Finite-differences - mesh drift and superconvergence

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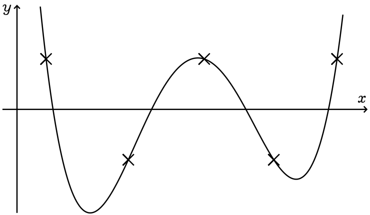
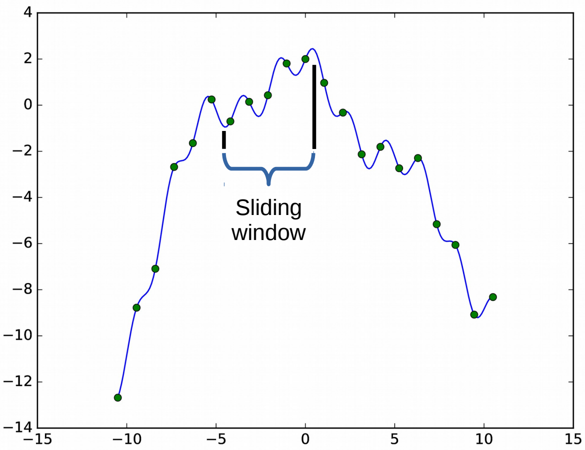


A few reminders on finite-differences



A few reminders on finite-differences

What we know

- a set of n distinct points: $x_1 < x_2 < ...x_n$
- the values of f at those points: $f(x_1), f(x_2), ...f(x_n)$

A few reminders on finite-differences

What we know

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- the values of f at those points: $f(x_1), f(x_2), \ldots f(x_n)$

What we would like to know

$$f^{(d)}(z) \text{ for some point } z$$

.

A few reminders on finite-differences

We carry out a Taylor expansion around z:

$$
\begin{aligned}
f(x_1) &= f(z) + f'(z)(x_1 - z) + \ldots + f^{(n-1)}\frac{(x_1 - z)^{n-1}}{(n-1)!} + \mathcal{O}(x_1^n) \\
f(x_2) &= f(z) + f'(z)(x_2 - z) + \ldots + f^{(n-1)}\frac{(x_2 - z)^{n-1}}{(n-1)!} + \mathcal{O}(x_2^n) \\
&\ldots \\
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\end{aligned}$$

- search for coefficients $a_i^d(x)$ such that $\sum_{i=1}^n a_i^d(z) f(x_i) = f^{(d)}(z) + \sum_{i=1}^n a_i^d(z)\mathcal{O}(x_i^n)$
- in other words, $\sum_{i=1}^n a_i^d(z)\frac{(x_i-z)^k}{k!} = \delta_k^d$

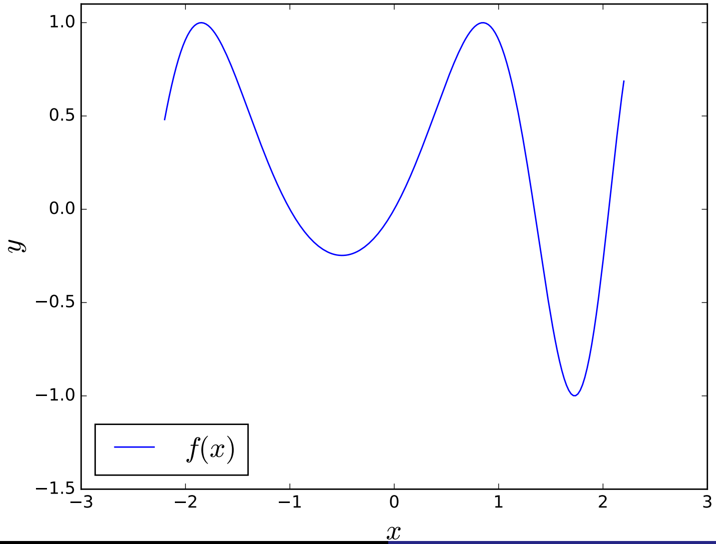
A few reminders on finite-differences

Solution

$$a_i^d(z) = L_i^{(d)}(z)$$

where $L_i(z)$ is the Lagrange interpolation polynomial such that $L_i(x_j) = \delta_i^j$ (e.g. Fornberg (1988), also see proof in the appendix).

