# Record of Things I Know - Taylor Expansions

Cris Cecka

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## 1 Cartesian Taylor Expansions

Consider a translation-invariant function of one $d$-dimensional vector:

$$f(\mathbf{r}_{ij}) = f(\mathbf{r}_i - \mathbf{r}_j)$$

Decomposing the vector $\mathbf{r}_{ij}$ into parts

$$\begin{aligned}
\mathbf{r}_{ij} &= \mathbf{r}_i - \mathbf{r}_i \\
&= (\mathbf{r}_i - \mathbf{r}_L) + (\mathbf{r}_L - \mathbf{r}_M) + (\mathbf{r}_M - \mathbf{r}_j) \\
&= \mathbf{r}_{iL} + \mathbf{r}_{LM} + \mathbf{r}_{Mj}
\end{aligned}$$

where $|\mathbf{r}_{LM}| \gg |\mathbf{r}_{iL} + \mathbf{r}_{Mj}|$. Then, the $p$-th order Taylor expansion of $f(\mathbf{r}_{ij})$ in the neighborhood of $\mathbf{r}_{LM}$ can be written as

$$f(\mathbf{r}_{ij}) = \sum_{|\mathbf{n}| \leq p} \frac{1}{\mathbf{n}!} (\mathbf{r}_{iL} + \mathbf{r}_{Mj})^{\mathbf{n}} (\partial^{\mathbf{n}} f)(\mathbf{r}_{LM})$$

where we use the following abbreviated multi-index notations:

$$\begin{aligned}
\mathbf{n} &= (n_0, n_1, \ldots, n_{d-1}) \\
\mathbf{n} \pm \mathbf{k} &= (n_0 \pm k_0, n_1 \pm k_1, \ldots, n_{d-1} \pm k_{d-1}) \\
\mathbf{n} < \mathbf{k} &= \forall i,\ n_i < k_i \\
|\mathbf{n}| &= n_0 + n_1 + \cdots + n_{d-1} \\
\mathbf{n}! &= n_0!\, n_1! \,\cdots\, n_{d-1}! \\
\mathbf{x}^{\mathbf{n}} &= x_0^{n_0}\, x_1^{n_1}\, \ldots\, x_{d-1}^{n_{d-1}} \\
\partial^{\mathbf{n}} &= \partial_0^{n_0}\, \partial_1^{n_1}\, \cdots\, \partial_{d-1}^{n_{d-1}}
\end{aligned}$$

Using the binomial theorem for $(\mathbf{r}_{iL} + \mathbf{r}_{Mj})^{\mathbf{n}}$, we have

$$\begin{aligned}
f(\mathbf{r}_{ij}) &= \sum_{|\mathbf{n}| \leq p} \frac{1}{\mathbf{n}!} (\mathbf{r}_{iL} + \mathbf{r}_{Mj})^{\mathbf{n}} (\partial^{\mathbf{n}} f)(\mathbf{r}_{LM}) \\
&= \sum_{|\mathbf{n}| \leq p} \frac{1}{\mathbf{n}!} (\partial^{\mathbf{n}} f)(\mathbf{r}_{LM}) \sum_{\mathbf{k} \leq \mathbf{n}} \frac{\mathbf{n}!}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!} \mathbf{r}_{iL}^{\mathbf{k}} \mathbf{r}_{Mj}^{\mathbf{n}-\mathbf{k}}
\end{aligned}$$

canceling $\mathbf{n}!$,

$$= \sum_{|\mathbf{n}| \leq p} \sum_{\mathbf{k} \leq \mathbf{n}} \frac{1}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!} \mathbf{r}_{iL}^{\mathbf{k}} \mathbf{r}_{Mj}^{\mathbf{n}-\mathbf{k}} (\partial^{\mathbf{n}} f)(\mathbf{r}_{LM})$$

