Review: Numerical Differentiation

Formulas using Taylor Series

Given *smooth function* $f(x)$, we can approximate the derivative $f'(x)$

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$$

- Recall for small h, the Taylor series expansion of $f(x_0 + h)$ is given by:

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(x_0) + \mathcal{O}(h^4). \tag{1}$$

- The Big-$\mathcal{O}$ notation is used to describe the error term in the Taylor series expansion. And it means that the error term is bounded by a constant times h^4!
- Therefore $D_h^+ f(x_0) \equiv \dfrac{f(x_0 + h) - f(x_0)}{h} \approx f'(x_0) + f''(x_0)\dfrac{h}{2}$. This is:
  - Forward difference formula
  - First-order approximation of $f'(x_0)$.
- Backward difference formula: $D_h^- f(x_0) \equiv \dfrac{f(x_0) - f(x_0 - h)}{h} = f'(x_0) + \dfrac{h}{2} f''(\xi)$, where $\xi \in [x_0 - h, x_0]$. We note this leads to

$$f'(x_0) = D_h^- f(x_0) + E_{\text{trunc}}(f, h), \;\; E_{\text{trunc}}(f, h) = \frac{h}{2} f''(\xi_1) \tag{2}$$

Here $E_{\text{trunc}}(f, h)$ is the **truncation error** for using the backward difference formula $D_h^- f(x_0)$ to approximate $f'(x_0)$.

- **Definition**: Truncation errors are the errors that result from using an approximation $Df(x, h)$ in place of an exact mathematical procedure $f'(x)$:

$$E(h) = |f'(x) - \mathrm{Df}(x, h)|, \tag{3}$$

where x is fixed. The approximation is p-th order accurate, means

$$|E(h)| \leq \mathrm{Ch}^p, \text{for some } C > 0, h \geq 0 \text{ sufficiently small.} \tag{4}$$

We use the notation

$$Df\left(x_0\right) = f'\left(x_0\right) + O\left(h^p\right) \tag{5}$$

- Plotting the error: assuming the error is $O(h^p)$, then the error should be proportional to h^p, i.e., $E(h) \approx Ch^p$, then

$$\log(|E(h)|) \approx \log(C) + p\log(h).$$

We can compute the error for different values of h and plot $\log(|E(h)|)$ versus $\log(h)$!

Central difference formula

- We note the Taylor series should give us:

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(x_0) + \mathcal{O}(h^4). \qquad (6)$$

- Then we have

$$D_0 f(x_0) \equiv \frac{1}{2}(D_h^+ f(x_0) + D_h^- f(x_0)) = \frac{f(x_0+h) - f(x_0-h)}{2h} \approx f'(x_0) + \frac{h^2}{6}K$$

- This central difference *stencil* is second order accurate.

Example: A second-order one sided finite difference formula for derivative:

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} + \frac{h^2}{3}f'''(\xi), \qquad (7)$$

where $\xi \in [x_0, x_0 + h]$. How do we derive (7)? We want to set

$$D_2 f(x_0) \equiv af(x_0) + bf(x_0+h) + cf(x_0+2h) = f'(x_0) + \mathcal{O}(h^2). \qquad (8)$$

and note

$$f(x_0+2h) = f(x_0) + \frac{2h}{1}f'(x_0) + \frac{(2h)^2}{2}f''(x_0) + \frac{(2h)^3}{6}f'''(x_0) + \mathcal{O}(h^4) \qquad (9)$$

So (8) is indeed

$$D_2 f(x_0) = (a{+}b{+}c)f(x_0){+}(b{+}2c)\frac{h}{1}f'(x_0){+}(b{+}4c)\frac{h^2}{2}f''(x_0){+}(b{+}8c)\frac{h^3}{6}f'''(x_0){+}\mathcal{O}(h^4).$$

Now we can see this leads to

$$a + b + c = 0, \;\; b + 2c = 1/h, \;\; b + 4c = 0,$$

which gives $a = \frac{-3}{2h}$, $b = \frac{4}{2h}$, and $c = -\frac{1}{2h}$.