Another way of looking at this



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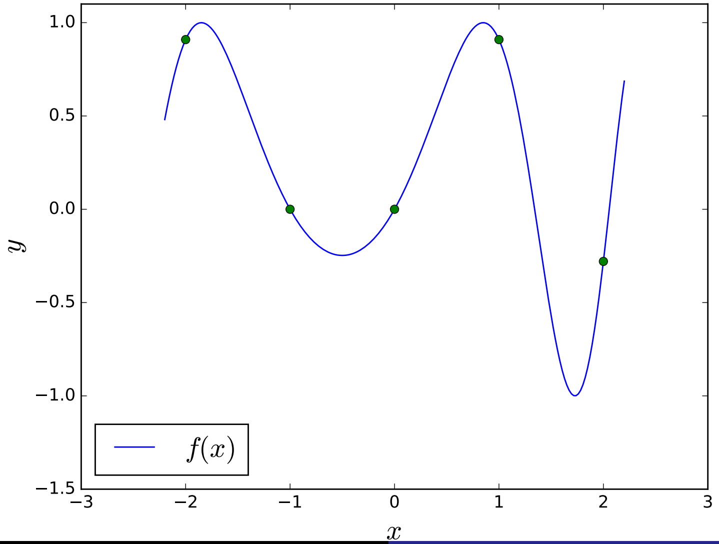

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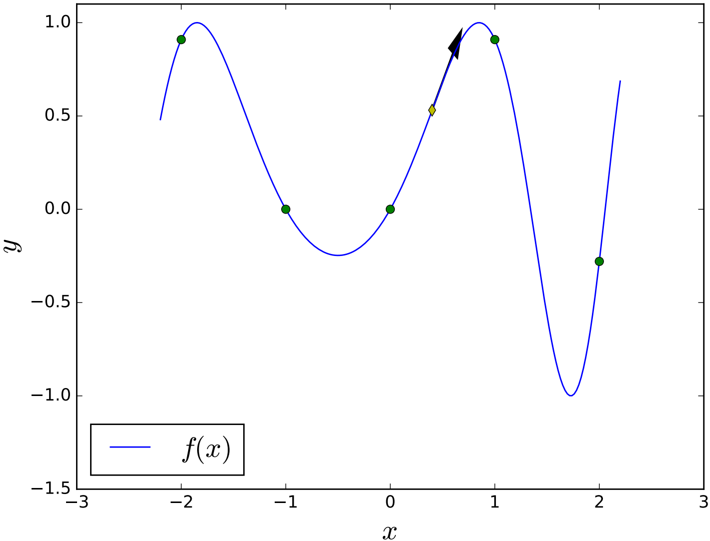

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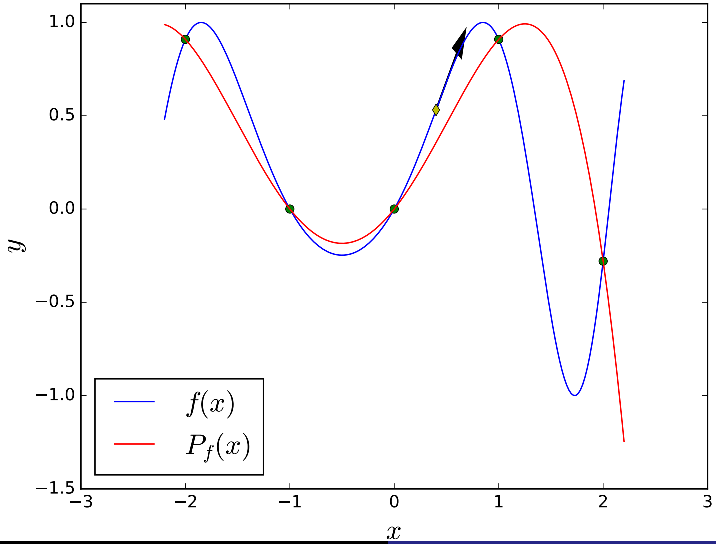

