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Problem 1

a) $f(x \pm \delta) \simeq f(x) + f'(x)\delta + \frac{1}{2} f''(x)\delta^2 \pm \frac{1}{6} f'''(x)\delta^3 \pm \dots$

$f_\delta' \approx [f(x+\delta) - f(x-\delta)]\frac{1}{2\delta}$

$\simeq [f(x) + f'(x)\delta + \frac{1}{2} f''(x)\delta^2 + \frac{1}{6} f'''(x)\delta^3 - f(x) + f'(x)\delta$

$- \frac{1}{2} f''(x)\delta^2 + \frac{1}{6} f'''(x)\delta^3]\frac{1}{2\delta}$

$\approx [2f'(x)\delta + \frac{2}{6} f'''(x)\delta^3 + \frac{2}{120} f^{(5)}(x)\delta^5]\frac{1}{2\delta}$

$f(x \pm 2\delta) \approx f(x) \pm 2f'(x)\delta + \frac{4}{2} f''(x)\delta^2 \pm \frac{2^3}{6} f'''(x)\delta^3 + \dots$

$f_{2\delta}' \approx [f(x+2\delta) - f(x-2\delta)]\frac{1}{2\delta}$

$\approx [f(x) + 2f'(x)\delta + \frac{4}{2} f''(x)\delta^2 + \frac{8}{6} f'''(x)\delta^3 - f(x) + 2f'(x)\delta$

$- \frac{4}{2} f''(x)\delta^2 + \frac{8}{6} f'''(x)\delta^3]\frac{1}{2\delta}$

$\approx [4f'(x)\delta + \frac{16}{6} f'''(x)\delta^3 + \frac{64}{120} f^{(5)}\delta^5]\frac{1}{2\delta}$

Cancel f''' terms:

$8f_\delta' - f_{2\delta}' = [8f(x+\delta) - 8f(x-\delta)]\frac{1}{2\delta} - [f(x+2\delta) + f(x-2\delta)]\frac{1}{2\delta}$

$\approx [16 f'(x)\delta + \frac{16}{6} f'''(x)]\frac{1}{2\delta} - [4f'(x)\delta + \frac{16}{6} f'''(x)]\frac{1}{2\delta}$

$\approx 12 f'(x)\delta$

$$\boxed{f'(x) = \frac{1}{12\delta}\left(8f(x+\delta) - 8f(x-\delta) - f(x+2\delta) + f(x-2\delta)\right)}$$

b) roundoff err ~ $\frac{\varepsilon f(x)}{\delta}$, truncation err ~ $f^{(5)}(x)\delta^4$

err ~ $\frac{\varepsilon f(x)}{\delta} + f^{(5)}(x)\delta^4$

derivative w.r.t $\delta \approx -\frac{\varepsilon f(x)}{\delta^2} + f^{(5)}(x)\delta^3 = 0$

$f^{(5)}(x)\delta^3 = \frac{\varepsilon f(x)}{\delta^2}$

$$f^{(s)}(x)\,\delta^s = \varepsilon f(x)$$

$$\boxed{\delta \approx \left(\frac{\varepsilon f(x)}{f^{(s)}(x)}\right)^{1/s} \quad \text{where } \varepsilon = 2^{-52}}$$

At $x=42$ $f(x) = e^x$ gave a derivative with fractional error of order 10^{-12}. for $f(x) = e^{0.01x}$ the fractional error was also of order 10^{-14}.

Problem 2

$$f'(x) \approx [f(x+dx) - f(x-dx)]\frac{1}{2dx}$$

$$\approx [f(x) + f'(x)dx + \tfrac{1}{2}f''(x)dx^2 + \tfrac{1}{6}f'''(x)dx^3 + \ldots - f(x) + f'(x)dx - \tfrac{1}{2}f''(x)dx^2 + \tfrac{1}{6}f'''(x)dx^3 \ldots]\frac{1}{2dx}$$

$$\approx [2f'(x)dx + \tfrac{1}{3}f'''(x)dx^3]\frac{1}{2dx}$$

$$f'(x) \approx f'(x) + \tfrac{1}{6}f'''(x)dx^2$$

$$\boxed{err \approx \frac{\varepsilon f(x)}{dx} + f'''(x)dx^2}$$

deriv w.r.t dx: $-\dfrac{\varepsilon f(x)}{dx^2} + f'''(x)dx = 0$

$$f'''(x)dx^3 = \varepsilon f(x)$$

$$\boxed{dx = \left(\frac{\varepsilon f(x)}{f'''(x)}\right)^{1/3} \sim \varepsilon^{1/3}}$$

$$f(x+dx) + f(x-dx) = [f(x) + \cancel{f'(x)dx} + \tfrac{1}{2}f''(x)dx^2 + \cancel{\tfrac{1}{6}f'''(x)dx^3} + f(x) - \cancel{f'(x)dx} + \tfrac{1}{2}f''(x)dx^2 - \cancel{\tfrac{1}{6}f'''(x)dx^3}\ldots]$$

$$= 2f(x) + f''(x)dx^2$$

$$f''(x) \approx \frac{f(x+dx) + f(x-dx) - 2f(x)}{dx^2}$$

$$f'''(x) = \frac{f''(x+dx) - f''(x-dx)}{2f(x)}$$

$$= \frac{\frac{f(x+2dx) - f(x) - 2f(x+dx)}{dx^2} - \frac{f(x) + f(x-2dx) - 2f(x-dx)}{dx^2}}{2dx}$$

$$\boxed{f'''(x) = \frac{f(x+2dx) - 2f(x+dx) - f(x-2dx) + 2f(x-dx)}{2dx^3}}$$

Problem 3

For error, used bootstrap resampling. Sampled 3 sets of points from lakeshore.txt data and did the same spline interpolation the samples as was done on the original points. The error is then estimated to be the variance on the spline at each point.