This method could be used to derive other finite difference formulas.

Example: A fourth-order central difference formula for derivative $f'(x_0)$:

$$f'(x_0) = \frac{-f(x_0 + 2h) + 8f(x_0 + h) - 8f(x_0 - h) + f(x_0 - 2h)}{12h} + \frac{h^4}{30}f^{(5)}(\xi),$$

where $\xi \in [x_0, x_0 + h]$.

Note: We can get higher order approximations by adding more neighboring points.

Centered formula for the second derivative: We note, the difference formula for the second derivative could be drived as $D_h^+(D_h^- f(x_0)) = \frac{1}{h}(D_h^- f(x_0 + h) - D_h^- f(x_0))$,

$$D^2 f(x_0) = D_h^+ D_h^- f(x_0) = \frac{\frac{f(x_0+h)-f(x_0)}{h} - \frac{f(x_0)-f(x_0-h)}{h}}{h}$$

And we can see that

$$f''(x_0) = \frac{f(x_0 - h) - 2f(x_0) + f(x_0 + h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi), \tag{10}$$

where $x_0 - h \le \xi \le x_0 + h$.

- (10) comes from adding the expressions for forward and backward difference formulas:

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f^{(4)}(\xi_1)$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f^{(4)}(\xi_2)$$

$$f(x_0 + h) + f(x_0 - h) = 2f(x_0) + h^2 f''(x_0) + \frac{h^4}{24} \left(f^{(4)}(\xi_1) + f^{(4)}(\xi_2) \right).$$

Richardson Extrapolation

- This is a method for generating higher order numerical methods using lower order ones.

Example 2: if we have a 2nd order accurate method for approximating the second derivative

- Central differences for second derivative $f''(x_0)$:

$$\begin{aligned} f''(x_0) &= \frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2} \\ &-\frac{h^2}{12}f^{(4)}(x_0)-\frac{h^4}{360}f^{(6)}(x_0)+\mathcal{O}(h^5) \end{aligned}$$

- If we use points one step further to the left and right, to expand in terms of $f(x_0 \pm 2h)$ (replace h by $2h$ in the formula above), we get;

$$\begin{aligned} f''(x_0) &= \frac{f(x_0-2h)-2f(x_0)+f(x_0+2h)}{(2h)^2} \\ &-\frac{(2h)^2}{12}f^{(4)}(x_0)-\frac{(2h)^4}{360}f^{(6)}(x_0)+\mathcal{O}(h^5) \end{aligned}$$

- Combine the two formulas to eliminate the leading error term $\mathcal{O}(h^2)$:

$$\begin{aligned}
3f''(x_0) \;&= 4\left(\frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2}\right) \\
&-\left(\frac{f(x_0-2h)-2f(x_0)+f(x_0+2h)}{4h^2}\right) \\
&-4\left(\frac{h^2}{12}f^{(4)}(x_0)-\frac{h^4}{360}f^{(6)}(x_0)\right) \\
&+\frac{4h^2}{12}f^{(4)}(x_0)+\frac{16h^4}{360}f^{(6)}(x_0)+\mathcal{O}(h^5)
\end{aligned}$$

$$\begin{aligned}
3f''(x_0) \;&= 4\left(\frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2}\right) \\
&-\left(\frac{f(x_0-2h)-2f(x_0)+f(x_0+2h)}{4h^2}\right) \\
&+\frac{4h^4}{360}f^{(6)}(x_0)+\frac{16h^4}{360}f^{(6)}(x_0)+\mathcal{O}(h^5) \\
3f''(x_0) \;&= 4\left(\frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{h^2}\right) \\
&-\left(\frac{f(x_0-2h)-2f(x_0)+f(x_0+2h)}{4h^2}\right) \\
&+\frac{h^4}{30}f^{(6)}(x_0)+\mathcal{O}(h^5)
\end{aligned}$$

- Finally

$$\begin{aligned}
f''(x_0) \;&= 4\left(\frac{f(x_0-h)-2f(x_0)+f(x_0+h)}{3h^2}\right) \\
&-\left(\frac{f(x_0-2h)-2f(x_0)+f(x_0+2h)}{12h^2}\right)+\frac{h^4}{90}f^{(6)}(\xi),
\end{aligned}$$

where $\xi \in [x_0-2h, x_0+2h]$.