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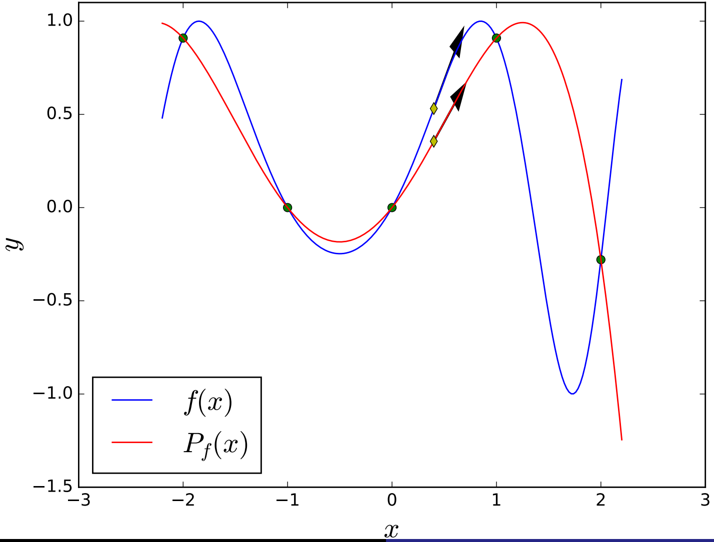

A few simple examples

For a uniform grid:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} + \mathcal{O}(x)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} + \mathcal{O}(x^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12(x_{i+1} - x_i)} + \mathcal{O}(x^4)$$

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(x_{i+1} - x_i)^2} + \mathcal{O}(x^2)$$

Mesh drift

Definition

- a numerical instability where even and odd grid points decouple
- it typically leads to a “jigsaw” type behaviour in the solution

Mesh drift – an example

An eigenvalue problem

$$\begin{aligned} v' &= -\omega u \\ u' &= \omega v \\ u(0) &= u(1) = 0 \end{aligned}$$

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Analytical solution

$$\begin{aligned} u(x) &= A\sin(\omega x) \\ v(x) &= A\cos(\omega x) \\ \omega &= k\pi, \text{ where } k \text{ is an integer} \end{aligned}$$

Mesh drift – an example

Numerical setup

$$
\begin{aligned}
-\omega u_i &= \frac{v_{i+1} - v_{i-1}}{2\Delta x}, & \omega v_i &= \frac{u_{i+1} - u_{i-1}}{2\Delta x}, & 2 \leq i \leq N-1, \\
-\omega u_N &= \frac{v_N - v_{N-1}}{\Delta x}, & \omega v_1 &= \frac{u_2 - u_1}{\Delta x}, \\
u_1 &= 0, & u_N &= 0,
\end{aligned}
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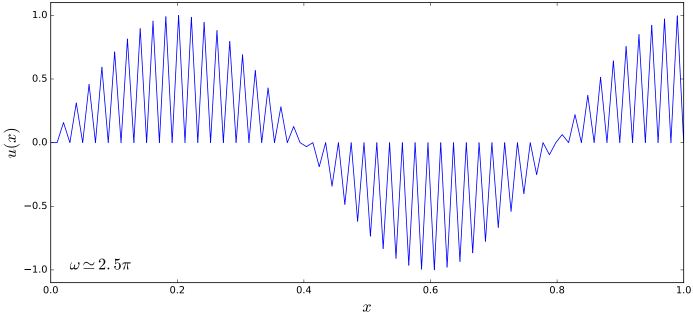

