p}$, writing

$$\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^T\, \Sigma^{-1}\, \boldsymbol{x}\right)}\, d\boldsymbol{x} = \int V(r)\, e^{-\frac{1}{2}\left([\boldsymbol{\delta}\ \boldsymbol{p}]^T \left(A^T\, \Sigma A\right)^{-1}\, [\boldsymbol{\delta}\ \boldsymbol{p}]\right)}\, d\boldsymbol{\delta}\, d\boldsymbol{p}$$

But this is just equivalent to taking the marginal distribution in $\boldsymbol{\delta}$ and multiplying by the integral over the $\boldsymbol{p}$ coordinates, which in fact means we only need to compute Σ_{δ}^{-1} and (once all normalization factors are accounted for) we get

$$
\begin{aligned}
\int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{x}^{T}\, \Sigma^{-1}\, \boldsymbol{x}\right)}\, d\boldsymbol{x} &= \sqrt{\frac{|2\pi\Sigma|}{|\pi\Sigma_{\delta}|}} \int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{\delta}^{T}\, \Sigma_{\delta}{}^{-1} \boldsymbol{\delta}\right)}\, d\boldsymbol{\delta} \\
&= \left(\sqrt{\pi^{(d-k)}\, \frac{|\Sigma|}{|\Sigma_{\delta}|}}\right) \int V(r)\, e^{-\frac{1}{2}\left(\boldsymbol{\delta}^{T}\, \Sigma_{\delta}{}^{-1} \boldsymbol{\delta}\right)}\, d\boldsymbol{\delta}
\end{aligned}
$$

When Factoring out the Overlap Element

Tests

Dealing with Watson Modes

When working with Gaussians constructed from Cartesian-displacement normal modes the approach above won't work as specified, since even though we have proper Gaussians in $(3N-6)$-dimensional normal modes space, we don't have them in proper $3N$ space as that would require a singular covariance matrix

The difficulty is then to figure out how many modes we can construct that *don't* change the bond length, this is equivalent to finding the set of solutions W such that

$$(L\,W_P)_1 = (L\,W_P)_2$$

where $(L\,W_P)_1$ is the $3{\times}(3N{-}6)$ matrix encoding how the Cartesian coordinates of atom 1 change and L_2 is the corresponding matrix for atom 2

This implies that

$$(L\,W_P)_1 - (L\,W_P)_2 = 0$$

but we also know that (using the A_δ from above)

$$
\begin{aligned}
(L\,W_P)_1 - (L\,W_P)_2 &= A_\delta\, L\, W_P \\
&= 0
\end{aligned}
$$

therefore W_P is simply a basis for the nullspace of $A_\delta\, L$ and the total transformation W_P we are truly interested

We can recognize now that this is equivalent to computing the SVD of $A_\delta\, L$ as

$$V\,S\,W = A_\delta\, L$$

where we will have k (up to 3) non-zero singular values corresponding to the columns of A that change the bond length (W_δ) and $3N{-}6{-}k$ columns of A that correspond to the dimensions that do not change the bond length (W_P)

Moreover, to actually determine how the bond lengths change, given a set of k displacements along these new modes, $\boldsymbol{q}$, we can note that we'll have an initial set of δ coordinates given by

$$\boldsymbol{\delta}_0 = A_\delta \boldsymbol{c}$$

where $\boldsymbol{c}$ is the vector of $3N$ coordinates and to get the change in these coordinates we simply note that the unit change is given by $A_\delta\, L W_\delta$ and so in total we have

$$r = |\boldsymbol{\delta}_0 + A_\delta\, L W_\delta \boldsymbol{q}|$$

and then to get derivatives with respect to the normal modes we start by writing $\boldsymbol{\delta} = A_\delta\, L W_\delta \boldsymbol{q}$ because we already have formulae for $\nabla_{\boldsymbol{\delta}^n} r$, and so we know

$$\begin{aligned}\nabla_{q^n} r &= \nabla_q \delta \odot^n \nabla_{\boldsymbol{\delta}^n} r \\ &= (A_\delta\, L W_\delta)^T \odot^n \nabla_{\boldsymbol{\delta}^n} r\end{aligned}$$

and then to get back to the normal mode derivatives we can write

$$\begin{aligned}\nabla_{l^n} r &= \nabla_L \delta \odot^n \nabla_{\boldsymbol{\delta}^n} r \\ &= \nabla_L q\, \nabla_q \delta \odot^n \nabla_{\boldsymbol{\delta}^n} r \\ &= W_\delta^{-1} (A_\delta\, L W_\delta)^T \odot^n \nabla_{\boldsymbol{\delta}^n} r \\ &= (A_\delta\, L)^T \odot^n \nabla_{\boldsymbol{\delta}^n} r\end{aligned}$$

which is actually something we could have known without needing the W_δ step but oh well...

