Potential Derivatives Series Expansions

With these rules in place we can write code to do this differentiation automatically, but for performance reasons and to show the procedure out we'll do up to the fourth derivatives by hand

General Layout

We have basically two types of terms here:

$$\nabla_Q x = \begin{pmatrix} \frac{\partial x_1}{\partial Q_1} & \cdots & \frac{\partial x_n}{\partial Q_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial x_1}{\partial Q_m} & \cdots & \frac{\partial x_n}{\partial Q_m} \end{pmatrix}$$

which is the Jacobian going from Cartesian coordinates to internal coordinate normal modes. We will also have higher order Jacobian type things.

$$\nabla_x V = \begin{pmatrix} \frac{\partial}{\partial x_1} & \cdots & \frac{\partial}{\partial x_n} \end{pmatrix} V$$

which is the gradient of V with respect to the Cartesian coordinates. We'll also have higher order derivatives here.

I will denote higher derivatives by adding an exponent to the dependent variable, e.g.

$$\nabla_{Q^2} x = \left(\frac{\partial}{\partial Q_1} \begin{pmatrix} \frac{\partial x_1}{\partial Q_1} & \cdots & \frac{\partial x_n}{\partial Q_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial x_1}{\partial Q_m} & \cdots & \frac{\partial x_n}{\partial Q_m} \end{pmatrix} \cdots \frac{\partial}{\partial Q_m} \begin{pmatrix} \frac{\partial x_1}{\partial Q_1} & \cdots & \frac{\partial x_n}{\partial Q_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial x_1}{\partial Q_m} & \cdots & \frac{\partial x_n}{\partial Q_m} \end{pmatrix} \right) =$$

$$\left(\begin{pmatrix} \frac{\partial^2 x_1}{\partial Q_1 Q_1} & \cdots & \frac{\partial^2 x_n}{\partial Q_1 Q_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 x_1}{\partial Q_1 Q_m} & \cdots & \frac{\partial^2 x_n}{\partial Q_1 Q_m} \end{pmatrix} \cdots \begin{pmatrix} \frac{\partial^2 x_1}{\partial Q_m Q_1} & \cdots & \frac{\partial^2 x_n}{\partial Q_m Q_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 x_1}{\partial Q_m Q_m} & \cdots & \frac{\partial^2 x_n}{\partial Q_m Q_m} \end{pmatrix} \right)$$

is the 3D tensor of second derivatives of Cartesian coordinates with respect to pairs of internal coordinate normal modes.

Derivatives to Target

Basically we'll want

$$\nabla_Q V = \begin{pmatrix} \frac{\partial}{\partial Q_1} & \cdots & \frac{\partial}{\partial Q_m} \end{pmatrix} V$$

$$\nabla_{Q^2} V = \begin{pmatrix} \frac{\partial^2}{\partial Q_1 Q_1} V & \cdots & \frac{\partial^2}{\partial Q_1 Q_m} V \\ \vdots & \ddots & \vdots \\ \frac{\partial^2}{\partial Q_1 Q_m} V & \cdots & \frac{\partial^2}{\partial Q_m Q_m} V \end{pmatrix}$$

and higher up to order 4.

We don't actually have these directly, though, so we'll need to build them using the chain rule a bunch from the components we do have.

First Derivatives

We want

$$\nabla_Q V = \begin{pmatrix} \frac{\partial}{\partial Q_1} & \cdots & \frac{\partial}{\partial Q_m} \end{pmatrix} V$$

By applying the chain rule and noting that V is a function of the Cartesian coordinates (x)

$$\begin{aligned} \nabla_Q V &= \nabla_Q x \odot \nabla_x V \\ &= x_Q\, V_x \end{aligned}$$

Second Derivatives

Here we take

$$\begin{aligned} \nabla_{Q^2} V &= \nabla_Q (\nabla_Q V) \\ &= (x_Q\, V_x)_Q \end{aligned}$$

Recalling the product rule we have here and letting

$$\begin{aligned} A &= x_Q \\ B &= V_x \end{aligned}$$

$$\begin{aligned} (AB)_Q &= A_Q\, B + \left(A (B_Q)^{2:1}\right)^{2:1} \\ &= x_{Q^2}\, V_x + \left(x_Q ((V_x)_Q)^{2:1}\right)^{2:1} \\ &= x_{Q^2}\, V_x + \left(x_Q (x_Q\, V_{x^2})^{2:1}\right)^{2:1} \end{aligned}$$

we can then see that this second term can be reduced, keeping in mind that for **A**, **B** two-dimensional tensors,

$$(AB)^{2:1} = \left(B^{2:1}\, A^{2:1}\right)$$

as this is just a transposition, so we get

$$\left(x_Q (x_Q\, V_{x^2})^{2:1}\right)^{2:1} = \left(\left((x_Q\, V_{x^2})^{2:1}\right)^{2:1} x_Q{}^{2:1}\right)$$

$$=x_Q\, V_{x^2}\, {x_Q}^{2:1}$$

and so

$$V_{Q^2}=x_{Q^2}\, V_x+x_Q\, V_{x^2}\, {x_Q}^{2:1}$$

Validation (Redo)

We'll check this termwise

$$\begin{aligned}(x_{Q^2}\, V_x)_{ij}&=(x_{Q^2})_{ij:}\cdot V_x\\&=\left(\left(\frac{\partial^2 x_n}{\partial Q_i\,\partial Q_j}\right)_{n=1,\ldots,N}\right)\cdot\left(\left(\frac{\partial V}{\partial x_n}\right)_{n=1,\ldots,N}\right)\\&=\sum_{n=1}^{N}\frac{\partial V}{\partial x_n}\,\frac{\partial^2 x_n}{\partial Q_i\,\partial Q_j}\end{aligned}$$

$$\begin{aligned}\left(\left(x_Q(x_Q\, V_{x^2})^{2:1}\right)^{2:1}\right)_{ij}&=\left(x_Q(x_Q\, V_{x^2})^{2:1}\right)_{ji}\\&=(x_Q)_{j:}\cdot\left((x_Q\, V_{x^2})^{2:1}\right)_{:i}\\&=(x_Q)_{j:}\cdot(x_Q\, V_{x^2})_{i:}\\&=(x_Q)_{j:}\cdot((x_{Q_{i:}})\cdot V_{x^2})\\&=\left(\frac{\partial x_m}{\partial Q_j}\right)_m\cdot\left(\left(\frac{\partial x_n}{\partial Q_i}\right)_n\cdot\left(\frac{\partial^2 V}{\partial x_n\,\partial x_m}\right)_n\right)_m\\&=\sum_{n=1}^{N}\sum_{m=1}^{N}\frac{\partial x_m}{\partial Q_j}\,\frac{\partial x_n}{\partial Q_i}\,\frac{\partial^2 V}{\partial x_n\,\partial x_m}\end{aligned}$$

Put together

$$\nabla_{Q^2}V=\sum_{n=1}^{N}\frac{\partial V}{\partial x_n}\,\frac{\partial^2 x_n}{\partial Q_i\,\partial Q_j}+\sum_{n=1}^{N}\sum_{m=1}^{N}\frac{\partial x_m}{\partial Q_j}\,\frac{\partial x_n}{\partial Q_i}\,\frac{\partial^2 V}{\partial x_n\,\partial x_m}$$