swap the sums by introducing a Kronecker delta and extending the range,

$$
\begin{aligned}
&= \sum_{|\mathbf{n}|\le p} \sum_{|\mathbf{k}|\le p} \frac{\delta_{\mathbf{k}\le\mathbf{n}}}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!} \mathbf{r}_{iL}^{\mathbf{k}} \mathbf{r}_{Mj}^{\mathbf{n}-\mathbf{k}} (\partial^{\mathbf{n}} f)(\mathbf{r}_{LM}) \\
&= \sum_{|\mathbf{k}|\le p} \sum_{|\mathbf{n}|\le p} \frac{\delta_{\mathbf{k}\le\mathbf{n}}}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!} \mathbf{r}_{iL}^{\mathbf{k}} \mathbf{r}_{Mj}^{\mathbf{n}-\mathbf{k}} (\partial^{\mathbf{n}} f)(\mathbf{r}_{LM})
\end{aligned}
$$

redefining $\mathbf{n}-\mathbf{k}$ to $\mathbf{n}$,

$$
= \sum_{|\mathbf{k}|\le p} \sum_{|\mathbf{n}+\mathbf{k}|\le p} \frac{\delta_{\mathbf{k}\le\mathbf{n}+\mathbf{k}}}{\mathbf{n}!\mathbf{k}!} \mathbf{r}_{iL}^{\mathbf{k}} \mathbf{r}_{Mj}^{\mathbf{n}} (\partial^{\mathbf{n}+\mathbf{k}} f)(\mathbf{r}_{LM})
$$

recognizing that $|\mathbf{n}+\mathbf{k}| = |\mathbf{n}| + |\mathbf{k}|$,

$$
= \sum_{|\mathbf{k}|\le p} \sum_{|\mathbf{n}|\le p-|\mathbf{k}|} \frac{1}{\mathbf{n}!\mathbf{k}!} \mathbf{r}_{iL}^{\mathbf{k}} \mathbf{r}_{Mj}^{\mathbf{n}} (\partial^{\mathbf{n}+\mathbf{k}} f)(\mathbf{r}_{LM})
$$

and rearranging,

$$
= \sum_{|\mathbf{k}|\le p} \frac{1}{\mathbf{k}!} \mathbf{r}_{iL}^{\mathbf{k}} \sum_{|\mathbf{n}|\le p-|\mathbf{k}|} (\partial^{\mathbf{n}+\mathbf{k}} f)(\mathbf{r}_{LM}) \frac{1}{\mathbf{n}!} \mathbf{r}_{Mj}^{\mathbf{n}}
$$

Then, the matrix-vector product

$$
r_i = \sum_j f(\mathbf{r}_{ij}) c_j
$$

can be computed via the following steps

$$
\begin{aligned}
M_{\mathbf{n}} &= \sum_j \frac{1}{\mathbf{n}!} \mathbf{r}_{Mj}^{\mathbf{n}} c_j && (S2M) \\
L_{\mathbf{n}} &= \sum_{|\mathbf{k}|\le p-|\mathbf{n}|} (\partial^{\mathbf{k}+\mathbf{n}} f)(\mathbf{r}_{LM}) M_{\mathbf{k}} && (M2L) \\
r_i &= \sum_{|\mathbf{k}|\le p} \frac{1}{\mathbf{k}!} \mathbf{r}_{iL}^{\mathbf{k}} L_{\mathbf{k}} && (L2T)
\end{aligned}
$$

## 2 Multilevel Expansion

The vectors $\mathbf{r}_{iL}$ and $\mathbf{r}_{Mj}$ can be further decomposed as:

$$
\begin{aligned}
\mathbf{r}_{Mj} &= \mathbf{r}_{Mm} + \mathbf{r}_{mj} \\
\mathbf{r}_{iL} &= \mathbf{r}_{i\ell} + \mathbf{r}_{\ell L}
\end{aligned}
$$

and the binomial theorem applied to derive the multipole-to-multipole operator:

$$
\begin{aligned}
M_{\mathbf{n}} &= \sum_j \frac{1}{\mathbf{n}!}\mathbf{r}_{Mj}^{\mathbf{n}} c_j \\
&= \sum_j \frac{1}{\mathbf{n}!}(\mathbf{r}_{Mm} + \mathbf{r}_{mj})^{\mathbf{n}} c_j \\
&= \sum_j \sum_{\mathbf{k}\le\mathbf{n}} \frac{1}{\mathbf{n}!}\frac{\mathbf{n}!}{(\mathbf{n}-\mathbf{k})!\mathbf{k}!}\mathbf{r}_{Mm}^{\mathbf{k}}\mathbf{r}_{mj}^{\mathbf{n}-\mathbf{k}} c_j \\
&= \sum_{\mathbf{k}\le\mathbf{n}} \frac{1}{\mathbf{k}!}\mathbf{r}_{Mm}^{\mathbf{k}} \widetilde{M}_{\mathbf{n}-\mathbf{k}}
\end{aligned}
$$