- Common denominator

$$f''(x_0) = \frac{-f(x_0-2h)+16f(x_0-h)-30f(x_0)+16f(x_0+h)-f(x_0+2h)}{12h^2} + \frac{h^4}{90}f^{(6)}(\xi).$$

- Fourth order accuracy!

Disadvantages

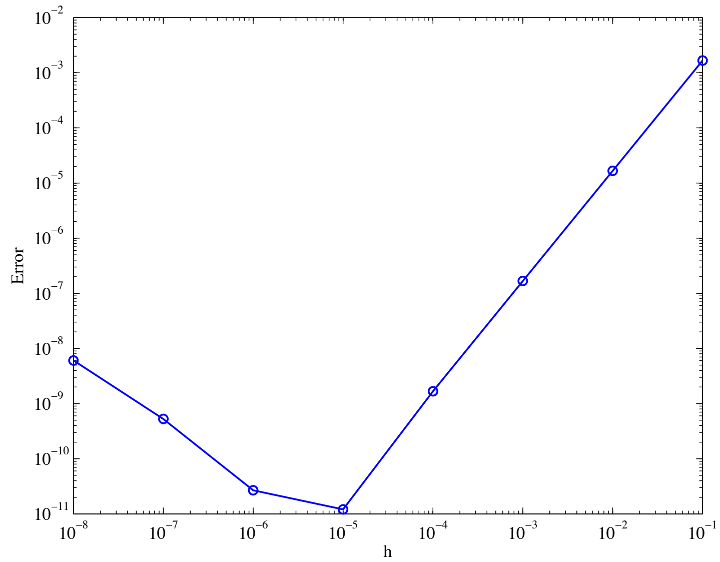
- Requires a wider stencil, i.e. more points, $f(x_0)$, $f(x_0+h)$, $f(x_0-h)$, $f(x_0+2h)$, and $f(x_0-2h)$.
- f needs to have nice, bounded higher order derivatives.

Roundoff and data errors

Example: Consider the centered difference approximation of $f'(0)$ for $f(x) = e^x$,

$$f'(x_0) = \frac{f(x_0+h)-f(x_0-h)}{2h} = \frac{e^h - e^{-h}}{2h}$$

- Error increases if $h < 10^{-5}$
- Problem is cancellation error.




```
clc;
clear all;
clf;

set(0,'DefaultAxesFontName', 'Times New Roman');
axes('FontSize',12);

n = 8;
h = zeros(n,1);
error = zeros(n,1);
hVal = 0;

for i=1:n
    hVal = 0.1*10^(-(i-1));
    h(i) = hVal;
    Dh = (exp(hVal)-exp(-hVal))/(2.0*hVal);
    error(i) = abs(Dh-1);
end

loglog(h,error,'-bo','LineWidth',1.25);
xlabel('h');
ylabel('Error');
```

Error analysis: Let $\bar{f} \equiv \mathrm{fl}(f(x))$ be the floating point representation for $f(x)$.

- Let $\bar{f}(x) = f(x) + e_r(x)$, where $e_r(x)$ is roundoff error bounded by machine epsilon, $\epsilon_m \leq 1 \times 10^{-16}$.