Problem 4

For $f(x) = \cos(x)$ the polynomial fit is inaccurate with an error $\sim 10^{-3}$ and a fit that visually is wrong. The spline and rational were both accurate with errors of $\sim 10^{-6}$ and $\sim 10^{-8}$ respectively.

For $f(x) = \frac{1}{1+x^2}$ & polynomial was again inaccurate with error $\sim 10^{-1}$. The spline was accurate with error $\sim 10^{-5}$.

For linalg.inv the rational was inaccurate with error $\sim 10^{-1}$. But when using linalg.pinv the fit became accurate with error $\sim 10^{-16}$, making it the best fit. The massive improvement from switching from inv to pinv can be understood by looking at p and q.

Rational fit: $y = \dfrac{\bar{x}\,p}{1+\bar{x}'q}$ $\quad |x| = (1+x+x^2+\dots x^n)$

$\quad |x'| = (x+x^2+x^3+\dots x^m)$

for $y = \dfrac{1}{1+x^2}$

$$y = \frac{1p_0 + xp_1 + \dots}{1 + xq_0 + x^2 q_1 + \dots} \implies \begin{array}{l} p = [1,0,0,0\dots 0] \\ q = [0,1,0,0,0\dots 0] \end{array}$$

When using inv (for $n=4$, $m=5$) $p[0]$ was 0.6 and the other values were not all zero or near zero. For $q[1]$ the value was 0! This would clearly not produce an accurate fit. For pinv $p[0]$ is 1 and the other values are of order 10^{-15}, so near zero. For $q[1]$ 0.67, close to one and the other values are generally of order 10^{-15}, near zero. This explains why pinv worked better since values that needed to be near zero were set small.

The error in the Lorentzian function from the rational function fit must take into account that the Lorentzian is itself a rational function. $f(x) = \dfrac{1}{1+x^2}$ $\begin{array}{l} \rightarrow \text{polynomial} \\ \rightarrow \text{2nd degree taylor} \end{array}$

error comes from Taylor's remainder theorem for $1+x^2$:

$$err_{truncation} = |R_2(x)| = \frac{f'''(x)}{3!} x^3 \Big|_{-1}^{1} = \left|\frac{f'''(x)}{6}\right|$$

the roundoff error is $\frac{\varepsilon f(x)}{dx}$

for $dx = \left(\frac{\varepsilon f(x)}{f'''(x)}\right)^{1/3}$ derived from prob 2

$$err = \frac{\varepsilon f(x) f'''(x)^{1/3}}{\varepsilon^{1/3} f(x)^{1/3}} + f'''(x)\left(\frac{\varepsilon f(x)}{f'''(x)}\right)^{2/3}$$

$$= \varepsilon^{2/3} f(x)^{2/3} f'''(x)^{1/3} + \varepsilon^{2/3} f(x)^{2/3} f'''(x)^{1/3}$$

$$err \sim \varepsilon^{2/3} f(x)^{2/3} f'''(x)^{1/3}$$

$$f'(x) = \frac{d}{dx}\frac{1}{1+x^2} = \frac{-2x}{(x^2+1)^2}$$

$$f''(x) = \frac{d}{dx}\left(-\frac{2x}{(x^2+1)^2}\right) = \frac{d}{dx} \cdot \frac{2x(x^2+1)^2}{(x^2+1)^4}$$

$$= -2\,\frac{(x^2+1)^2 - 2x(x^2+1)(2x)}{(x^2+1)^4} = -2\,\frac{(x^2+1)^2 - 4x^2(x^2+1)}{(x^2+1)^4}$$

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

$$f'''(x) = \frac{d}{dx}\frac{2(3x^2-1)}{(x^2+1)^3} = 2\,\frac{\frac{d}{dx}(3x^2-1)(x^2+1)^3}{(x^2+1)^6}$$

$$= 2\,\frac{(6x)(x^2+1)^3 - (3x^2-1)3(x^2+1)^2(2x)}{(x^2+1)^6}$$

$$= 2\,\frac{6x(x^2+1) - 6x(3x^2-1)}{(x^2+1)^4} = -\frac{24x(x^2-1)}{(x^2+1)^4}$$

Using this predicted error, the predicted err was $\sim 10^{-19}$, meaning pinv of 10^{-16} was closest to this. But the true error is still off by an average of 10^{3} for $n=4$, $m=5$.