

Numerical methods: basics and linear regression

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1. Numbers, approximations and errors
2. Interpolation
3. Least-square regression

Numbers, approximations and errors

It is better to be vaguely right than exactly wrong

Carveth Read, "Logic: Deductive and Inductive" (1898)

Double precision, floating point numbers

Most scientific computations represent real numbers using double precision floating-point numbers:

- Single precision → 32 bits = 4 Bytes
- Double precision → 64 bits = 8 Bytes

This is a binary version of the scientific or engineering notation:

- $c = +2.99792458 \times 10^8 \text{ m s}^{-1}$ scientific notation
- $c = +0.299792458 \times 10^9$ or $+0.299792458E09 \text{ m s}^{-1}$ engineering notation, **use this second notation to initialize your variables!**

Floating-point numbers are represented as

$$x_f = (-1)^s \times 1.f \times 2^{e-b}$$

Double precision numbers are stored contiguously (2 words of 32 bits):

- The sign s is stored as a single bit
- The exponent e is stored in the next 11 bits ($0 \leq e \leq 2047$). The actual exponent is $e - b$, with the bias $b = 1023$
- The fractional part of the mantissa f is stored in the remaining 52 bits

Double precision numbers have approximately 16 decimal places of precision and magnitudes in the range

$$4.9 \dots \times 10^{-324} \rightarrow 1.8 \dots \times 10^{308}$$

Representation scheme for IEEE doubles

Number name	Values of s , e , and f	Value of double
Normal	$0 < e < 2047$	$(-1)^s \times 2^{e-1023} \times 1.f$
Subnormal	$e = 0, f \neq 0$	$(-1)^s \times 2^{-1022} \times 0.f$
Signed zero	$e = 0, f = 0$	$(-1)^s \times 0.0$
$+\infty$	$s = 0, e = 2047, f = 0$	+INF
$-\infty$	$s = 1, e = 2047, f = 0$	-INF
Not a number	$s = u, e = 2047, f \neq 0$	NaN

Figure 1: IEEE representation

Exercise

Write a program that determines the underflow and overflow limits.

→ Take a number, keep dividing or multiplying until it becomes 0 or INF

Machine precision

The floating-point representation used to store numbers in a computer is of limited precision.

Machine precision, ϵ_m is the maximum positive number that can be added to the number stored as 1 without changing it:

$$1_{comp} + \epsilon_m := 1_{comp}$$

For example $1.0 + 10^{-16} \rightarrow 1.0$ for a double precision number.

The computer representation of a number can then be written as:

$$x_c = x(1 \pm \epsilon_x)$$

where the error $|\epsilon_x| \leq \epsilon_m$

Exercise

Write a program to determine the machine precision (for double precision numbers)

Subtractive Cancellation

Let's consider the subtraction of two numbers $a = b - c$. In the computer representation this can be approximately written as

$$a_c \simeq b_c - c_c \simeq b(1 + \epsilon_b) - c(1 + \epsilon_c) \simeq a \left(1 + \frac{b}{a} \epsilon_b - \frac{c}{a} \epsilon_c \right)$$

→ For example, if $b \gg c$ then $a \sim b$ and $a_c \sim a(1 + \epsilon_b)$

→ But if $b \sim c$

$$a_c \simeq a \left[1 + \frac{b}{a} (\epsilon_b - \epsilon_c) \right]$$

The errors do not necessarily cancel out and we cannot assume any sign for the errors. Moreover, the error is multiplied by the large number $\frac{b}{a}$ (remember that $b \sim c \rightarrow a \sim 0$).

Exercise

Explore subtractive cancellation for the function

$$f(x) = \frac{1 - \sqrt{1 - t(x)^2}}{t(x)}$$

where

$$t(x) = e^{-\pi x}$$

Interpolation

- Data (mathematical functions, etc.) are represented as discrete sets of points.
- It is often the case that we need information on the data or a function (or its derivatives) at intermediate points, where we do not have the actual values.
- Interpolation is a method to obtain new data points from the discrete set of known data points.

Direct Method i

It can be proven that given $n + 1$ data points it is always possible to find a polynomial of order/degree n to pass through/reproduce the $n + 1$ points.