Third Derivatives

$$\begin{aligned}V_{Q^3}&=\left(x_{Q^2}\, V_x+\left(x_Q(x_Q\, V_{x^2})^{2:1}\right)^{2:1}\right)_Q\\&=(x_{Q^2}\, V_x)_Q+\left(\left(x_Q(x_Q\, V_{x^2})^{2:1}\right)^{2:1}\right)_Q\\&=(x_{Q^2}\, V_x)_Q+\left(\left(x_Q(x_Q\, V_{x^2})^{2:1}\right)_Q\right)^{3:2}\end{aligned}$$

At this point we'll split into two terms. The first is pretty straightforward

$$\begin{aligned}(x_{Q^2}\, V_x)_Q&=x_{Q^3}\, V_x+\left(x_{Q^2}((V_x)_Q)^{2:1}\right)^{3:1}\\&=x_{Q^3}\, V_x+\left(x_{Q^2}(x_Q\, V_{x^2})^{2:1}\right)^{3:1}\end{aligned}$$

The second is more complicated so we'll use the procedure as before

$$\begin{aligned}A&=x_Q\\B&=(x_Q\, V_{x^2})^{2:1}\\(AB)_Q&=A_Q\, B+\left(A(B_Q)^{2:1}\right)^{a:1}\end{aligned}$$

$$
\begin{aligned}
&= x_{Q^2}(x_Q\, V_{x^2})^{2:1} + \left(x_Q\left(\left((x_Q\, V_{x^2})^{2:1}\right)_Q\right)^{2:1}\right)^{2:1} \\
\left(\left((x_Q\, V_{x^2})^{2:1}\right)_Q\right)^{2:1} &= \left((x_Q\, V_{x^2})_Q{}^{3:2}\right)^{2:1} \\
&= (x_Q\, V_{x^2})_Q{}^{3:1} \\
&= \left(x_{Q^2}\, V_{x^2} + \left(x_Q\left(V_{x^2 Q}\right)^{2:1}\right)^{2:1}\right)^{3:1} \\
&= (x_{Q^2}\, V_{x^2})^{3:1} + \left(\left(x_Q\left(V_{x^2 Q}\right)^{2:1}\right)^{2:1}\right)^{3:1} \\
&= (x_{Q^2}\, V_{x^2})^{3:1} + \left(x_Q\left(V_{x^2 Q}\right)^{2:1}\right)^{2:1,3:1} \\
&= (x_{Q^2}\, V_{x^2})^{3:1} + \left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1,3:1} \\
\left(x_Q\left(\left((x_Q\, V_{x^2})^{2:1}\right)_Q\right)^{2:1}\right)^{2:1} &= \left(x_Q\left((x_{Q^2}\, V_{x^2})^{3:1} + \left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1,3:1}\right)\right)^{2:1} \\
&= \left(x_Q(x_{Q^2}\, V_{x^2})^{3:1}\right)^{2:1} + \left(x_Q\left(\left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1,3:1}\right)\right)^{2:1}
\end{aligned}
$$

Then sticking these parts together we get

$$
V_{Q^3} = x_{Q^3}\, V_x + \left(x_{Q^2}(x_Q\, V_{x^2})^{2:1}\right)^{3:1} + x_{Q^2}(x_Q\, V_{x^2})^{2:1} + \left(x_Q(x_{Q^2}\, V_{x^2})^{3:1}\right)^{2:1} + \left(x_Q\left(\left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1,3:1}\right)\right)^{2:1}
$$

Intuitive Description

Ignoring the index jockeying, this is

$$
V_{Q^3} = x_{Q^3}\, V_x + x_{Q^2}\, x_Q\, V_{x^2} + x_{Q^2}\, x_Q\, V_{x^2} + x_Q\, x_{Q^2}\, V_{x^2} + x_Q\, x_Q\, x_Q\, V_{x^3}
$$

Simplification

We can reduce these terms

$$
\begin{aligned}
\left(x_{Q^2}(x_Q\, V_{x^2})^{2:1}\right)^{3:1} &= \left((x_Q\, V_{x^2})^{2:1}\right)^{2:1} x_{Q^2}{}^{3:1} \\
&= x_Q\, V_{x^2}\, x_{Q^2}{}^{3:1} \\
x_{Q^2}(x_Q\, V_{x^2})^{2:1} &= x_{Q^2}\, V_{x^2}{}^{2:1}\, x_Q{}^{2:1} \\
&= x_{Q^2}\, V_{x^2}\, x_Q{}^{2:1} \text{ (by symmetry)} \\
\left(x_Q(x_{Q^2}\, V_{x^2})^{3:1}\right)^{2:1} &= \left(x_Q\, V_{x^2}{}^{2:1}\, x_{Q^2}{}^{3:1}\right)^{2:1} \\
\left(x_Q\left(\left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1,3:1}\right)\right)^{2:1} &= \left(x_Q\left(\left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1}\right)^{3:1}\right)^{2:1} \\
\left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1} &= \left(x_Q\left(V_{x^3}{}^{1:3}\, x_Q{}^{2:1}\right)^{3:2}\right)^{2:1} \\
&= \left(\left(V_{x^3}{}^{1:3}\, x_Q{}^{2:1}\right)^{3:2,1:3} x_Q{}^{2:1}\right)^{3:2} \\
&= \left(\left(V_{x^3}{}^{1:3}\, x_Q{}^{2:1}\right)^{3:1} x_Q{}^{2:1}\right)^{3:2} \\
&= \left(x_Q\, V_{x^3}\, x_Q{}^{2:1}\right)^{3:2} \\
\left(\left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1}\right)^{3:1} &= \left(\left(x_Q\, V_{x^3}\, x_Q{}^{2:1}\right)^{3:2}\right)^{3:1} \\
&= \left(x_Q\, V_{x^3}\, x_Q{}^{2:1}\right)^{2:1} \\
\left(x_Q\left(\left(x_Q(x_Q\, V_{x^3})^{2:1}\right)^{2:1,3:1}\right)\right)^{2:1} &= \left(x_Q\left(x_Q\, V_{x^3}\, x_Q{}^{2:1}\right)^{2:1}\right)^{2:1} \\
&= \left(x_Q\, V_{x^3}\, x_Q{}^{2:1}\right)^{2:3} x_Q{}^{2:1}
\end{aligned}
$$

Yielding

$$V_{Q^3}=x_{Q^3}\,V_x+x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}+x_{Q^2}\,V_{x^2}\,{x_Q}^{2:1}+\left(x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}\right)^{2:1}+\left(x_Q\,V_{x^3}\,{x_Q}^{2:1}\right)^{2:3}{x_Q}^{2:1}$$

$(x_Q\,V_{x^3}\,{x_Q}^{2:1})^{2:3}\,{x_Q}^{2:1}$: dot(VQxx, xQ, xQ, axes=[[2, 1], [1, 1]])

