# Computational Methods and Modelling

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Lecture 4

Curve Fitting and Interpolation

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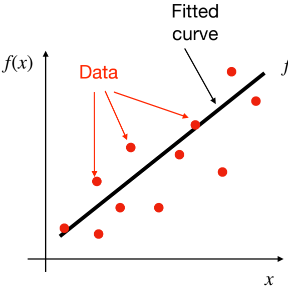
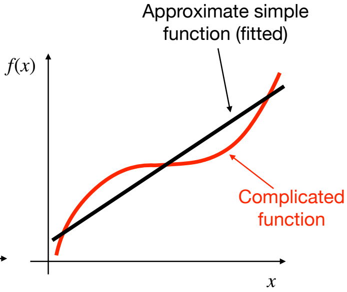
**Motivation:**

- Data is often available at discrete point along a continuum, but we may require estimates at points between the discrete values.
- We may require a simplified version of a complicated function: Compute values of the function at a number of discrete values fit a simpler function to these values.

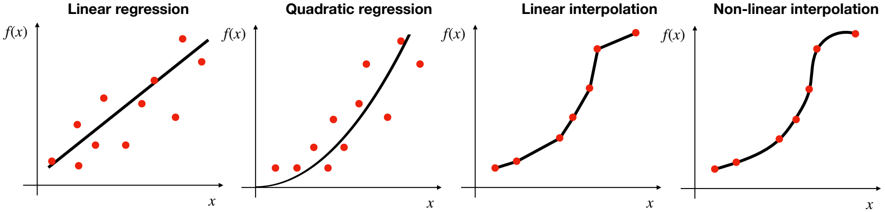


# Regression and Interpolation

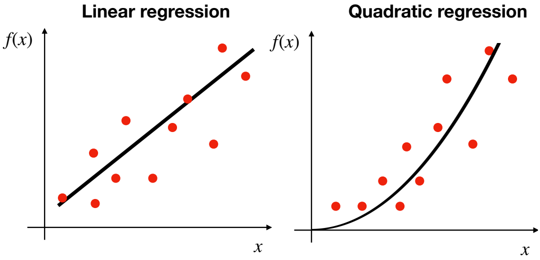
**Two general approaches:**

- Regression
  - If discrete exhibits a significant error or "noise".
  - We make no effort to intersect every point. Rather, the curve is designed to follow the pattern of the points taken as a group.
  - Example: *least-squares regression*.
- Interpolation
  - Data is known to be precise.
  - Fit a curve (or a series of curves) that passes directly through each of the points.



# Least-squares regression

- Derive an approximating function that fits the shape or general trend of the data without necessarily matching the individual points
- Possible approach: determine the line by visually inspecting the plotted data and then sketch a best line through the points. Although such "eyeball" approach has commonsense appeal and is valid for back-of-the-envelope calculations, they are deficient because they are arbitrary.
- Some criterion must be devised to establish a basis for the fit. One way to do this is to derive a curve that minimizes the discrepancy between the data points and the curve.
- A technique for accomplishing this objective is the **least-squares regression**.



# Linear regression

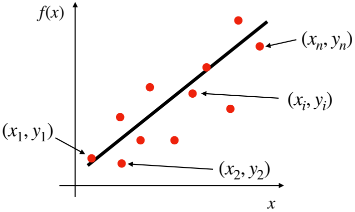
- The simplest example of regression is fitting a straight line to a set of paired observations: $(x_1, y_1)$, $(x_2, y_2)$, ... ,$(x_n, y_n)$.
- The mathematical expression for the straight line is:

$$y = a_0 + a_1 x + e \tag{1}$$

  - $a_0$ and $a_1$ are coefficients representing the intercept and the slope
  - $e$ is the error, or residual, between the model and the observations and can be represented also as:

$$e = y - a_0 - a_1 x \tag{2}$$

- The error, or residual, is the discrepancy between the true value and the approximate value, $a_0 + a_1 x$.



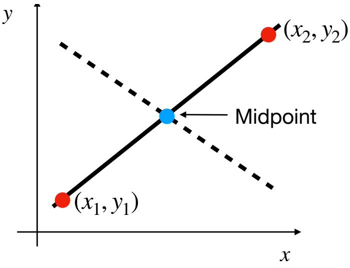
# Criteria for the best fit of a straight line

**We need a strategy to minimize the error $e$. Let's consider different strategies.**

- One strategy is to **minimize the sum of the errors for all the available data**:

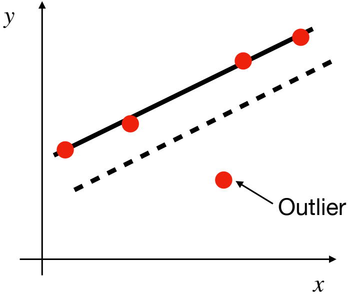
$$\sum_{i=1}^{n} e_i = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) \tag{3}$$

- This is an inadequate criterion.
- Example on the right with only two data points: obviously, the best fit is the solid line connecting the two points.
- Any straight line passing through the midpoint results in a minimum value of Eq. 3, equal to zero because the errors cancel.



