2072U Computational Science I
Winter 2022

Week	Topic
1	Introduction
1–2	Solving nonlinear equations in one variable
3–4	Solving systems of (non)linear equations
5–6	Computational complexity
6–8	Interpolation and least squares
8–10	Integration & differentiation
10–12	Additional Topics

1. What conditions, how fast, how accurate?
2. Interpolation error
3. Computational complexity
4. Taylor polynomials

Key questions:

- Polynomial interpolation: what conditions, how fast, how accurate?
- What are Taylor polynomials?
- What are the differences between Taylor and interpolating polynomials?

The three questions:

1. When does it work?
2. How fast does it work?
3. How accurate is the result?

Theorem (Polynomial interpolation error)

Let $\{x_k\}_{k=0}^{n}$ be distinct interpolation nodes in $I \subset \mathbb{R}$ and let f be $n+1$ times continuously differentiable in I. Then, $\forall x \in I$, $\exists \xi \in I$ such that

$$E_n(x) := f(x) - \Pi_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{k=0}^{n} (x - x_k),$$

where Π_n is the unique polynomial interpolant of degree at most n that interpolates the data $\{(x_k, f(x_k))\}_{k=0}^{n}$.

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- What theorem says: size of error controlled by
  - size of $f^{(n+1)}(\xi)$
  - size of $\prod_{k=0}^{n}(x - x_k)$
- This error comes on top of the error of linear solving.

Because we can't know ξ unless we know the error, for practical application we use the theorem to find an upper bound on the error. In particular, the theorem implies:

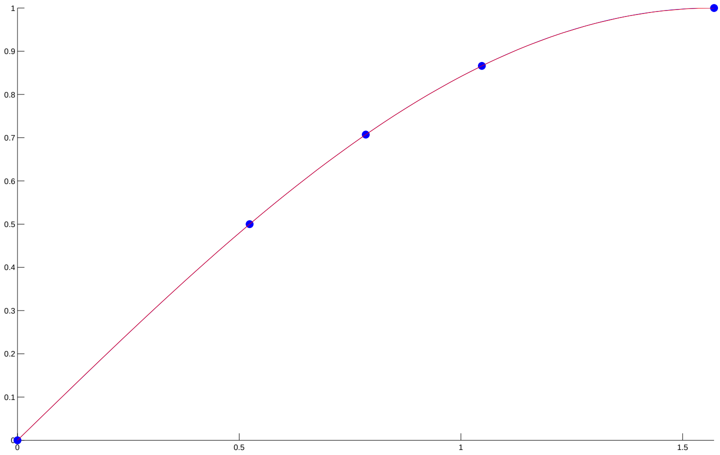
$$|E_n(x)| := |f(x) - \Pi_n(x)| \leq \max_{x \in I} \frac{\left|f^{(n+1)}(x)\right|}{(n+1)!} \prod_{k=0}^{n} |x - x_k|,$$

Back to the last example:

x	0	$\pi/6$	$\pi/4$	$\pi/3$	$\pi/2$
$\sin(x)$	0	$1/2$	$1/\sqrt{2}$	$\sqrt{3}/2$	1

these exact values can be used to approximate $sin(x)$ by a polynomial:

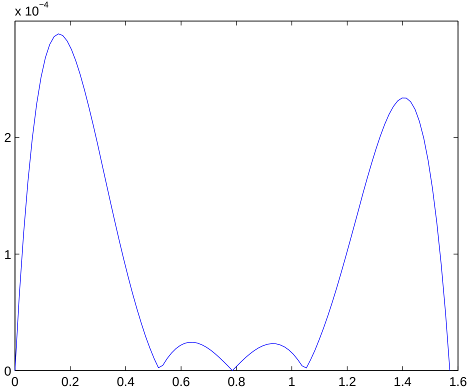
$$
\begin{aligned}
sin(x) \approx 0.9956261\, x + 0.021372984\, x^2 - 0.2043407\, x^3 \\
+ 0.02879711\, x^4 \qquad (\text{for } 0 < x < \pi/2)
\end{aligned}
$$