Validation

We validate termwise

$$\begin{aligned}
(x_{Q^3}\,V_x)_{ijk} &= (x_{Q^3})_{ijk:}\cdot V_x\\
&= \sum_{n=1}^{N}\frac{\partial V}{\partial x_n}\,\frac{\partial^3 x_n}{\partial Q_i\,\partial Q_j\,\partial Q_k}\\
\left(x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}\right)_{ijk} &= (x_Q\,V_{x^2})_{i:}\,\left({x_{Q^2}}^{3:1}\right)_{:jk}\\
&= x_{Q_{i:}}\,V_{x^2::}\,x_{Q^2jk:}\\
&= \left(\left(\frac{\partial x_n}{\partial Q_i}\right)_n\cdot\left(\frac{\partial^2 V}{\partial x_n\,\partial x_m}\right)_n\right)_m\cdot\left(\frac{\partial^2 x_m}{\partial Q_j\,\partial Q_k}\right)_m\\
&= \sum_{n=1}^{N}\sum_{m=1}^{N}\frac{\partial^2 x_m}{\partial Q_j\,\partial Q_k}\,\frac{\partial x_n}{\partial Q_i}\,\frac{\partial^2 V}{\partial x_n\,\partial x_m}\\
\left(x_{Q^2}\,V_{x^2}\,{x_Q}^{2:1}\right)_{ijk} &= x_{Q^2ij:}\left(V_{x^2}\,{x_Q}^{2:1}\right)_{:k}\\
&= x_{Q^2ij:}\,V_{x^2::}\,\left({x_Q}^{2:1}\right)_{:k}\\
&= x_{Q^2ij:}\,V_{x^2::}\,x_{Qk:}\\
&= \left(\frac{\partial^2 x_m}{\partial Q_i\,\partial Q_j}\right)_m\cdot\left(\left(\frac{\partial x_n}{\partial Q_k}\right)_n\cdot\left(\frac{\partial^2 V}{\partial x_n\,\partial x_m}\right)_n\right)_m\\
&= \sum_{n=1}^{N}\sum_{m=1}^{N}\frac{\partial^2 x_m}{\partial Q_i\,\partial Q_j}\,\frac{\partial x_n}{\partial Q_k}\,\frac{\partial^2 V}{\partial x_n\,\partial x_m}\\
\left(\left(x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}\right)^{2:1}\right)_{ijk} &= \left(x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}\right)_{jik}\\
&= x_{Q_{j:}}\,V_{x^2::}\,x_{Q^2ik:}\\
&= \left(\left(\frac{\partial x_n}{\partial Q_j}\right)_n\cdot\left(\frac{\partial^2 V}{\partial x_n\,\partial x_m}\right)_n\right)_m\cdot\left(\frac{\partial^2 x_m}{\partial Q_i\,\partial Q_k}\right)_m\\
&= \sum_{n=1}^{N}\sum_{m=1}^{N}\frac{\partial^2 x_m}{\partial Q_i\,\partial Q_k}\,\frac{\partial x_n}{\partial Q_j}\,\frac{\partial^2 V}{\partial x_n\,\partial x_m}\\
\left(x_Q\left(x_Q\,V_{x^3}\,{x_Q}^{2:1}\right)^{2:1}\right)_{ijk} &= x_{Q_{i:}}\left(\left(x_Q\,V_{x^3}\,{x_Q}^{2:1}\right)^{2:1}\right)_{:jk}\\
&= x_{Q_{i:}}\left(x_Q\,V_{x^3}\,{x_Q}^{2:1}\right)_{j:k}\\
&= x_{Q_{i:}}\,x_{Q_{j:}}\,V_{x^3:::}\left({x_Q}^{2:1}\right)_{:k}\\
&= x_{Q_{i:}}\,x_{Q_{j:}}\,V_{x^3:::}\,x_{Q_{k:}}\\
&= x_{Q_{i:}}\,x_{Q_{j:}}\,x_{Q_{k:}}\,V_{x^3:::}\\
&= \left(\frac{\partial x_n}{\partial Q_i}\right)_n\cdot\left(\left(\frac{\partial x_m}{\partial Q_j}\right)_m\cdot\left(\left(\frac{\partial x_l}{\partial Q_k}\right)_l\cdot\left(\frac{\partial^3 V}{\partial x_n\,\partial x_m\,\partial x_l}\right)_l\right)_m\right)_n
\end{aligned}$$

$$=\sum_{n=1}^{N}\sum_{m=1}^{N}\sum_{l=1}^{N}\frac{\partial x_n}{\partial Q_i}\frac{\partial x_m}{\partial Q_j}\frac{\partial x_l}{\partial Q_k}\frac{\partial^3 V}{\partial x_l\,\partial x_m\,\partial x_l}$$

We can see this matches up with what we would expect to get

$$V_{Q^3}=\sum_{n=1}^{N}\frac{\partial V}{\partial x_n}\frac{\partial^3 x_n}{\partial Q_i\,\partial Q_j\,\partial Q_k}+$$
$$\sum_{n=1}^{N}\sum_{m=1}^{N}\frac{\partial^2 V}{\partial x_n\,\partial x_m}\left(\frac{\partial^2 x_m}{\partial Q_j\,\partial Q_k}+\frac{\partial^2 x_m}{\partial Q_i\,\partial Q_j}+\frac{\partial^2 x_m}{\partial Q_i\,\partial Q_k}\right)+\sum_{n=1}^{N}\sum_{m=1}^{N}\sum_{l=1}^{N}\frac{\partial^3 V}{\partial x_l\,\partial x_m\,\partial x_l}\frac{\partial x_n}{\partial Q_i}\frac{\partial x_m}{\partial Q_j}\frac{\partial x_l}{\partial Q_k}$$

Mixing Q and x

There are cases where we have $\nabla_Q(\nabla_{x^2} V) = V_{Q\,x^2} = x_Q\, V_{x^3}$ so we might want an expression that makes use of that, giving us

$$V_{Q^3}=x_{Q^3}\,V_x+x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}+x_{Q^2}\,V_{x^2}\,{x_Q}^{2:1}+\left(x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}\right)^{2:1}+\left(x_Q\,V_{x^3}\,{x_Q}^{2:1}\right)^{2:3}{x_Q}^{2:1}$$

Fourth Derivatives

We're going to have many, many terms to deal with here so we won't even bother to write out the entire expression but instead go term-wise from the start

Round 2

$$V_{Q^4}=\left(x_{Q^3}\,V_x+x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}+x_{Q^2}\,V_{x^2}\,{x_Q}^{2:1}+\left(x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}\right)^{2:1}+x_Q\left(x_Q\,V_{x^3}\,{x_Q}^{2:1}\right)^{2:1}\right)_Q$$

Terms

X Derivative

$$\begin{aligned}(x_{Q^3}\,V_x)_Q&=x_{Q^4}\,V_x+\left(x_{Q^3}((V_x)_Q)^{2:1}\right)^{4:1}\\&=x_{Q^4}\,V_x+\left(x_{Q^3}(x_Q\,V_{x^2})^{2:1}\right)^{4:1}\end{aligned}\tag{1}$$