Then to get what we really need,

$$\nabla_{l^n} f(r) = T([\nabla_l r, \nabla_{l^2} r, \ldots], [\nabla_r f, \nabla_{r^2} f, \ldots])$$

where T is just a standard tensor derivative conversion obtained by mapping out all of the necessary transformations

Alternate Derivative Issues

We really have

$$A_\delta\, L = \nabla_\delta q$$

but can we say

Angles

Angles are given by

$$\theta_{ijk} = \tan^{-1}\left(\frac{|a \times b|}{|a|\,|b|}, \frac{a \cdot b}{|a|\,|b|}\right) \text{ where } a = x_j - x_i \text{ and } b = x_k - x_i$$

Therefore to get a change we either need a change in $\hat{a}$ or $\hat{b}$, which means to *avoid* changing the bond length we need to either shift every coordinate by the same amount or we need to displace along $\hat{a}$ or $\hat{b}$, we can set up a simple basis for this by taking every possible vector we can think of that doesn't change the angle and orthogonalizing this, leading in general to a basis of about 5 vectors that don't change the angle

We can then project this basis *out* of the normal modes and compute the nullspace for this to find both the proper angle-changing modes and the corresponding complement

Generic Form

Tests

Gram-Schmidt Orthogonalized Gaussians

Given two distributed Gaussians, ϕ_1, ϕ_2 we can obviously orthogonalize this system by writing

$$\varphi_2 = \phi_2 - \langle \phi_1 | \phi_2 \rangle \, \phi_1$$

which has corresponding norm

$$\begin{aligned} \langle \varphi_2 | \varphi_2 \rangle &= \langle \phi_2 | \phi_2 \rangle - \langle \phi_1 | \phi_2 \rangle \langle \phi_1 | \phi_2 \rangle + \langle \phi_1 | \phi_2 \rangle - \langle \phi_1 | \phi_2 \rangle \langle \phi_1 | \phi_1 \rangle \\ &= 1 - \langle \phi_1 | \phi_2 \rangle^2 \end{aligned}$$

and then if we want to introduce a third Gaussian, ϕ_3, we can orthogonalize this relative to the initial set of Gaussians by writing

$$\varphi_3 = \phi_3 - \langle \phi_1 | \phi_3 \rangle \, \phi_1 - \langle \phi_2 | \phi_3 \rangle \, \phi_2$$

or we can orthogonalize relative the the new set by

$$\varphi_3 = \phi_3 - \langle \phi_1 | \phi_3 \rangle \, \phi_1 - \frac{\langle \varphi_2 | \phi_3 \rangle}{\langle \varphi_2 | \varphi_2 \rangle} \, \varphi_2$$

Partial Orthog Reduction

which almost orthogonal to φ_2, that being a simple linear combination of ϕ_1 and ϕ_2, therefore this has a norm given by (reduction done as I went)

$$\langle \varphi_3 | \varphi_3 \rangle = 1 - \langle \phi_1 | \phi_3 \rangle^2 - \langle \phi_2 | \phi_3 \rangle^2 + 2 \langle \phi_1 | \phi_3 \rangle \langle \phi_2 | \phi_3 \rangle \langle \phi_1 | \phi_2 \rangle$$

and introducing a n-th function, the orthogonalization is obvious but the normalization comes out to

$$\langle \varphi_3 | \varphi_3 \rangle = 1 - \sum_{i<4} \langle \phi_i | \phi_4 \rangle^2 + \sum_{j<4} \langle \phi_i | \phi_4 \rangle \sum_{i<4 \neq j} \langle \phi_j | \phi_4 \rangle \langle \phi_i | \phi_j \rangle$$