Mesh drift – an example

Numerical setup 2

- use 4^{th} order scheme:

$$f'(x_i) \simeq \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12(x_{i+1} - x_i)}$$

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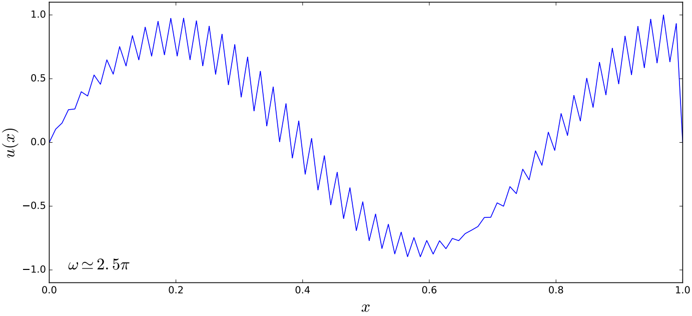

Mesh drift – an example

Numerical setup 3

- use 2^{nd} order scheme + non uniform grid

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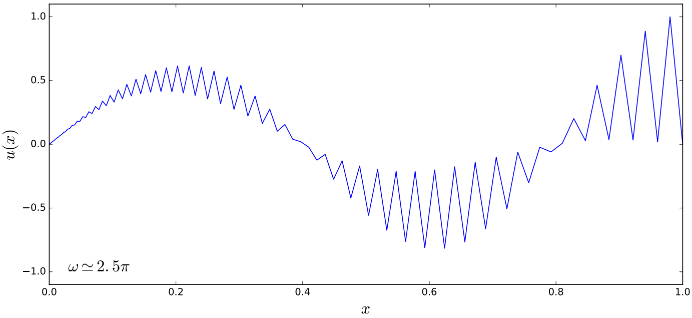

Causes of mesh drift

What are not the causes

- finite-difference expressions with only even or odd grid points
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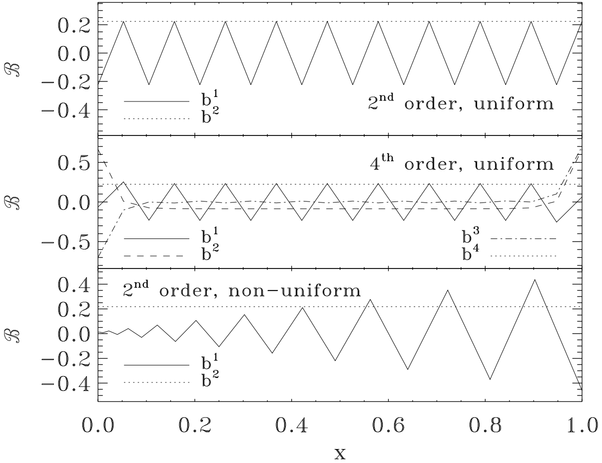
What are the causes