First Term

$$\begin{aligned}\left(x_Q\,V_{x^2}\,{x_{Q^2}}^{3:1}\right)_Q&=x_{Q^2}\,V_{x^2}\,{x_{Q^2}}^{3:1}+\left(x_Q\left(\left(V_{x^2}\,{x_{Q^2}}^{3:1}\right)_Q\right)^{2:1}\right)^{2:1}\\&=x_{Q^2}\,V_{x^2}\,{x_{Q^2}}^{3:1}+\left(x_Q\left(x_Q\,V_{x^3}\,{x_{Q^2}}^{3:1}\right)^{2:1}\right)^{2:1}+\left(x_Q\left(\left(V_{x^2}\left({x_{Q^3}}^{4:2}\right)^{2:1}\right)^{3:1}\right)^{2:1}\right)^{2:1}\end{aligned}$$

we can then try to reduce the second and third terms

$$\begin{aligned}\left(x_Q\left(x_Q\,V_{x^3}\,{x_{Q^2}}^{3:1}\right)^{2:1}\right)^{2:1}&=\left(x_Q(x_Q\,V_{x^3})^{2:1}\right)^{2:1}{x_{Q^2}}^{3:1}\\&=\left(x_Q\,{V_{x^3}}^{2:3}\,{x_Q}^{2:1}\right)^{3:2}{x_{Q^2}}^{3:1}\\&=\left(x_Q\,V_{x^3}\,{x_Q}^{2:1}\right)^{3:2}{x_{Q^2}}^{3:1}\\&=x_Q\left(V_{x^3}\,{x_Q}^{2:1}\right)^{3:2}{x_{Q^2}}^{3:1}\end{aligned}$$

$$
\begin{aligned}
&= x_Q\left(x_Q V_{x^3}{}^{3:1}\right)^{2:1} x_{Q^2}{}^{3:1}\\
&= x_Q(x_Q V_{x^3})^{2:1} x_{Q^2}{}^{3:1}
\end{aligned}
$$

$$
\begin{aligned}
\left(x_Q\left(\left(V_{x^2}\left(x_{Q^3}{}^{4:2}\right)^{2:1}\right)^{3:1}\right)^{2:1}\right)^{2:1} &= \left(x_Q\left(V_{x^2}\left(x_{Q^3}{}^{4:2}\right)^{2:1}\right)^{3:1\,2:1}\right)^{2:1}\\
&= \left(x_Q\left(V_{x^2} x_{Q^3}{}^{4:1}\right)^{2:3}\right)^{2:1}\\
&= \left(x_Q V_{x^2} x_{Q^3}{}^{4:1\,2:3}\right)^{2:1}\\
&= \left(x_{Q^3} V_{x^2}{}^{2:1} x_Q{}^{2:1}\right)^{1:2,3:4}\\
&= \left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)^{1:2,3:4}
\end{aligned}
$$

so

$$\left(x_Q V_{x^2} x_{Q^2}{}^{3:1}\right)_Q = x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1} + x_Q(x_Q V_{x^3})^{2:1} x_{Q^2}{}^{3:1} + \left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)^{1:2,3:4} \tag{2}$$

Second Term

$$
\begin{aligned}
\left(x_{Q^2} V_{x^2} x_Q{}^{2:1}\right)_Q &= x_{Q^3} V_{x^2} x_Q{}^{2:1} + \left(x_{Q^2}\left(V_{x^2} x_Q{}^{2:1}\right)_Q{}^{2:1}\right)^{3:1}\\
&= x_{Q^3} V_{x^2} x_Q{}^{2:1} + \left(x_{Q^2}\left(x_Q V_{x^3} x_Q{}^{2:1}\right)^{2:1}\right)^{3:1} + \left(x_{Q^2}\left(V_{x^2} x_{Q^2}{}^{3:2\,2:1}\right)^{3:1\,2:1}\right)^{3:1}
\end{aligned}
$$

again, we'll reduce the terms

$$\left(x_{Q^2}\left(x_Q V_{x^3} x_Q{}^{2:1}\right)^{2:1}\right)^{3:1} = \left(x_{Q^2}\left(V_{x^3} x_Q{}^{2:1}\right)^{2:3} x_Q{}^{2:1}\right)^{4:1}$$

$$
\begin{aligned}
\left(x_{Q^2}\left(V_{x^2} x_{Q^2}{}^{3:2\,2:1}\right)^{3:1\,2:1}\right)^{3:1} &= \left(x_{Q^2}\left(V_{x^2} x_{Q^2}{}^{3:1}\right)^{2:3}\right)^{3:1}\\
&= \left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1,2:3}\right)^{3:1}\\
&= \left(x_{Q^2} V_{x^2}{}^{2:1} x_{Q^2}{}^{3:1}\right)^{1:4}\\
&= \left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1}\right)^{1:4}
\end{aligned}
$$

so

$$\left(x_{Q^2} V_{x^2} x_Q{}^{2:1}\right)_Q = x_{Q^3} V_{x^2} x_Q{}^{2:1} + \left(x_{Q^2}\left(V_{x^3} x_Q{}^{2:1}\right)^{2:3} x_Q{}^{2:1}\right)^{4:1} + \left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1}\right)^{1:4} \tag{3}$$

Third Term

This is basically the same as the first term but with an extra transposition

$$
\begin{aligned}
\left(\left(x_Q V_{x^2} x_{Q^2}{}^{3:1}\right)^{2:1}\right)_Q &= \left(x_Q V_{x^2} x_{Q^2}{}^{3:1}\right)_Q{}^{3:2}\\
&= \left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1} + \left(x_Q\left(x_Q V_{x^3} x_{Q^2}{}^{3:1}\right)^{2:1}\right)^{2:1} + \left(x_Q\left(\left(V_{x^2}\left(x_{Q^3}{}^{4:2}\right)^{2:1}\right)^{3:1}\right)^{2:1}\right)^{2:1}\right)^{3:2}
\end{aligned}
$$

then we can reuse the reductions from before

$$
\begin{aligned}
\left(\left(x_Q\left(x_Q V_{x^3} x_{Q^2}{}^{3:1}\right)^{2:1}\right)^{2:1}\right)^{3:2} &= \left(x_Q(x_Q V_{x^3})^{2:1} x_{Q^2}{}^{3:1}\right)^{3:2}\\
&= x_Q\left((x_Q V_{x^3})^{2:1} x_{Q^2}{}^{3:1}\right)^{3:2}
\end{aligned}
$$

$$\left(x_Q\left(\left(V_{x^2}\left(x_{Q^3}{}^{4:2}\right)^{2:1}\right)^{3:1}\right)^{2:1}\right)^{2:1\,3:2} = \left(\left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)^{1:2,3:4}\right)^{3:2}$$

$$=\left(x_{Q^3}\ V_{x^2}\ x_Q{}^{2:1}\right)^{1:2,4:2}$$

so

$$\left(\left(x_Q\ V_{x^2}\ x_{Q^2}{}^{3:1}\right)^{2:1}\right)_Q=\left(x_{Q^2}\ V_{x^2}\ x_{Q^2}{}^{3:1}\right)^{3:2}+x_Q\left((x_Q\ V_{x^3})^{2:1}\ x_{Q^2}{}^{3:1}\right)^{3:2}+\left(x_{Q^3}\ V_{x^2}\ x_Q{}^{2:1}\right)^{1:2,4:2} \tag{4}$$