Direct Method

Given $n + 1$ data points the direct method assumes the following polynomial:

$$y = f(x) = a_0 + a_1x + a_2x^2 + \dots + a_nx^n$$

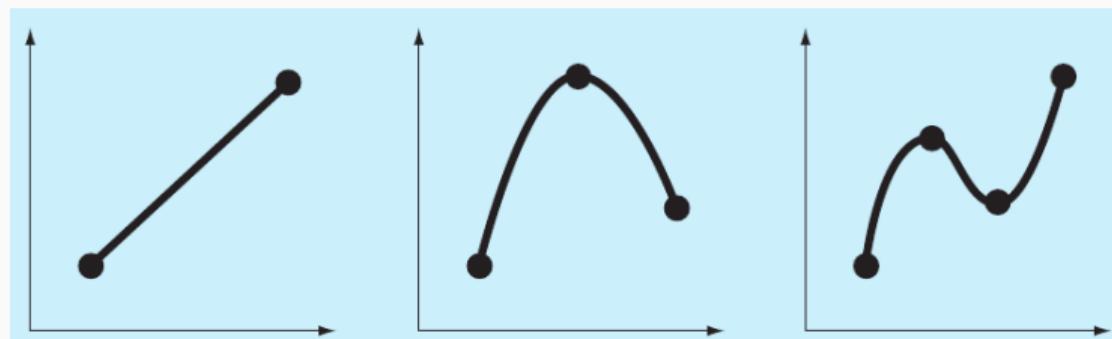


Figure 2: Examples of interpolating polynomials

Direct Method ii

With $n + 1$ values for x and the $n + 1$ corresponding values for y (i.e. the data set), we can solve for coefficients a_0, a_1, \dots, a_n by solving the $n + 1$ simultaneous linear equations.

For example, given two data points (x_0, y_0) and (x_1, y_1) , we can use the polynomial (linear function)

$$y = f(x) = a_0 + a_1x$$

to pass through the two data points:

$$y_0 = a_0 + a_1x_0$$

$$y_1 = a_0 + a_1x_1$$

Solving for a_0 and a_1 gives the analytical expression of the function $f(x)$, which can be used as the basis for interpolation - estimating the missing data points y in-between x_0 and x_1 .

Newton's divided-difference interpolating polynomial i

Given a set of $n + 1$ data points

$$(x_0, y_0), \dots, (x_j, y_j), \dots, (x_k, y_k)$$

where no two x_j are the same, the Newton interpolation polynomial is a linear combination of Newton basis polynomials:

$$N(x) := \sum_{j=0}^k a_j n_j(x)$$

with the Newton basis polynomials defined as

$$n_j(x) := \prod_{i=0}^{j-1} (x - x_i)$$

for $j > 0$ and $n_0(x) \equiv 1$.

Newton's divided-difference interpolating polynomial ii

The coefficients of the polynomial are defined as

$$a_j := [y_0, \dots, y_j]$$

where

$$[y_0, \dots, y_j]$$

is the notation for **divided differences**.

Example of divided differences

$$[y_0] = y_0$$

$$[y_0, y_1] = \frac{y_1 - y_0}{x_1 - x_0}$$

$$[y_0, y_1, y_2] = \frac{[y_1, y_2] - [y_0, y_1]}{x_2 - x_0} = \frac{\frac{y_2 - y_1}{x_2 - x_1} - \frac{y_1 - y_0}{x_1 - x_0}}{x_2 - x_0} = \frac{y_2 - y_1}{(x_2 - x_1)(x_2 - x_0)} - \frac{y_1 - y_0}{(x_1 - x_0)(x_2 - x_0)}$$

$$[y_0, y_1, y_2, y_3] = \frac{[y_1, y_2, y_3] - [y_0, y_1, y_2]}{x_3 - x_0}$$

Newton's divided-difference interpolating polynomial iii

Thus Newton polynomial can be written as

$$N(x) = [y_0] + [y_0, y_1](x - x_0) + \cdots + [y_0, \dots, y_k](x - x_0)(x - x_1) \cdots (x - x_{k-1})$$

Given two data points Newton's polynomial takes the form

$$y = f(x) = a_0 + a_1(x - x_0)$$

with the coefficients

$$a_0 = y_0$$

$$a_1 = \frac{y_1 - y_0}{x_1 - x_0}$$

The first derivative of the function at $x = x_0$ is $f'(x_0) = a_1 = \frac{y_1 - y_0}{x_1 - x_0}$, which is the *forward* divided difference.

Lagrange interpolating polynomial i

This is another form for the interpolating polynomial and it is essentially a reformulation of Newton polynomial in order to avoid the computation of divided differences.