- finite-difference expressions which allow oscillatory solutions to

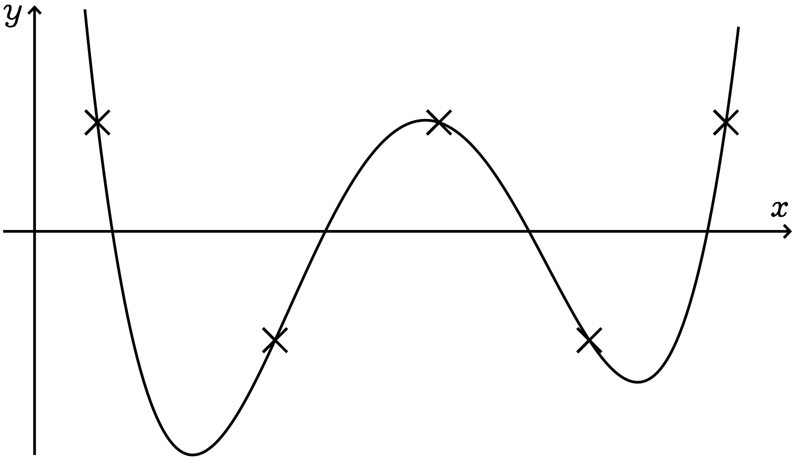
$$f' = 0$$

Causes of mesh drift

Solutions of $f' = 0$



Causes of mesh drift



Remedies for mesh drift

1. **Numerical viscosity**: introduce terms with higher order derivatives to damp oscillations
2. **Staggered grid**: different variables are defined on different grids
3. **Alternate grid**: keep variables on the same grid, but enforce differential equations on a different grid

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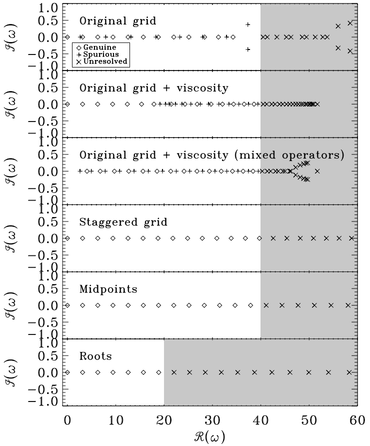
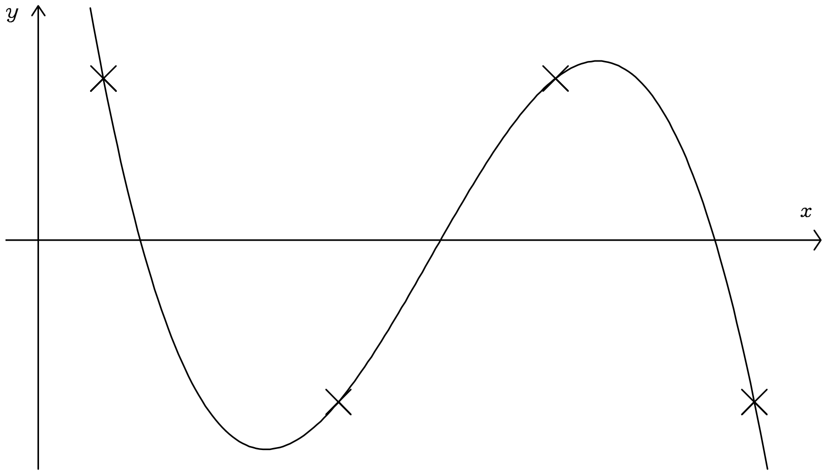


Remedies of mesh drift



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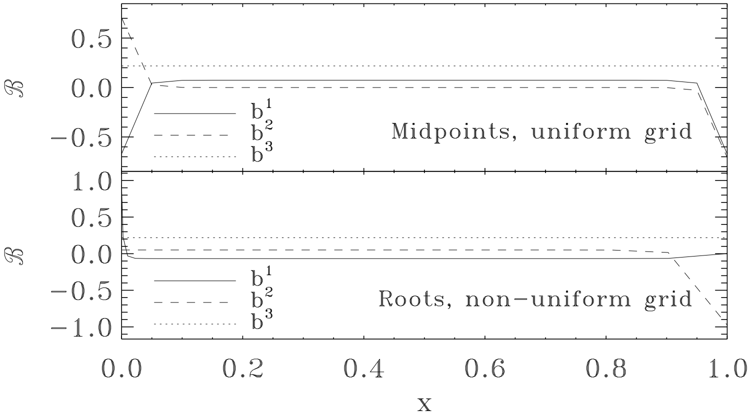

Remedies for mesh drift

The alternate grid strategy also lends itself to “superconvergence” ...