and the local-to-local operator:

$$
\begin{aligned}
r_i &= \sum_{|\mathbf{k}|\le p} \frac{1}{\mathbf{k}!}\mathbf{r}_{iL}^{\mathbf{k}} L_{\mathbf{k}} \\
&= \sum_{|\mathbf{k}|\le p} \frac{1}{\mathbf{k}!}(\mathbf{r}_{i\ell} + \mathbf{r}_{\ell L})^{\mathbf{k}} L_{\mathbf{k}} \\
&= \sum_{|\mathbf{k}|\le p} \sum_{\mathbf{n}\le\mathbf{k}} \frac{1}{\mathbf{k}!}\frac{\mathbf{k}!}{(\mathbf{k}-\mathbf{n})!\mathbf{n}!}\mathbf{r}_{i\ell}^{\mathbf{n}}\mathbf{r}_{\ell L}^{\mathbf{k}-\mathbf{n}} L_{\mathbf{k}} \\
&= \sum_{|\mathbf{k}|\le p} \sum_{|\mathbf{n}|\le p} \delta_{\mathbf{n}\le\mathbf{k}} \frac{1}{(\mathbf{k}-\mathbf{n})!\mathbf{n}!}\mathbf{r}_{i\ell}^{\mathbf{n}}\mathbf{r}_{\ell L}^{\mathbf{k}-\mathbf{n}} L_{\mathbf{k}} \\
&= \sum_{|\mathbf{n}|\le p} \frac{1}{\mathbf{n}!}\mathbf{r}_{i\ell}^{\mathbf{n}} \widetilde{L}_{\mathbf{n}}
\end{aligned}
$$

where

$$
\widetilde{L}_{\mathbf{n}} = \sum_{\substack{\mathbf{k}\ge\mathbf{n} \\ |\mathbf{k}|\le p}} \frac{1}{(\mathbf{k}-\mathbf{n})!}\mathbf{r}_{\ell L}^{\mathbf{k}-\mathbf{n}} L_{\mathbf{k}}
$$

and redefining $\mathbf{k}-\mathbf{n}$ to $\mathbf{k}$,

$$
= \sum_{|\mathbf{k}|\le p-|\mathbf{n}|} \frac{1}{\mathbf{k}!}\mathbf{r}_{\ell L}^{\mathbf{k}} L_{\mathbf{n}+\mathbf{k}}
$$

So, in summary, we have the five tree operators:

$$\widetilde{M}_{\mathbf{n}} = \sum_{j} \frac{1}{\mathbf{n}!} \mathbf{r}_{mj}^{\mathbf{n}} c_j \tag{S2M}$$

$$M_{\mathbf{n}} = \sum_{\mathbf{k} \leq \mathbf{n}} \frac{1}{\mathbf{k}!} \mathbf{r}_{Mm}^{\mathbf{k}} \widetilde{M}_{\mathbf{n}-\mathbf{k}} \tag{M2M}$$

$$L_{\mathbf{n}} = \sum_{|\mathbf{k}| \leq p - |\mathbf{n}|} (\partial^{\mathbf{n}+\mathbf{k}} f)(\mathbf{r}_{LM}) M_{\mathbf{k}} \tag{M2L}$$

$$\widetilde{L}_{\mathbf{n}} = \sum_{|\mathbf{k}| \leq p - |\mathbf{n}|} \frac{1}{\mathbf{k}!} \mathbf{r}_{\ell L}^{\mathbf{k}} L_{\mathbf{n}+\mathbf{k}} \tag{L2L}$$

$$r_i = \sum_{|\mathbf{k}| \leq p} \frac{1}{\mathbf{k}!} \mathbf{r}_{i\ell}^{\mathbf{k}} \widetilde{L}_{\mathbf{k}} \tag{L2T}$$