- Let $\bar{D}_h = \dfrac{\bar{f}(x_0+h) - \bar{f}(x_0-h)}{2h}$.

$$\begin{aligned}
|\bar{D}_h - D_h| &= \left| \frac{\bar{f}(x_0+h) - \bar{f}(x_0-h)}{2h} - \frac{f(x_0+h) - f(x_0-h)}{2h} \right| \\
&= \left| \frac{e_r(x_0+h) - e_r(x_0-h)}{2h} \right| \\
&\leq \left| \frac{e_r(x_0+h)}{2h} \right| + \left| \frac{e_r(x_0-h)}{2h} \right| \leq \frac{\epsilon_m}{h}.
\end{aligned}$$

- If $|f'''(\xi)| \leq M$ in $[x_o - h, x_0 + h]$,

$$\begin{aligned}
|f'(x_0) - \bar{D}_h| &= \left|(f'(x_0) - D_h) + \left(D_h - \bar{D}_h\right)\right| \\
&\leq |f'(x_0) - D_h| + \left|D_h - \bar{D}_h\right| \leq \frac{h^2 M}{6} + \frac{\epsilon_m}{h}.
\end{aligned}$$

- If h is small, ϵ_m/h term dominates.

- Should not choose h to close to the rounding unit.

- Remember that roundoff error is not smooth.

Differentiating noisy data: Noise will be magnified by $1/h$.

- For the kth derivative, it will be magnified by $1/h^k$.

- Options are to filter out high frequency noise or use a least squares fit of the data before differentiating.

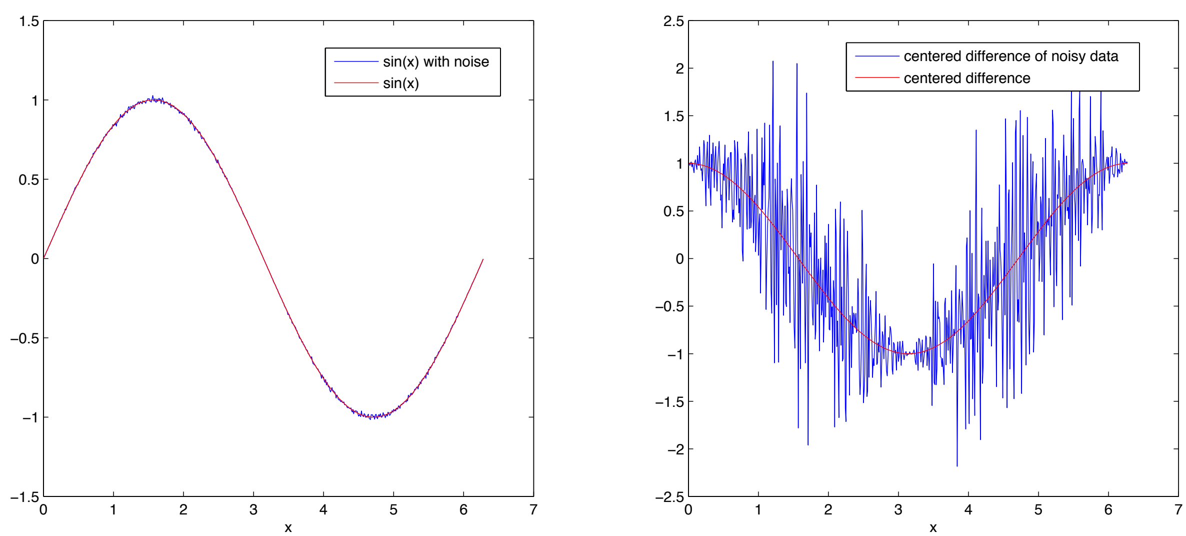
```
% Example 14.6 -- Figure 14.3 : differentiating noisy data

x = 0:.01:2*pi;
l = length(x);
sinx = sin(x);
sinp = (1+.01*randn(1,l)).*sinx;

cosx = (sinx(3:l)-sinx(1:l-2))/.02;
cosp = (sinp(3:l)-sinp(1:l-2))/.02;
err_f = max(abs(sinx-sinp))
err_fp = max(abs(cosx-cosp))

subplot(1,2,1)
plot(x,sinp,x,sinx,'r')
legend('sin(x) with noise', 'sin(x)');
xlabel('x')
%title('sin (x) with 1% noise')

subplot(1,2,2)
plot(x(2:l-1),cosp,x(2:l-1),cosx,'r')
xlabel('x')
legend('centered difference of noisy data', ...
    'centered difference ');
%title('cos (x) by noisy numerical differentiation')
```



