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. Interpolation of data
2. Polynomial interpolation
3. Polynomial interpolation in a monomial basis
4. What conditions, how fast, how accurate?

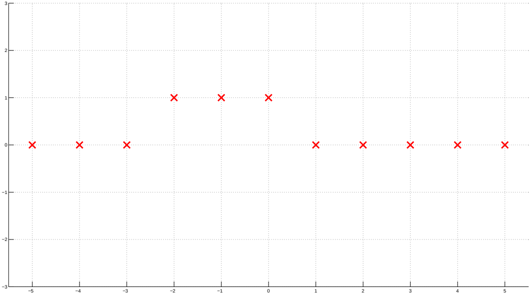
Key questions:

- What is an interpolant?
- How is the interpolation problem defined?
- What does polynomial interpolation mean?
- How is the solution of a polynomial interpolation problem found?
- What is a Vandermonde matrix?
- Our 3 questions: What conditions, how fast, how accurate?

Interpolation problem

Given $n+1$ data points $\{(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)\}$ with x_k distinct ($k = 0 : n$), determine a function $\tilde{f}$ that satisfies

$$\tilde{f}(x_k) = y_k \qquad (k = 0 : n).$$



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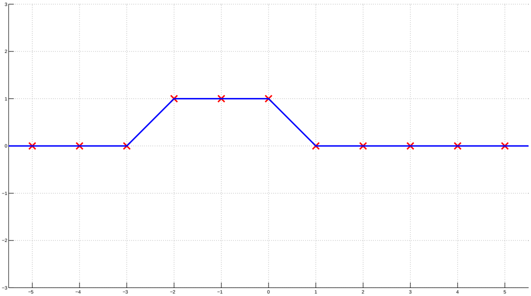

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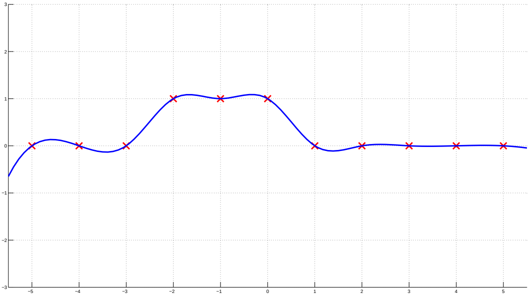

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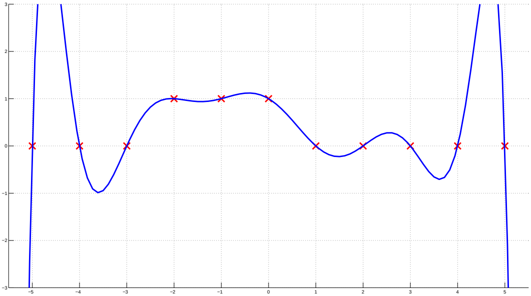

Remarks:

- $\tilde{f}$ is called an interpolating function or interpolant.
- x_k are interpolation points or nodes or abscissa.
- $\tilde{f}$ provides values for points in between the x_k
- Desirable to have $\tilde{f}$ smooth, differentiable, easy to compute.

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- Example: linear interpolation using SciPy's `interp1d`

Other classes of interpolating functions

Polynomial interpolant:

$$\tilde{f}(x) = \sum_{k=0}^{n} a_k x^k = a_0 + a_1 x + \cdots + a_n x^n$$

Trigonometric interpolant:

$$\tilde{f}(x) = \sum_{k=-M}^{M} c_k e^{ikx} \qquad (M = \lfloor n/2 \rfloor)$$

$$= c_{-M} e^{-iMx} + \cdots + c_0 + \cdots + c_n e^{iMx}$$

Rational interpolant:

$$\tilde{f}(x) = \frac{\sum_{j=0}^{k} a_j x^j}{\sum_{\ell=0}^{n-k-1} a_{k+\ell+1} x^\ell} \qquad (k < n)$$

$$= \frac{a_0 + a_1 x^1 + \cdots + a_k x^k}{a_{k+1} + a_{k+2} x^1 + \cdots + a_n x^{n-k-1}}$$

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- ϕ_k are basis functions, a_k are coefficients.
- For $\tilde{f} = \sum_{k=0}^{n} a_k \phi_k$, a_k depend linearly on data y_k $(k = 0 : n)$.
- For rational interpolation, different linear equations result.

Recall: Interpolation problem

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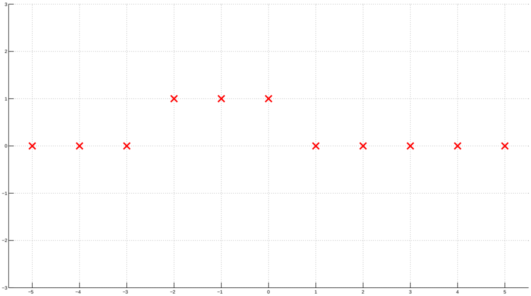

Polynomial interpolation problem

Given $n+1$ data points $\{(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)\}$ with x_k distinct ($k = 0:n$), determine a polynomial function Π_n of degree at most n that satisfies

$$\Pi_n(x_k) = y_k \qquad (k = 0:n).$$

In the case where the value y_k represents the value of a continuous function f sampled at $x = x_k$ ($k = 0:n$), the interpolating polynomial (or interpolant) is denoted $\Pi_n f$.

- n is (maximum) degree of interpolant.
- $n+1$ is number of data points.

Polynomial interpolation

- Polynomials easy to evaluate, differentiate, etc.
- Π_n lies in vector space of polynomials of degree at most n.
- $n+1$ coefficients to determine as $\deg(\Pi_n) \leq n$.

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

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- Gives $n+1$ equations in the $n+1$ unknowns a_k
- Reduces to linear algebra: solution of linear system of equations.