Fourth Term

$$\begin{aligned}
\left(x_Q\left(x_Q\ V_{x^3}\ x_Q{}^{2:1}\right)^{2:1}\right)_Q&=x_{Q^2}\left(x_Q\ V_{x^3}\ x_Q{}^{2:1}\right)^{2:1}+\left(x_Q\left(\left(x_Q\ V_{x^3}\ x_Q{}^{2:1}\right)^{2:1}\right)_Q{}^{2:1}\right)^{2:1}\\
&=x_{Q^2}\left(x_Q\ V_{x^3}\ x_Q{}^{2:1}\right)^{2:1}+\left(x_Q\left(\left(x_Q\ V_{x^3}\ x_Q{}^{2:1}\right)_Q{}^{3:2}\right)^{2:1}\right)^{2:1}\\
\left(x_Q\ V_{x^3}\ x_Q{}^{2:1}\right)_Q&=x_{Q^2}\ V_{x^3}\ x_Q{}^{2:1}+\left(x_Q\left(V_{x^3}\ x_Q{}^{2:1}\right)_Q{}^{2:1}\right)^{2:1}\\
&=x_{Q^2}\ V_{x^3}\ x_Q{}^{2:1}+\left(x_Q\left(x_Q\ V_{x^4}\ x_Q{}^{2:1}\right)^{2:1}\right)^{2:1}+\left(x_Q\left(V_{x^3}\ x_{Q^2}{}^{3:2^{2:1}}\right)^{3:1^{2:1}}\right)^{2:1}\\
\left(x_Q\left(x_Q\ V_{x^3}\ x_Q{}^{2:1}\right)^{2:1}\right)_Q&=x_{Q^2}(x_Q\ V_{x^3}\ x_Q{}^{2:1})^{2:1}+\\
&\quad\left(x_Q(x_{Q^2}\ V_{x^3}\ x_Q{}^{2:1})^{3:2^{2:1}}\right)^{2:1}+\\
&\quad\left(x_Q\left(x_Q(x_Q\ V_{x^4}\ x_Q{}^{2:1})^{2:1}\right)^{2:1^{3:2^{2:1}}}\right)^{2:1}+\\
&\quad\left(x_Q\left(x_Q\left(V_{x^3}\ x_{Q^2}{}^{3:2^{2:1}}\right)^{3:1^{2:1}}\right)^{2:1^{3:2^{2:1}}}\right)^{2:1}
\end{aligned}$$

finally we'll try to reduce these

$$\begin{aligned}
\left(x_Q\left(x_{Q^2}\ V_{x^3}\ x_Q{}^{2:1}\right)^{3:2^{2:1}}\right)^{2:1}&=\left(x_Q\left(x_{Q^2}\ V_{x^3}\ x_Q{}^{2:1}\right)^{3:1}\right)^{2:1}\\
&=\left(x_Q(x_Q\ V_{x^3})^{2:1}\ x_{Q^2}{}^{3:1}\right)^{2:4,2:1}\\
\left(x_Q\left(x_Q\left(x_Q\ V_{x^4}\ x_Q{}^{2:1}\right)^{2:1}\right)^{2:1^{3:2^{2:1}}}\right)^{2:1}&=\left(x_Q\left(x_Q(x_Q\ V_{x^4})^{2:1}\right)^{1\leftrightarrow 3}\right)^{2:1}\ x_Q{}^{2:1}\\
&=\left(x_Q\left(x_Q\left(V_{x^4}{}^{2:4}\ x_Q{}^{2:1}\right)^{3:4}\right)^{2:1}\right)^{2:1}\ x_Q{}^{2:1}\\
\text{Hypothesis:}&\\
&=x_Q\left(x_Q\left(x_Q(x_Q\ V_{x^4})^{1:4}\right)^{1:4}\right)^{1:4}\\
\left(x_Q\left(x_Q\left(V_{x^3}\ x_{Q^2}{}^{3:2^{2:1}}\right)^{3:1^{2:1}}\right)^{2:1^{3:2^{2:1}}}\right)^{2:1}&=\left(x_Q\left(x_Q\ V_{x^3}\ x_{Q^2}{}^{3:1}\right)^{1:3}\right)^{2:1}
\end{aligned}$$

so

$$\begin{aligned}
\left(x_Q\left(x_Q\ V_{x^3}\ x_Q{}^{2:1}\right)^{2:1}\right)_Q=x_{Q^2}(x_Q\ V_{x^3}\ x_Q{}^{2:1})^{2:1}&+\\
\left(x_Q(x_Q\ V_{x^3})^{2:1}\ x_{Q^2}{}^{3:1}\right)^{2:4,2:1}&+\\
x_Q\left(x_Q\left(x_Q(x_Q\ V_{x^4})^{1:4}\right)^{1:4}\right)^{1:4}&+\\
\left(x_Q(x_Q\ V_{x^3}\ x_{Q^2}{}^{3:1})^{1:3}\right)^{2:1}&
\end{aligned} \tag{5}$$

Validation

We have a full 15 terms

V_x

$$(x_{Q^4} V_x)_{ijkl} = x_{Q^4 ijkl:} V_{x:} \tag{1}$$

V_{x^2}

$$\begin{aligned}\left(\left(x_{Q^3}(x_Q V_{x^2})^{2:1}\right)^{4:1}\right)_{ijkl} &= \left(x_{Q^3}(x_Q V_{x^2})^{2:1}\right)_{jkli} \\ &= x_{Q^3 jkl:}\left((x_Q V_{x^2})^{2:1}\right)_{:i} \\ &= x_{Q^3 jkl:}(x_Q V_{x^2})_{i:} \\ &= x_{Q^3 jkl:} V_{x^2 ::} x_{Q i:} \\ &= x_{Q i:} x_{Q^3 jkl:} V_{x^2}\end{aligned} \tag{2}$$

$$\begin{aligned}\left(\left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)^{1:2,4:2}\right)_{ijkl} &= \left(\left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)^{1:2}\right)_{iklj} \\ &= \left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)_{kilj} \\ &= x_{Q^3 kil:} V_{x^2 ::} x_{Q j:} \\ &= x_{Q j:} x_{Q^3 kil:} V_{x^2}\end{aligned} \tag{3}$$

$$\begin{aligned}\left(\left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)^{1:2,3:4}\right)_{ijkl} &= \left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)_{jilk} \\ &= x_{Q^3 jil:} V_{x^2 ::}\left(x_Q{}^{2:1}\right)_{:k} \\ &= x_{Q^3 jil:} V_{x^2 ::} x_{Q k:} \\ &= x_{Q k:} x_{Q^3 jil:} V_{x^2}\end{aligned} \tag{4}$$