Superconvergence

Definition

- usually, finite-differences for n points are accurate to order $n - d$, where d is the order of the derivative
- in some cases, it is accurate to a higher order – this is called "superconvergence" (e.g. Sadiq & Viswanath 2013)

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- usually, finite-differences for n points are accurate to order $n - d$, where d is the order of the derivative
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Question: is it possible to cause superconvergence by carefully choosing the point, z, where you calculate the finite differences?

Superconvergence

Answer: yes!

We carry out a Taylor expansion around z:

$$
\begin{aligned}
f(x_1) &= f(z) + \ldots + f^{(n-1)}\frac{(x_1-z)^{n-1}}{(n-1)!} + f^{(n)}\frac{(x_1-z)^n}{n!} + \mathcal{O}(x_1^{n+1}) \\
f(x_2) &= f(z) + \ldots + f^{(n-1)}\frac{(x_2-z)^{n-1}}{(n-1)!} + f^{(n)}\frac{(x_2-z)^n}{n!} + \mathcal{O}(x_2^{n+1}) \\
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\end{aligned}
$$

- the FD coefficients verify $\sum_{i=1}^n a_i^d(z) f(x_i) = f^{(d)}(z) + R$, where:

$$R = \underbrace{\sum_{i=1}^n a_i^d(z) f^{(n)}(z)\frac{(x_i-z)^n}{n!}}_{R_n(z)} + \sum_{i=1}^n a_i^d(z)\mathcal{O}\left((x_i-z)^{n+1}\right)$$

- superconvergence if $R_n(z) = 0$

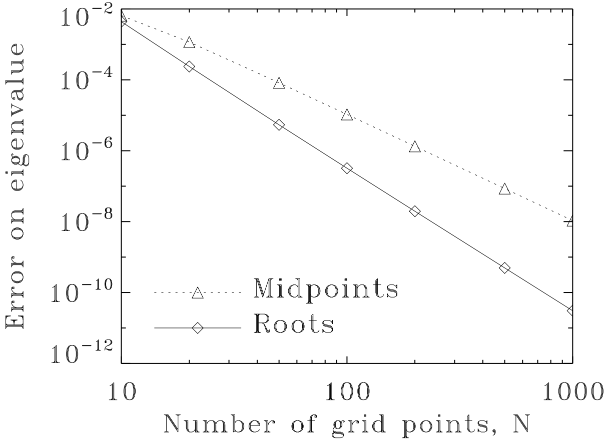
Superconvergence

- it can be shown that (see appendix):

$$R_n(z) = -\frac{f^{(n)}(z)}{n!} Q^{(d)}(z) \text{ where } Q(z) = \prod_{i=1}^{n} (z - x_i)$$

- hence, by choosing one of the roots of $Q^{(d)}(z)$, superconvergence is achieved
- furthermore, mesh drift continues to be suppressed

Superconvergence



Conclusion

- suppression of mesh-drift through alternate grid strategy (i.e. the variables are defined on one grid, but the equations are enforced on another grid)
- superconvergence can be achieved systematically and combines nicely with the suppression of mesh-drift
- for more details, see Reese (2013, A&A 555, A148) and references therein

Derivation of finite-difference coefficients

We carry out a Taylor expansion around z:

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- search for coefficients $a_i^d(x)$ such that $\sum_{i=1}^n a_i^d(z) f(x_i) = f^{(d)}(z) + \sum_{i=1}^n a_i^d(z) \mathcal{O}(x_i^n)$
- in other words, $\sum_{i=1}^n a_i^d(z) \frac{(x_i - z)^k}{k!} = \delta_k^d$

Derivation of finite-difference coefficients

In matrix form, this can be expressed as follows:

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 - z & x_2 - z & \dots & x_n - z \\ \vdots & \vdots & \ddots & \vdots \\ \frac{(x_1-z)^{n-1}}{(n-1)!} & \frac{(x_2-z)^{n-1}}{(n-1)!} & \dots & \frac{(x_n-z)^{n-1}}{(n-1)!} \end{bmatrix} \begin{bmatrix} a_1^0 & a_1^1 & \dots & a_1^{n-1} \\ a_2^0 & a_2^1 & \dots & a_2^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_n^0 & a_n^1 & \dots & a_n^{n-1} \end{bmatrix} = \mathcal{I}$$

where $\mathcal{I}$ is the identity matrix.