1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
0.5
1
1.5

Maximum Error

$$
\begin{aligned}
|f(x) - \Pi_n(x)| &\le \max_{x \in I} \frac{\left|f^{(n+1)}(x)\right|}{(n+1)!} \prod_{k=0}^{n} |x - x_k|, \\
|\sin(x) - \Pi_4(x)| &\le \max_{x \in I} \frac{\left|f^{(5)}(x)\right|}{5!} |x| \left|x - \frac{\pi}{6}\right| \left|x - \frac{\pi}{4}\right| \left|x - \frac{\pi}{3}\right| \left|x - \frac{\pi}{2}\right| \\
&\le \max_{x \in I} \frac{|\cos(x)|}{5!} |x| \left|x - \frac{\pi}{6}\right| \left|x - \frac{\pi}{4}\right| \left|x - \frac{\pi}{3}\right| \left|x - \frac{\pi}{2}\right| \\
&\le
\end{aligned}
$$



The difference between $\sin(x)$ and $\Pi_4(x)$ is less than 3×10^{-4} on $[0, \pi/2]$.

Three conclusions we can draw from the error formula:

1. Functions with *small higher derivatives* are well-approximated by interpolating polynomials.
   Such functions are *smooth*. The smoothest functions are the polynomials.
2. We can choose the location of the interpolation nodes to minimize the error (see CSII).
   In fact, it turns out that *equidistant* nodes are bad. Good sets of interpolation nodes have more nodes near the boundaries.
3. *Extra*polation is far more dangerous than *inter*polation.
   The upper bound for the error of extrapolation grows without bound – as x^{n+1}.

Recall: To compute the polynomial interpolant, we can solve $V\mathbf{a} = \mathbf{y}$:

$$\underbrace{\begin{bmatrix} 1 & x_0^1 & \cdots & x_0^{n-1} & x_0^n \\ 1 & x_1^1 & \cdots & x_1^{n-1} & x_1^n \\ 1 & x_2^1 & \cdots & x_2^{n-1} & x_2^n \\ \vdots & \vdots & & \vdots & \vdots \\ 1 & x_n^1 & \cdots & x_n^{n-1} & x_n^n \end{bmatrix}}_{V} \underbrace{\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}}_{\mathbf{a}} = \underbrace{\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{\mathbf{y}}$$

To compute FLOPS, we need to consider

- cost of building the matrix (see Assignment 3)
- cost of solving the system

Is there a more efficient approach?
Is there another approach that doesn't lead to badly conditioned systems?

Recall: The interpolant is written as:

$$\Pi_n(x) = \sum_{k=0}^{n} a_k \phi_k(x) = a_0\phi_0(x) + a_1\phi_1(x) + \cdots + a_n\phi_n(x)$$

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Instead of using monomial basis $\phi_k(x) = x^k$, use:

Newton polynomial basis

$$\phi_0(x) = 1 \qquad \phi_1(x) = x - x_0 \qquad \phi_2(x) = (x - x_0)(x - x_1) \quad \ldots$$

$$\phi_n(x) = (x - x_0)(x - x_1)\ldots(x - x_{n-1})$$

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With this basis, the resulting system of linear equations for the coefficients $\{a_k\}_{k=0}^{n}$ is $M\mathbf{a} = \mathbf{y}$, where

- the matrix M is now triangular
- the matrix M depends on the interpolation points x_k

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Write out interpolation conditions $\Pi_n(x_k) = y_k$ for new basis

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- $\vdots$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & \cdots \\ 1 & (x_1 - x_0) & 0 & 0 & \cdots \\ 1 & (x_2 - x_0) & (x_2 - x_0)(x_2 - x_1) & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}}_{M} \underbrace{\begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}}_{\mathbf{a}} = \underbrace{\begin{bmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}}_{\mathbf{y}}$$

Theorem (Taylor's Theorem with Lagrange Remainder)

If $f^{(n)}$ is continuous in the interval $[a, b]$ and if $f^{(n+1)}$ exists on the open interval (a, b), then for any points c and x in $[a, b]$ there exists a ξ between c and x such that

$$\begin{aligned} f(x) &= T_n(x) + R_n(x), \quad \textit{with} \\ T_n(x) &= \textit{nth Taylor polynomial} \\ &= \sum_{k=0}^{n} \frac{f^{(k)}(c)}{k!}(x-c)^k \quad \textit{and} \\ R_n(x) &= \textit{remainder or truncation error} \\ &= \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1} \end{aligned}$$

Example of a Taylor polynomial: e.g., $f(x) = e^x$, $c = 0$, $n = 3$

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- $R_3(x) = \frac{f^{(4)}(\xi)}{4!}x^4 = \frac{e^{\xi}}{24}x^4$

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For this function, we can consider the *series*

$$\exp(x) = \sum_{k=0}^{\infty} \frac{1}{k!}x^k$$

This series converges for any $x \in \mathbb{R}$.
We say it has an *infinite radius of convergence*.