Polynomial interpolation

Theorem (Existence/Uniqueness of polynomial interpolation:)

If all interpolation nodes are distinct the interpolant exists. If we select the polynomial interpolant of the lowest possible order, it is unique.

Interpolation in power (monomial) basis:

- Choose $\phi_k(x) = x^k$, and thus write polynomial Π_n as

$$\begin{aligned}
\Pi_n(x) &= \sum_{k=0}^{n} a_k x^k \\
&= a_0 x^0 + a_1 x^1 + a_2 x^2 + \cdots + a_{n-1} x^{n-1} + a_n x^n \\
&= a_0 + x^1 a_1 + x^2 a_2 + \cdots + x^{n-1} a_{n-1} + x^n a_n
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- Write out interpolation conditions $\Pi_n(x_k) = y_k$ $(k = 0 : n)$

$$\begin{array}{ccccccccccc}
1 \cdot a_0 & + & x_0^1 \cdot a_1 & + & \cdots & + & x_0^{n-1} \cdot a_{n-1} & + & x_0^n \cdot a_n & = & y_0 \\
1 \cdot a_0 & + & x_1^1 \cdot a_1 & + & \cdots & + & x_1^{n-1} \cdot a_{n-1} & + & x_1^n \cdot a_n & = & y_1 \\
1 \cdot a_0 & + & x_2^1 \cdot a_1 & + & \cdots & + & x_2^{n-1} \cdot a_{n-1} & + & x_2^n \cdot a_n & = & y_2 \\
\vdots & & \vdots & & & & \vdots & & \vdots & = & \vdots \\
1 \cdot a_0 & + & x_n^1 \cdot a_1 & + & \cdots & + & x_n^{n-1} \cdot a_{n-1} & + & x_n^n \cdot a_n & = & y_n
\end{array}$$

Vandermonde system

- In matrix form, $V\mathbf{a} = \mathbf{y}$ where

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

- Matrix $V \in \mathbb{R}^{(n+1)\times(n+1)}$ is Vandermonde matrix
- $(n+1) \times (n+1)$ linear system of equations to solve for $\mathbf{a}$

Example of polynomial interpolation

- Consider data $(1.0, 2.0)$, $(1.1, 2.5)$, and $(1.2, 1.5)$
- In this case, $n = 2$ and data $\{(x_k, y_k)\}_{k=0}^{n}$ are

k	0	1	2
x_k	1.0	1.1	1.2
y_k	2.0	2.5	1.5

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- Interpolation conditions are

$$\begin{aligned}
\Pi_2(x_0) &= 1 \cdot a_0 + 1.0 \cdot a_1 + 1.00 \cdot a_2 = 2, \\
\Pi_2(x_1) &= 1 \cdot a_0 + 1.1 \cdot a_1 + 1.21 \cdot a_2 = 2.5, \\
\Pi_2(x_2) &= 1 \cdot a_0 + 1.2 \cdot a_1 + 1.44 \cdot a_2 = 1.5
\end{aligned}$$

Example of polynomial interpolation (cont.)

- Write system as $V\mathbf{a} = \mathbf{y}$

$$V\mathbf{a} = \begin{bmatrix} 1 & 1.0 & 1.00 \\ 1 & 1.1 & 1.21 \\ 1 & 1.2 & 1.44 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 2.5 \\ 1.5 \end{bmatrix} = \mathbf{y}$$

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- Solving the 3×3 linear system yields

$$\mathbf{a} = [a_0, a_1, a_2]^T = [-85.5, 162.5, -75]^T$$

- Resulting polynomial interpolant is

$$\begin{aligned} \Pi_2(x) &= \sum_{k=0}^{2} a_k x^k \\ &= -85.5 + 162.5x - 75x^2 \end{aligned}$$

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Proof of the theorem on existence and uniqueness:

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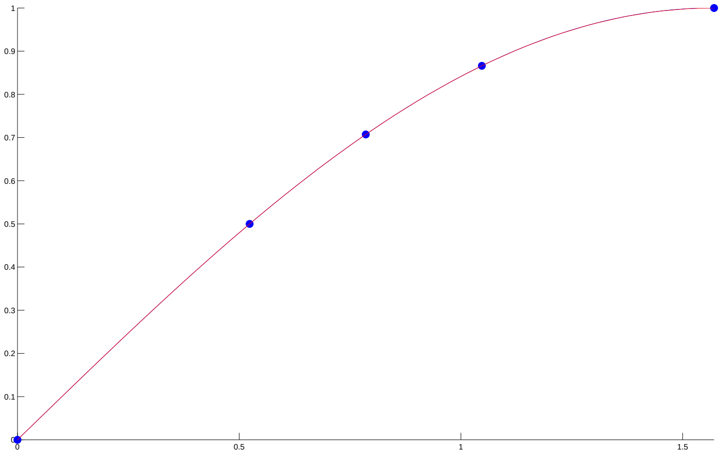
- However, this polynomial is of order n, so it can have no more than n zeros.
- This contradicts the assumption that the Vandermonde matrix is sigular. Therefore, it is non-singular.

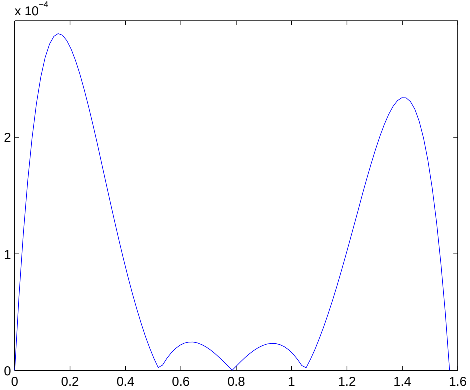
Another example:

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:

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


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



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

The three questions:

1. When does it work?

2. How fast does it work?

3. How accurate is the result?