The Lagrange form specifies the interpolation polynomial as:

$$f_n(x) := \sum_{i=0}^n L_i(x)f(x_i)$$

$$L_i(x) := \prod_{\substack{0 \leq m \leq n \\ m \neq i}} \frac{x - x_m}{x_i - x_m} = \frac{(x - x_0)}{(x_i - x_0)} \cdots \frac{(x - x_{i-1})}{(x_i - x_{i-1})} \frac{(x - x_{i+1})}{(x_i - x_{i+1})} \cdots \frac{(x - x_n)}{(x_i - x_n)}$$

where n is the order of the polynomial.

Example

For two data points, the polynomial of order $n = 1$ is

$$\begin{aligned}f_1(x) &= L_0 f(x_0) + L_1 f(x_1) \\&= \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)\end{aligned}$$

The first derivative also matches that of the divided difference method:

$$\begin{aligned}f'(x) &= \frac{f(x_0)}{x_0 - x_1} + \frac{f(x_1)}{x_1 - x_0} \\&= \frac{f(x_1) - f(x_0)}{x_1 - x_0}\end{aligned}$$

Note that $L_i(x) = 1$ at $x = x_i$ and zero for all other sample points.

Lagrange interpolating polynomial iii

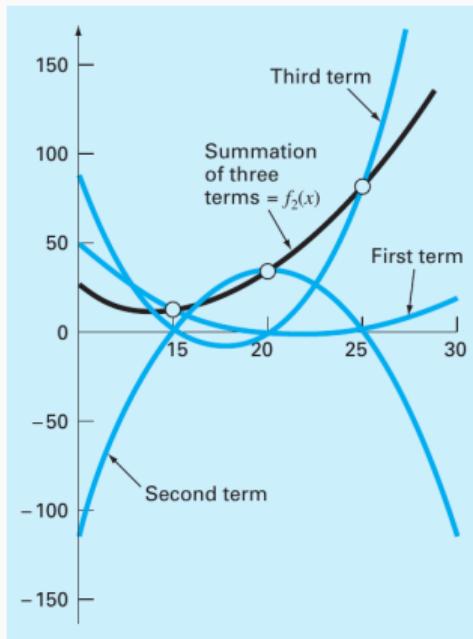


Figure 3: Example of a second order polynomial in Lagrange form: $f_2(x) = L_0(x)f(x_0) + L_1(x)f(x_1) + L_2(x)f(x_2)$

- Direct method requires more computational effort for large number of data points $n + 1$ and can yield inaccurate results
- Newton and Lagrange methods have similar computational effort. Lagrange is easier to program.
- Use Newton if the order of the polynomial is not known a priori, Lagrange otherwise.

Discussion on interpolation ii

Fitting high-order polynomials can lead to oscillatory behaviour

→ need for piecewise interpolation or other methods

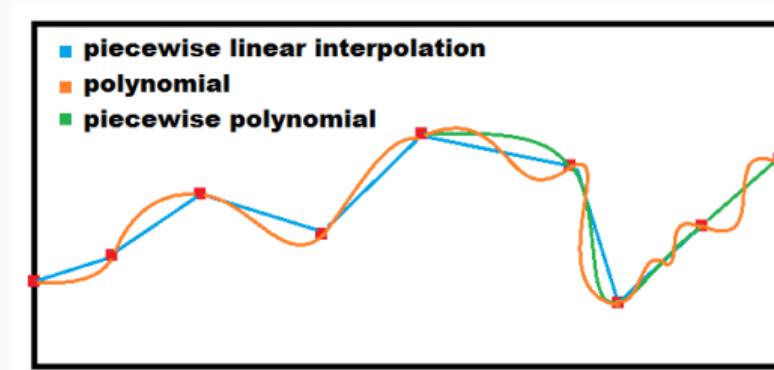


Figure 4: Example of piecewise interpolation

See jupyter notebook

You can explore polynomial interpolation and Runge's phenomenon in the jupyter notebook

Runge_phenomenon.ipynb

Discussion on interpolation iii

A commonly used technique is spline interpolation. In this case the function used to interpolate is a piecewise polynomial called a spline.

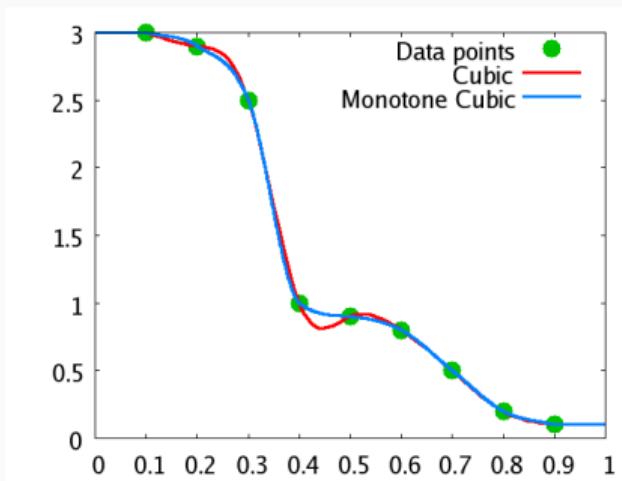


Figure 5: Monotonic cubic interpolation using cubic Hermite splines

Least-square regression

Introduction

Fitting a polynomial to a set of data is not always a good idea, especially experimental data!