Second example: Taylor polynomials for $\sin x$:

$$\sin x = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} x^{2k+1} \qquad (x \in \mathbb{R})$$

again with an infinite radius of convergence.

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$$S_7(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!}$$

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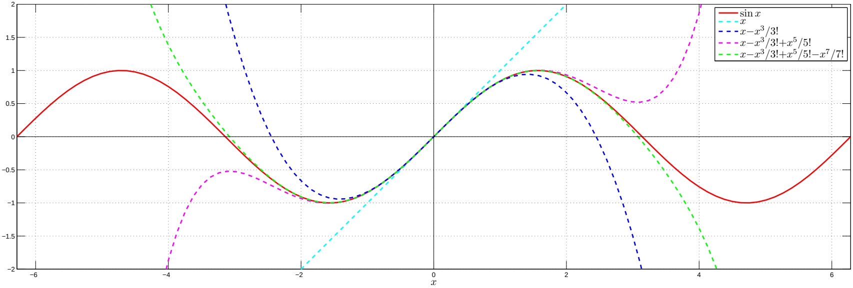
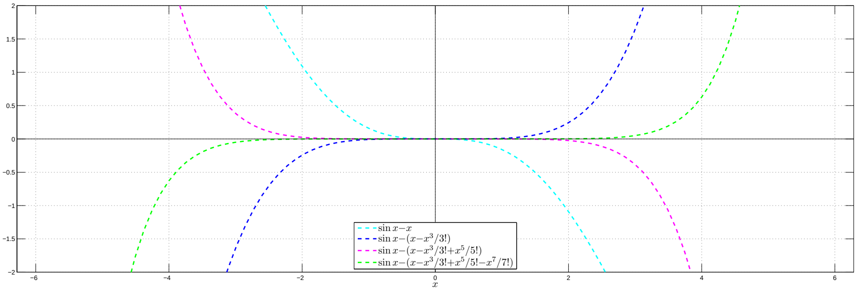
$$S_7(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} = x\left(1 + \frac{x^2}{2 \cdot 3}\left(-1 + \frac{x^2}{4 \cdot 5}\left(1 - \frac{x^2}{6 \cdot 7}\right)\right)\right)$$

Nested form of polynomials simplifies evaluation.

$\sin x$ and Taylor polynomials



Taylor polynomial errors for $\sin x$



Third example: $f(x) = \ln(1+x)$.

$$f^{(1)}(x) = \frac{1}{1+x} \qquad f^{(3)}(x) = \frac{2}{(1+x)^3}$$
$$f^{(2)}(x) = \frac{-1}{(1+x)^2} \qquad f^{(k)}(x) = \frac{(-1)^{k+1}(k-1)!}{(1+x)^k}$$

so $f^{(1)}(0) = 1$, $f^{(2)}(0) = -1$, $f^{(3)}(0) = 2, \ldots,$
$f^{(k)}(0) = (-1)^{k+1}(k-1)!$ and

$$\ln(1+x) = \sum_{k=1}^{n} \frac{(-1)^{k+1}}{k} x^k + R_n(x), \;\; R_n(x) = \frac{(-1)^n x^{n+1}}{(n+1)(1+\xi)^{n+1}}$$

This series converges for $-1 < x < 1$, we say the radius of convergence is 1.

Summary for Taylor polynomials:

- The Taylor polynomial exists is f is sufficiently smooth.
- We have an expression for the remainder.
- The computation of Taylor polynomials requires the computation of derivatives. Not many functions have such simple derivatives as in out examples!
- Properties of f at $x = c$ completely determine $T_n(x)$, so all information comes from $x = c$. The Taylor polynomial is useful as a local approximation only.
- For $|x - c|$ large, many terms needed for convergence.

In contrast, polynomial interpolation is useful on a whole domain.