$$\begin{aligned}\left(x_{Q^3} V_{x^2} x_Q{}^{2:1}\right)_{ijkl} &= x_{Q^3 ijk:} V_{x^2 ::}\left(x_Q{}^{2:1}\right)_{:l} \\ &= x_{Q^3 ijk:} V_{x^2 ::} x_{Q l:} \\ &= x_{Q l:} x_{Q^3 ijk:} V_{x^2}\end{aligned} \tag{5}$$

$$\begin{aligned}\left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1}\right)_{ijkl} &= x_{Q^2 ij:} V_{x^2 ::} x_{Q^2 kl:} \\ &= x_{Q^2 ij:} x_{Q^2 kl:} V_{x^2}\end{aligned} \tag{6}$$

$$\begin{aligned}\left(\left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1}\right)^{3:2}\right)_{ijkl} &= \left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1}\right)_{ikjl} \\ &= x_{Q^2 ik:} V_{x^2 ::} x_{Q^2 jl:} \\ &= x_{Q^2 ik:} x_{Q^2 jl:} V_{x^2}\end{aligned} \tag{7}$$

$$\begin{aligned}\left(\left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1}\right)^{1:4}\right)_{ijkl} &= \left(x_{Q^2} V_{x^2} x_{Q^2}{}^{3:1}\right)_{lijk} \\ &= x_{Q^2 li:} V_{x^2 ::} x_{Q^2 jk:} \\ &= x_{Q^2 jk:} x_{Q^2 li:} V_{x^2}\end{aligned} \tag{8}$$

V_{x^3}

$$
\begin{aligned}
\left(x_Q (x_Q\, V_{x^3})^{2:1}\, {x_{Q^2}}^{3:1}\right)_{ijkl} &= x_{Q_{i:}} \left((x_Q\, V_{x^3})^{2:1}\right)_{:j:} \left({x_{Q^2}}^{3:1}\right)_{:kl} \\
&= x_{Q_{i:}} (x_Q\, V_{x^3})_{j::}\, x_{Q^2 kl:} \\
&= x_{Q_{i:}}\, x_{Q_{j:}}\, V_{x^3}\, x_{Q^2 kl:} \\
&= x_{Q_{i:}}\, x_{Q_{j:}}\, x_{Q^2 kl:}\, V_{x^3}
\end{aligned} \tag{9}
$$

$$
\begin{aligned}
\left(x_Q \left((x_Q\, V_{x^3})^{2:1}\, {x_{Q^2}}^{3:1}\right)^{3:2}\right)_{ijkl} &= x_{Q_{i:}} \left(\left((x_Q\, V_{x^3})^{2:1}\, {x_{Q^2}}^{3:1}\right)^{3:2}\right)_{:jkl} \\
&= x_{Q_{i:}} \left((x_Q\, V_{x^3})^{2:1}\, {x_{Q^2}}^{3:1}\right)_{:kjl} \\
&= x_{Q_{i:}} \left((x_Q\, V_{x^3})^{2:1}\right)_{:k:}\, x_{Q^2 :jl} \\
&= x_{Q_{i:}}\, x_{Q_{k:}}\, V_{x^3 :::} \\
&= x_{Q_{i:}}\, x_{Q_{k:}}\, x_{Q^2 :jl}\, V_{x^3}
\end{aligned} \tag{10}
$$

$$
\begin{aligned}
\left(\left(x_{Q^2} \left(V_{x^3}\, {x_Q}^{2:1}\right)^{3:4}\, {x_Q}^{2:1}\right)^{4:1}\right)_{ijkl} &= \left(x_{Q^2} \left(V_{x^3}\, {x_Q}^{2:1}\right)^{2:3}\, {x_Q}^{2:1}\right)_{jkli} \\
&= x_{Q^2 jk:} \left(\left(V_{x^3}\, {x_Q}^{2:1}\right)^{2:3}\right)_{:l:}\, x_{Q_{i:}} \\
&= x_{Q^2 jk:} \left(V_{x^3}\, {x_Q}^{2:1}\right)_{::l}\, x_{Q_{i:}} \\
&= x_{Q_{i:}}\, x_{Q_{l:}}\, x_{Q^2 jk:}\, V_{x^3}
\end{aligned} \tag{11}
$$

$$
\begin{aligned}
\left(\left(x_Q \left(x_Q\, V_{x^3}\, {x_{Q^2}}^{3:1}\right)^{1:3}\right)^{2:1}\right)_{ijkl} &= \left(x_Q \left(x_Q\, V_{x^3}\, {x_{Q^2}}^{3:1}\right)^{1:3}\right)_{jikl} \\
&= x_{Q_{j:}} \left(\left(x_Q\, V_{x^3}\, {x_{Q^2}}^{3:1}\right)^{1:3}\right)_{:ikl} \\
&= x_{Q_{j:}} \left(x_Q\, V_{x^3}\, {x_{Q^2}}^{3:1}\right)_{k:il} \\
&= x_{Q_{j:}}\, x_{Q_{k:}}\, V_{x^3 :::}\, x_{Q^2 il:} \\
&= x_{Q_{j:}}\, x_{Q_{k:}}\, x_{Q^2 il:}\, V_{x^3}
\end{aligned} \tag{12}
$$

$$
\begin{aligned}
\left(\left(x_Q (x_Q\, V_{x^3})^{2:1}\, {x_{Q^2}}^{3:1}\right)^{2:4,2:1}\right)_{ijkl} &= \left(x_Q (x_Q\, V_{x^3})^{2:1}\, {x_{Q^2}}^{3:1}\right)_{jlik} \\
&= x_{Q_{j:}}\, x_{Q_{l:}}\, V_{x^3}\, x_{Q^2 ik:}
\end{aligned} \tag{13}
$$

$$
\begin{aligned}
\left(x_{Q^2} \left(x_Q\, V_{x^3}\, {x_Q}^{2:1}\right)^{2:1}\right)_{ijkl} &= x_{Q^2 ij:} \left(x_Q\, V_{x^3}\, {x_Q}^{2:1}\right)_{k:l} \\
&= x_{Q_{k:}}\, x_{Q_{l:}}\, x_{Q^2 ij:}\, V_{x^3}
\end{aligned} \tag{14}
$$

V_{x^4}

$$
\begin{aligned}
\left(x_Q \left(x_Q \left(x_Q (x_Q\, V_{x^4})^{1:4}\right)^{1:4}\right)^{1:4}\right)_{ijkl} &= x_{Q_{i:}} \left(\left(x_Q \left(x_Q (x_Q\, V_{x^4})^{1:4}\right)^{1:4}\right)^{1:4}\right)_{:jkl} \\
&= x_{Q_{i:}}\, x_{Q_{l:}} \left(\left(x_Q (x_Q\, V_{x^4})^{1:4}\right)^{1:4}\right)_{::jk} \\
&= x_{Q_{i:}}\, x_{Q_{l:}}\, x_{Q_{k:}} \left((x_Q\, V_{x^4})^{1:4}\right)_{:::j} \\
&= x_{Q_{i:}}\, x_{Q_{l:}}\, x_{Q_{k:}}\, x_{Q_{j:}}\, V_{x^4 ::::} \\
&= x_{Q_{i:}}\, x_{Q_{j:}}\, x_{Q_{k:}}\, x_{Q_{l:}}\, V_{x^4}
\end{aligned} \tag{15}
$$