Method of polynomial approximation

Example: Find a one-sided approximation to $f'(x_0)$ based on $f(x_0)$, $f(x_0+h)$ and $f(x_0+2h)$.

1. Approximate $f(x)$ by a degree-2 polynomial $p(x)$ with the given 3 points. Use Newton polynomial.

$$p(x) = c_0 + c_1(x - x_0) + c_2(x - x_0)(x - (x_0 + h)) \tag{11}$$

$$\begin{aligned} p(x_0) &= c_0 = f(x_0) && (12) \\ p(x_0 + h) &= c_0 + c_1 h = f(x_0 + h) && (13) \\ p(x_0 + 2h) &= c_0 + c_1(2h) + c_2(2h)(h) = f(x_0 + 2h) && (14) \end{aligned}$$

Solve the system with substitution or divided differences

$$c_0 = f(x_0)$$
$$c_1 = \frac{f(x_0 + h) - f(x_0)}{h}$$
$$c_2 = \frac{\frac{f(x_0+2h)-f(x_0+h)}{h} - \frac{(f(x_0+h)-f(x_0))}{h}}{2h} = \frac{f(x_0 + 2h) - 2f(x_0 + h) + f(x_0)}{2h^2}$$

Put together

$$p(x) = c_0 + c_1(x - x_1) + c_2(x - x_1)(x - x_2) = f(x_0) + \frac{f(x_0 + h) - f(x_0)}{h}(x - x_0)$$
$$+\frac{f(x_0 + 2h) - 2f(x_0 + h) + f(x_0)}{2h^2}(x - x_0)(x - x_0 - h)$$

2. Approximate $f'(x_0)$ by

$$p'(x_0) = c_1 + c_2(x_0 - x_1) + c_2(x_0 - x_2) = c_1 + c_2(-h)$$
$$= \frac{f(x_0 + h) - f(x_0)}{h} - \frac{f(x_0 + 2h) - 2f(x_0 + h) + f(x_0)}{2h}$$
$$= \frac{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h}$$

Finite difference differentiation matrices

- Let $x_i \in [a, b]$ such that $x_0 = a$, $x_1 = a + h$, $x_i = a + ih$, $\ldots$, $x_n = b$.
- $h = (b - a)/n$.
- $f(x_i) = f_i$ is the given data.
- If we want to approximate the derivative $f'(x_i)$ using centered differences,

$$f_1' = \frac{f_2 - f_0}{2h}, \quad f_i' = \frac{f_{i+1} - f_{i-1}}{2h}, \quad f_{n-1}' = \frac{f_n - f_{n-2}}{2h}.$$

- Then we can write the operator in matrix-vector form $\mathbf{f}' = D\mathbf{f}$, where

$$\mathbf{f} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix} = \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{bmatrix}, \quad D = \frac{1}{2h} \begin{bmatrix} -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \end{bmatrix}.$$

- Dimensions of vectors and matrices?

- $\mathbf{f}'$ is uniquely determined from $\mathbf{f}$.

- Using backward differences and the condition $f(x_0) = 0$,

$$\begin{bmatrix} f'(x_1) \\ f'(x_2) \\ \vdots \\ f'(x_n) \end{bmatrix} = \frac{1}{h} \begin{bmatrix} 1 & & & \\ -1 & 1 & & \\ & \ddots & \ddots & \\ & & -1 & 1 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix}.$$

- If we are given $\mathbf{f}'$ and the initial condition, then we can solve the linear system for $\mathbf{f}$.