A better strategy is to derive an approximating function that fits the shape or general trend of the data.

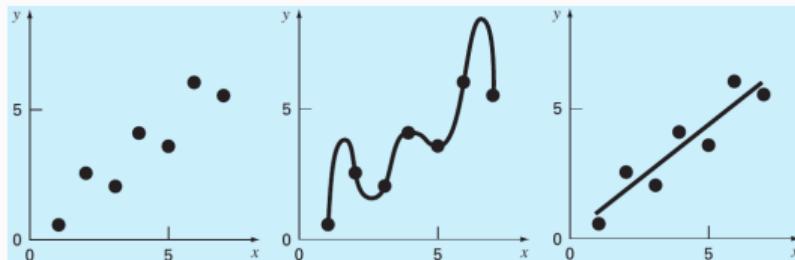


Figure 6: Least-squares fit vs polynomial interpolation

Linear regression i

The simplest is to fit a straight line $f(x) = a_0 + a_1x$ to a set of data $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$:

$$y_i = f(x_i) + \epsilon_i = a_0 + a_1x_i + \epsilon_i$$

where ϵ , the error or residual, is the discrepancy between the true value of y_i (the data) and the model $f(x)$:

$$\epsilon_i = y_i - (a_0 + a_1x_i)$$

One strategy that provides the "best fit" to the data is to minimize the sum of the squares of the residuals:

$$S(a_0, a_1) = \sum_{i=1}^n (\epsilon_i)^2 = \sum_{i=1}^n (y_i - f(x_i))^2 = \sum_{i=1}^n [y_i - a_0 - a_1x_i]^2$$

We can minimize the function $S(a_0, a_1)$ by setting the gradient to zero:

$$\frac{\partial S}{\partial a_0} = -2 \sum_{i=1}^n (y_i - a_0 - a_1x_i) = 0$$

$$\frac{\partial S}{\partial a_1} = -2 \sum_{i=1}^n [(y_i - a_0 - a_1x_i)x_i] = 0$$

Linear regression ii

Let's rewrite the first equation as:

$$-\sum_{i=1}^n y_i + \sum_{i=1}^n a_0 + \sum_{i=1}^n a_1 x_i = 0 \rightarrow -\sum_{i=1}^n y_i + n a_0 + \sum_{i=1}^n a_1 x_i = 0 \rightarrow a_0 n + a_1 \sum_{i=1}^n x_i = \sum_{i=1}^n y_i$$

and the second as:

$$-\sum_{i=1}^n y_i x_i + \sum_{i=1}^n a_0 x_i + \sum_{i=1}^n a_1 x_i^2 = 0 \rightarrow a_0 \sum_{i=1}^n x_i + a_1 \sum_{i=1}^n x_i^2 = \sum_{i=1}^n x_i y_i$$

The unknown a_0 and a_1 are then given by:

$$a_1 = \frac{n \sum_{i=1}^n x_i y_i - \sum_{i=1}^n x_i \sum_{i=1}^n y_i}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2}$$

$$a_0 = \frac{\sum_{i=1}^n x_i^2 \sum_{i=1}^n y_i - \sum_{i=1}^n x_i \sum_{i=1}^n x_i y_i}{n \sum_{i=1}^n x_i^2 - (\sum_{i=1}^n x_i)^2}$$

Using a more compact notation, which makes it easier for programming the method, let's define:

$$\bar{x} = \frac{\sum_{i=1}^n x_i}{n}$$

$$\bar{y} = \frac{\sum_{i=1}^n y_i}{n}$$

$$S_1 = \sum_{i=1}^n x_i y_i - n \bar{x} \bar{y}$$

$$S_2 = \sum_{i=1}^n x_i^2 - n \bar{x}^2$$

then

$$a_1 = \frac{S_1}{S_2}$$

$$a_0 = \bar{y} - a_1 \bar{x}$$

Exercise

Write a program that performs a fit to data using linear regression and use it to study the solar wind data from the ULYSSE satellite.