Mixing Q and x

Here we have both $V_{Q\,x^2} = x_Q\, V_3$ and $V_{Q^2\,x^2} = x_Q (x_Q\, V_{x^4})^{1:2}$ which gives us new term expressions

$$(x_{Q^3}\ V_x)_Q = x_{Q^4}\ V_x + \left(x_{Q^3}(x_Q\ V_{x^2})^{2:1}\right)^{4:1} \tag{1}$$

$$\left(x_Q\ V_{x^2}\ {x_{Q^2}}^{3:1}\right)_Q = x_{Q^2}\ V_{x^2}\ {x_{Q^2}}^{3:1} + x_Q(V_{Q\ x^2})^{2:1}\ {x_{Q^2}}^{3:1} + \left(x_{Q^3}\ V_{x^2}\ {x_Q}^{2:1}\right)^{1:2,3:4} \tag{2}$$

$$\left(x_{Q^2}\ V_{x^2}\ {x_Q}^{2:1}\right)_Q = x_{Q^3}\ V_{x^2}\ {x_Q}^{2:1} + \left(x_{Q^2}\ {V_{Q\ x^2}}^{1:2}\ {x_Q}^{2:1}\right)^{4:1} + \left(x_{Q^2}\ V_{x^2}\ {x_{Q^2}}^{3:1}\right)^{1:4} \tag{3}$$

$$\left(\left(x_Q\ V_{x^2}\ {x_{Q^2}}^{3:1}\right)^{2:1}\right)_Q = \left(x_{Q^2}\ V_{x^2}\ {x_{Q^2}}^{3:1}\right)^{3:2} + x_Q\left({V_{Q\ x^2}}^{2:1}\ {x_{Q^2}}^{3:1}\right)^{3:2} + \left(x_{Q^3}\ V_{x^2}\ {x_Q}^{2:1}\right)^{1:2,4:2} \tag{4}$$

$$\begin{aligned}\left(x_Q\left(x_Q\ V_{x^3}\ {x_Q}^{2:1}\right)^{2:1}\right)_Q = {} & x_{Q^2}(V_{Q\ x^2}\ {x_Q}^{2:1})^{2:1} + \\ & \left(x_Q\ {V_{Q\ x^2}}^{2:1}\ {x_{Q^2}}^{3:1}\right)^{2:4,2:1} + \\ & x_Q\left(x_Q\ {V_{Q^2\ x^2}}^{1:4}\right)^{1:4} + \\ & \left(x_Q(V_{Q\ x^2}\ {x_{Q^2}}^{3:1})^{1:3}\right)^{2:1}\end{aligned} \tag{5}$$

We need to keep in mind that we're working with things that are still functions of x

Termwise Expansion

We can also ask for this in terms of its diagonal elements, i.e.

$$(V_{Q^4})_{ii} = \partial_{x_i}(V_{Q^3})_i$$

This will allow us to construct the elements of the tensors that we need in a more targeted fashion. First off, then

$$\begin{aligned}(V_{Q^3})_i = {} & \left(x_{Q^3}\ V_x + x_Q\ V_{x^2}\ {x_{Q^2}}^{3:1} + x_{Q^2}\ V_{x^2}\ {x_Q}^{2:1} + \left(x_Q\ V_{x^2}\ {x_{Q^2}}^{3:1}\right)^{2:1} + x_Q\left(x_Q\ V_{x^3}\ {x_Q}^{2:1}\right)^{2:1}\right)_i \\ = {} & (x_{Q^3}\ V_x)_i + \\ & (x_Q\ V_{x^2}\ {x_{Q^2}}^{3:1})_i + \\ & (x_{Q^2}\ V_{x^2}\ {x_Q}^{2:1})_i + \\ & \left((x_Q\ V_{x^2}\ {x_{Q^2}}^{3:1})^{2:1}\right)_i + \\ & \left(x_Q(x_Q\ V_{x^3}\ {x_Q}^{2:1})^{2:1}\right)_i \\ = {} & x_{{Q^3}_i}\ V_x + \\ & x_{Q_i}\ V_{x^2}\ {x_{Q^2}}^{3:1} + \\ & x_{{Q^2}_i}\ V_{x^2}\ {x_Q}^{2:1} + \\ & x_Q\ V_{{x^2}_i}\ {x_{Q^2}}^{3:1} + \\ & x_{Q_i}(x_Q\ V_{x^3}\ {x_Q}^{2:1})^{2:1}\end{aligned}$$

(This too might be helpful if we're very space constrained and even 3D tensors are hard to store)

Then we can apply the plain univariate derivative to this

$$
\begin{aligned}
\partial_{Q_i}(V_{Q^3})_i = {} & \partial_{Q_i}\left(x_{Q^3 i}\, V_x\right) + \\
& \partial_{Q_i}(x_{Q i}\, V_{x^2}\, {x_{Q^2}}^{3:1}) + \\
& \partial_{Q_i}\left(x_{Q^2 i}\, V_{x^2}\, {x_Q}^{2:1}\right) + \\
& \partial_{Q_i}(x_Q\, V_{x^2 i}\, {x_{Q^2}}^{3:1}) + \\
& \partial_{Q_i}\left(x_{Q_i}(x_Q\, V_{x^3}\, {x_Q}^{2:1})^{2:1}\right) \\
= {} & \partial_{Q_i} x_{Q^3 i}\, V_x + x_{Q^3 i}\, \partial_{Q_i} V_x + \\
& \partial_{Q_i} x_{Q i}\, V_{x^2}\, {x_{Q^2}}^{3:1} + x_{Q i}\, \partial_{Q_i} V_{x^2}\, {x_{Q^2}}^{3:1} + x_{Q i}\, V_{x^2}\, \partial_{Q_i} {x_{Q^2}}^{3:1} + \\
& \partial_{Q_i} x_{Q^2 i}\, V_{x^2}\, {x_Q}^{2:1} + x_{Q^2 i}\, \partial_{Q_i} V_{x^2}\, {x_Q}^{2:1} + x_{Q^2 i}\, V_{x^2}\, \partial_{Q_i} {x_Q}^{2:1} + \\
& \partial_{Q_i} x_Q\, V_{x^2 i}\, {x_{Q^2}}^{3:1} + x_Q\, \partial_{Q_i} V_{x^2 i}\, {x_{Q^2}}^{3:1} + x_Q\, V_{x^2 i}\, \partial_{Q_i} {x_{Q^2}}^{3:1} + \\
& \partial_{Q_i} x_{Q_i}(x_Q\, V_{x^3}\, {x_Q}^{2:1})^{2:1} + x_{Q_i}(\partial_{Q_i} x_Q\, V_{x^3}\, {x_Q}^{2:1})^{2:1} + \\
& \quad x_{Q_i}(x_Q\, \partial_{Q_i} V_{x^3}\, {x_Q}^{2:1})^{2:1} + x_{Q_i}(x_Q\, V_{x^3}\, \partial_{Q_i} {x_Q}^{2:1})^{2:1} \\
= {} & x_{Q^4 ii}\, V_x + x_{Q^3 i}\, x_{Q i}\, V_{x^2} + \\
& x_{Q^2 ii}\, V_{x^2}\, {x_{Q^2}}^{3:1} + x_{Q i}\, x_{Q i}\, V_{x^3}\, {x_{Q^2}}^{3:1} + x_{Q i}\, V_{x^2}\, {x_{Q^3 i}}^{3:1} + \\
& x_{Q^3 ii}\, V_{x^2}\, {x_Q}^{2:1} + x_{Q^2 i}\, x_{Q i}\, V_{x^2}\, {x_Q}^{2:1} + x_{Q^2 i}\, V_{x^2}\, {x_{Q^2 i}}^{2:1} + \\
& x_{Q^2 i}\, V_{x^2 i}\, {x_{Q^2}}^{3:1} + x_Q\, x_{Q i}\, V_{x^3 i}\, {x_{Q^2}}^{3:1} + x_Q\, V_{x^2 i}\, {x_{Q^3 i}}^{3:1} + \\
& x_{Q^2 ii}(x_Q\, V_{x^3}\, {x_Q}^{2:1})^{2:1} + x_{Q_i}\left(x_{Q^2 i}\, V_{x^3}\, {x_Q}^{2:1}\right)^{2:1} + \\
& \quad x_{Q_i}(x_Q\, x_{Q i}\, V_{x^4}\, {x_Q}^{2:1})^{2:1} + x_{Q_i}\left(x_Q\, V_{x^3}\, {x_{Q^2 i}}^{2:1}\right)^{2:1}
\end{aligned}
$$