# Criteria for the best fit of a straight line

- Another strategy for fitting a best line could be the **minimax criterion**
- We choose the line that minimizes the maximum distance among the points.
- This strategy is not good for regression because it gives undue influence to an outlier (a single point with a large error).



# Criteria for the best fit of a straight line

- A strategy that overcomes these shortcomings is to **minimize the sum of the squares of the residuals**:

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i)^2 \tag{4}$$

- This criterion has a number of advantages, including the fact that it yields a unique line for a given set of data.
- Least square regression can also be applied to non-linear fits (parabolic, exponential, ...).

- We want to use the following model to fit some data:

$$y = a_0 + a_1 x \tag{5}$$

- This means we have to determine $a_0$ and $a_1$ such that the least-square error (Eq. 4) is minimised.
- This can be done with the following approach:
  - Differentiate Eq. 4 with respect to each coefficient:

$$\frac{\partial S_r}{\partial a_0} = -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i) \tag{6}$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum_{i=1}^{n} [(y_i - a_0 - a_1 x_i) x_i] \tag{7}$$

  - Setting these derivatives equal to zero will result in a minimum $Sr$:

$$0 = \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} a_0 - \sum_{i=1}^{n} a_1 x_i \tag{8}$$

$$0 = \sum_{i=1}^{n} y_i x_i - \sum_{i=1}^{n} a_0 x_i - \sum_{i=1}^{n} a_1 x_i^2 \tag{9}$$

# Least-Squares Fit of a Straight Line II

- Realizing that $\sum_{i=1}^{n} a_0 = na_0$ and grouping the terms, we obtain the two equations for the two unknowns ($a_0$ and $a_1$):

$$na_0 + \left(\sum_{i=1}^{n} x_i\right) a_i = \sum_{i=1}^{n} y_i \tag{10}$$

$$\left(\sum_{i=1}^{n} x_i\right) a_0 + \left(\sum_{i=1}^{n} x_i^2\right) a_1 = \sum_{i=1}^{n} x_i y_i \tag{11}$$

- which give the solution for $a_0$ and $a_1$:

$$a_1 = \frac{n \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n \sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \tag{12}$$

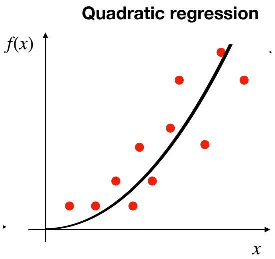
$$a_0 = \bar{y} - a_1 \bar{x} \tag{13}$$

where $\bar{y} = \left(\sum_{i=1}^{n} y_i\right)/n$ and $\bar{x} = \left(\sum_{i=1}^{n} x_i\right)/n$ are the means of y and x, respectively.

# Polynomial regression

- Some data, although exhibiting a marked pattern such as seen in the figure, is poorly represented by a straight line.
- A curve would be better suited to fit the data (a parabola in the case of the figure).
- A second-order polynomial (quadratic, parabola) has the form:

$$y = a_0 + a_1 x + a_2 x^2 + e \tag{14}$$




- More generally, it is possible to fit polynomials of any order $m$ to the data using **polynomial regression**:

$$y = a_0 + a_1 x + a_2 x^2 + \ldots + a_m x^m + e \tag{15}$$

# Quadratic regression

- For this case the sum of the squares of the residuals is:

$$S_r = \sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i - a_2 x_i^2)^2 \tag{16}$$

- With the same procedure employed in the linear case, we take the derivatives with respect to each of the unknown coefficients of the polynomial and equate them to zero:
- Setting these derivatives equal to zero will result in a minimum $Sr$:

$$\frac{\partial S_r}{\partial a_0} = -2 \sum_{i=1}^{n} (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0 \tag{17}$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum_{i=1}^{n} x_i (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0 \tag{18}$$

$$\frac{\partial S_r}{\partial a_2} = -2 \sum_{i=1}^{n} x_i^2 (y_i - a_0 - a_1 x_i - a_2 x_i^2) = 0 \tag{19}$$

# Quadratic regression II

- We can rearrange the terms and obtain three equations for the three unknown coefficients:

$$n a_0 + \left( \sum_{i=1}^{n} x_i \right) a_i + \left( \sum_{i=1}^{n} x_i^2 \right) a_2 = \sum_{i=1}^{n} y_i \tag{20}$$

$$\left( \sum_{i=1}^{n} x_i \right) a_0 + \left( \sum_{i=1}^{n} x_i^2 \right) a_1 + \left( \sum_{i=1}^{n} x_i^3 \right) a_2 = \sum_{i=1}^{n} x_i y_i \tag{21}$$

$$\left( \sum_{i=1}^{n} x_i^2 \right) a_0 + \left( \sum_{i=1}^{n} x_i^3 \right) a_1 + \left( \sum_{i=1}^{n} x_i^4 \right) a_2 = \sum_{i=1}^{n} x_i^2 y_i \tag{22}$$

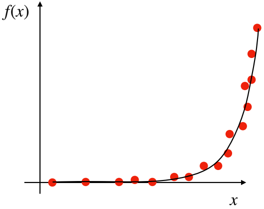
- The above three equations are linear and have three unknowns: $a_0$, $a_1$, and $a_2$.
- The coefficients of the unknowns can be calculated directly from the observed data.