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where $\mathcal{I}$ is the identity matrix.

However, a matrix and its inverse commute:

$$\begin{bmatrix} a_1^0 & a_1^1 & \dots & a_1^{n-1} \\ a_2^0 & a_2^1 & \dots & a_2^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ a_n^0 & a_n^1 & \dots & a_n^{n-1} \end{bmatrix} \begin{bmatrix} 1 & 1 & \dots & 1 \\ x_1 - z & x_2 - z & \dots & x_n - z \\ \vdots & \vdots & \ddots & \vdots \\ \frac{(x_1-z)^{n-1}}{(n-1)!} & \frac{(x_2-z)^{n-1}}{(n-1)!} & \dots & \frac{(x_n-z)^{n-1}}{(n-1)!} \end{bmatrix} = \mathcal{I}$$

Derivation of finite-difference coefficients

In algebraic form, this becomes: $\sum_{k=0}^{n-1} a_i^k \frac{(x_j-z)^k}{k!} = \delta_i^j$

We introduce the polynomial: $P(x) = \sum_{k=0}^{n-1} a_i^k \frac{(x-z)^k}{k!}$

From the above properties, $\left\{ \begin{array}{lcll} P(x_i) & = & 1 & \\ P(x_j) & = & 0 & \forall j \neq i \end{array} \right.$

From this we recognise the Lagrange interpolation polynomial:

$$P(x) = L_i(x) = \frac{\prod_{j \neq i}(x - x_j)}{\prod_{j \neq i}(x_i - x_j)}$$

The a_i^d coefficients simply come from the Taylor expansion of P around z:

$$a_i^d = L_i^{(d)}(z)$$

Proof for $R_n(z)$

We carry out a Taylor expansion around z:

$$\begin{aligned}
f(x_1) &= f(z) + \ldots + f^{(n-1)}\frac{(x_1-z)^{n-1}}{(n-1)!} + f^{(n)}\frac{(x_1-z)^n}{n!} + \mathcal{O}(x_1^{n+1}) \\
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\end{aligned}$$

- the FD coefficients verify $\sum_{i=1}^n a_i^d(z)f(x_i) = f^{(d)}(z) + R$, where:

$$R(z) = \underbrace{\sum_{i=1}^n a_i^d(z) f^{(n)}(z)\frac{(x_i-z)^n}{n!}}_{R_n(z)} + \sum_{i=1}^n a_i^d(z)\mathcal{O}\left((x_i-z)^{n+1}\right)$$

Proof for $R_n(z)$

- we calculate $R(z)$ for the function $f_0(x) = x^n$
- one has: $R = -f_0^{(d)}(z) + \sum_{i=1}^n a_i^d(z) x_i^n$
- furthermore, $a_i^d(z) = L_i^{(d)}(z)$
- let us define the polynomial $P(x) = -x^n + \sum_{i=1}^n L_i(x) x_i^n$
- it turns out that $P^{(d)}(z) = R$
- furthermore: $P(x_i) = -x_i^n + x_i^n = 0, \qquad 1 \leq i \leq n$
- but, P is of degree n with a leading coefficient of -1
- hence: $P(x) = -\prod_{i=1}^n (x - x_i)$
- however: $R = \sum_{i=1}^n a_i^d(z) f_0^{(n)}(z) \frac{(x_i - z)^n}{n!} = \sum_{i=1}^n a_i^d(z)(x_i - z)^n$,
- hence:

$$\sum_{i=1}^n a_i^d(z)(x_i - z)^n = P^{(d)}(z)$$