Full Orthog Reduction

and generically we can write this as

$$\varphi_k = \phi_k - \sum_{i=1}^{k-1} \left\langle \overline{\varphi_i} \middle| \phi_k \right\rangle \varphi_i$$

$$\left\langle \overline{\varphi_i} \middle| \phi_k \right\rangle = \frac{\left\langle \varphi_i \middle| \phi_k \right\rangle}{\left\langle \varphi_i \middle| \varphi_i \right\rangle}$$

which inductively is

$$\begin{aligned}
\varphi_1 &= \phi_1 \\
\varphi_2 &= \phi_2 - \left\langle \phi_1 \middle| \phi_2 \right\rangle \phi_1 \\
\varphi_3 &= \phi_3 - \left\langle \phi_1 \middle| \phi_3 \right\rangle \phi_1 - \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \varphi_2 \\
&= \phi_3 - \left\langle \phi_1 \middle| \phi_3 \right\rangle \phi_1 - \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \phi_2 + \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \left\langle \phi_1 \middle| \phi_2 \right\rangle \phi_1 \\
&= \phi_3 - \left(\left\langle \phi_1 \middle| \phi_3 \right\rangle + \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \left\langle \phi_1 \middle| \phi_2 \right\rangle \right) \phi_1 - \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \phi_2 \\
\varphi_4 &= \phi_4 - \left\langle \phi_1 \middle| \phi_4 \right\rangle \phi_1 - \left\langle \overline{\varphi_2} \middle| \phi_4 \right\rangle \varphi_2 - \left\langle \overline{\varphi_3} \middle| \phi_4 \right\rangle \varphi_3 \\
&= \phi_4 - \left(\left\langle \phi_1 \middle| \phi_3 \right\rangle + \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \left\langle \phi_1 \middle| \phi_2 \right\rangle \right) \phi_1 - \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \phi_2 \\
&\qquad - \left\langle \overline{\varphi_3} \middle| \phi_4 \right\rangle \left(\phi_3 - \left(\left\langle \phi_1 \middle| \phi_3 \right\rangle + \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \left\langle \phi_1 \middle| \phi_2 \right\rangle \right) \phi_1 - \left\langle \overline{\varphi_2} \middle| \phi_3 \right\rangle \phi_2 \right)
\end{aligned}$$

we'll note that we can also write

$$\begin{aligned}
\Gamma_k &= \phi_k - \sum_{i=1}^{k-1} \left\langle \phi_i \middle| \phi_k \right\rangle \phi_i \\
\varphi_k &= \Gamma_k - \sum_{i=1}^{k-1} \left\langle \overline{\Gamma_i} \middle| \phi_k \right\rangle \Gamma_i \\
&= \phi_k - \sum_{i=1}^{k-1} \left\langle \phi_i \middle| \phi_k \right\rangle \phi_i
\end{aligned}$$

Tests

Interpolations

The simplest treatment for the interpolation of the potential is the inverse-distance weighted interpolation, given by

$$V(x) = \frac{\sum_i V\left(\xi^{(i)}\right) \left| x - \xi^{(i)} \right|^{-p}}{\sum_i \left| x - \xi^{(i)} \right|^{-p}}$$

We will take advantage of the fact, however, that at every point we have a local quadratic expansion, i.e. we can write

$$V\left(x;\,\xi^{(i)}\right) = V\left(\xi^{(i)}\right) + \nabla_x V\left(\xi^{(i)}\right)\odot\left(x-\xi^{(i)}\right) + \frac{1}{2}\,\nabla_x V\left(\xi^{(i)}\right)\odot\left(x-\xi^{(i)}\right)^2$$

where $\odot$ is a total contraction and $\left(x-\xi^{(i)}\right)^2$ is the outer product of $\left(x-\xi^{(i)}\right)$ with itself.

Now we can do an inverse distance weighting of these Taylor series to give

$$V(x) = \frac{\sum_i V\left(x;\,\xi^{(i)}\right)\left|x-\xi^{(i)}\right|^{-p}}{\sum_i \left|x-\xi^{(i)}\right|^{-p}}$$

Derivatives

3rd Derivative Estimation

We can assume a Morse-like expansion along each mode to estimate the 3rd derivative at each interpolation point