Implementation

We'll provide a sample python implementation of this. Note that I didn't follow all the orderings directly since we can contract along axes that aren't the major ones and thus need fewer flips and things.

```
def get_derivs(x_derivs, V_derivs, mixed_XQ=False):
    """
    Returns the derivative tensors of the potential with respect to the normal modes
    (note that this is fully general and the "cartesians" and "normal modes" can be any coo

    :param x_derivs: The derivatives of the cartesians with respect to the normal modes
    :type x_derivs:
    :param V_derivs: The derivative of the potential with respect to the cartesians
    :type V_derivs:
    :param mixed_XQ: Whether the v_derivs[2] = V_Qxx and v_derivs[3] = V_QQxx or not
    :type mixed_XQ: bool
    """
    import numpy as np, functools as fp

    def dot(*t, axes=None):
```

```
  """
  Flexible tensordot
  """

  if len(t) == 1:
    return t[0]

  if any(isinstance(x, int) for x in t):
    return 0

  tdot = lambda a, b, **kw: (a.tensordot(b, **kw) if hasattr(a, "tensordot") else np.te
  td = lambda a, b: (0 if isinstance(a, int) or isinstance(b[0], int) else tdot(a, b[0]
  if axes is None:
    axes = [1] * (len(t)-1)

  return fp.reduce(td, zip(t[1:], axes), t[0])

def shift(a, *s):
  if isinstance(a, int):
    return a
  def shift_inds(n, i, j):
    if i<j:
        x = list(range(i)) + list(range(i+1, j+1)) + [i] + list(range(j+1, n))
    else:
        x = list(range(j)) + [i] + list(range(j, i)) + list(range(i+1, n))
    return x
  shiftIJ = lambda a, ij: np.transpose(a, shift_inds(a.ndim, *ij))
  return fp.reduce(shiftIJ, s, a)


# First Derivs
xQ = x_derivs[0]
Vx = V_derivs[0]
V_Q = dot(xQ, Vx)

# Second Derivs
xQQ = x_derivs[1]
Vxx = V_derivs[1]

xQ_Vxx = dot(xQ, Vxx)
V_QQ = dot(xQQ, Vx) + dot(xQ_Vxx, xQ)

# Third Derivs
xQQQ = x_derivs[2]
Vxxx = V_derivs[2]

xQQ_Vxx = dot(xQQ, Vxx)

V_QQQ_1 = dot(xQQQ, Vx)
V_QQQ_2 = dot(xQ_Vxx, xQQ, axes=[[-1, -1]])
V_QQQ_3 = dot(xQQ_Vxx, xQ, axes=[[-1, -1]])
V_QQQ_4 = shift(V_QQQ_2, (1, 0))

if not mixed_XQ:
    VQxx = dot(xQ, Vxxx)
```

```
else:
    VQxx = Vxxx

V_QQQ_5 = dot(xQ, VQxx, xQ, axes=[[-1, -1], [-1, -1]])

V_QQQ = (
        V_QQQ_1 +
        V_QQQ_2 +
        V_QQQ_3 +
        V_QQQ_4 +
        V_QQQ_5
)

# Fourth Derivs
# For now we'll just generate everything rather than being particularly clever about it

xQQQQ = x_derivs[3]
Vxxxx = V_derivs[3]
V_QQQQ_1 = dot(xQQQQ, Vx) + dot(xQ, Vxx, xQQQ, axes=[[-1, 0], [-1, -1]])

xQQQ_Vxx_xQ = dot(xQQQ, Vxx, xQ, axes=[[-1, 0], [-1, -1]])
xQ_22_Vxxx = dot(xQ, Vxxx, axes=[[-1, 1]])
xQQ_Vxx_xQQ = dot(xQQ_Vxx, xQQ, axes=[[-1, -1]])
V_QQQQ_2 = (
        xQQ_Vxx_xQQ +
        dot(xQ_22_Vxxx, xQ, xQQ, axes=[[0, -1], [1, -1]]) +
        shift(xQQQ_Vxx_xQ, (0, 1), (2, 3))
)

V_QQQQ_3 = (
        xQQQ_Vxx_xQ +
        dot(xQ_22_Vxxx, xQQ, xQ, axes=[[0, 2], [1, 1]]) +
        shift(xQQ_Vxx_xQQ, (0, 3))
)

V_QQQQ_4 = (
        shift(xQQ_Vxx_xQQ, (1, 2)) +
        shift(dot(xQ, VQxx, xQQ, axes=[[1, 1], [2, 2]]), (2, 3)) +
        shift(xQQQ_Vxx_xQ, (0, 1), (3, 1))
)

if not mixed_XQ:
    VQQxx = dot(xQ, dot(xQ, Vxxxx), axes=[[1, 1]])
else:
    VQQxx = Vxxxx

V_QQQQ_5 = (
        dot(xQQ, VQxx, xQ, axes=[[2, 1], [3, 1]]) +
        shift(dot(xQQ, VQxx, xQ, axes=[[2, 2], [2, 1]]), (3, 1)) +
        shift(dot(xQ, VQxx, xQQ, axes=[[1, 1], [2, 2]]), (2, 0)) +
        dot(VQQxx, xQ, xQ, axes=[[2, 1], [2, 1]])
)

V_QQQQ = (
        V_QQQQ_1 +
```

```
        V_QQQQ_2 +
        V_QQQQ_3 +
        V_QQQQ_4 +
        V_QQQQ_5
)

return V_Q, V_QQ, V_QQQ, V_QQQQ
```