# General nonlinear regression

- There are many cases in engineering where nonlinear models must be fit to data.
- These models have a nonlinear dependence on their parameters. For example an exponential:

$$f(x) = a_0(1 - e^{-a_1 x}) + error \tag{23}$$

- For the general nonlinear case, it is not always possible to find the coefficients ($a_0$ and $a_1$ in the exponential fit above) analytically with an algebraic manipulation of the equations like we did with the linear and polynomial fits.
- A numerical optimization method (e.g., Gauss-Newton method) is required to find the coefficients.

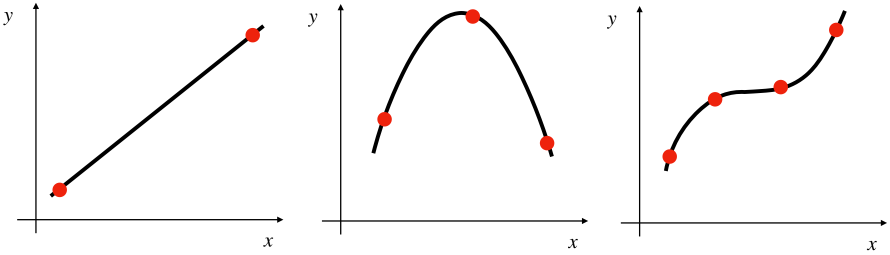


# Interpolation

- Often, it is needed to estimate intermediate values between precise data points.
- The most common method used for this purpose is polynomial interpolation.
- In general, a polynomial can be written as:

$$f(x) = a_0 + a_1 x + a_2 x^2 + ... + a_n x^n \tag{24}$$

- For $n+1$ data points, there is one and only one polynomial of order $n$ that passes through all the points.

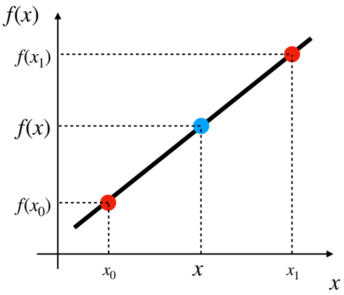


# Linear interpolation with Newton polynomials

- **Newton's divided-difference interpolating polynomial** is among the most popular and useful forms.
- The first order interpolation with a Newton polynomial is:

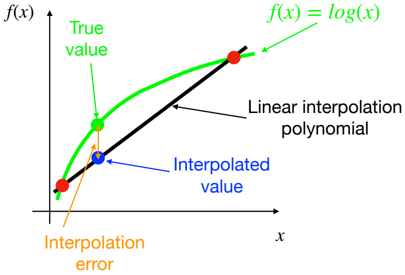
$$f(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0) \tag{25}$$

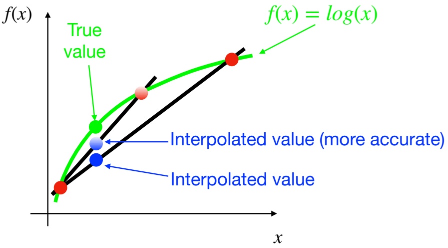
- Notice that besides representing the slope of the line connecting the points, the term $\frac{f(x_1)-f(x_0)}{x_1-x_0}$ is a finite-divided-difference approximation of the first derivative.
- In general, the smaller the interval between the data points, the better the approximation.



# Using interpolation to approximate a function

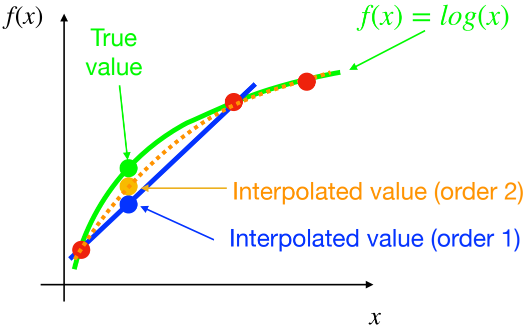
- Let's say we want to approximate a function, for example $f(x) = log(x)$ shown in the figure.
- We sample the function at two locations and use the linear interpolation to approximate the function between the two locations.
- If the two points are close, we obtain a better approximation (right figure).



# First and second order interpolation

- With first order interpolation, we approximate the underlying function with a straight line.
- With second order interpolation, we approximate the underlying function with a parabola.
- For second order interpolation, we need three points to construct a parabola that goes through them.
- Second order is more accurate (usually, not always).



# Splines

- Spline interpolation is a very flexible and powerful interpolation method.
- The interpolant is a special type of piecewise polynomial called a spline.
- Spline interpolation fits low-degree polynomials to small subsets of the values.
- The cubic spline is the most common. It can be made very accurate.
- Avoid the oscillatory behavior that occurs if we fit a single high-order polynomial using many data points.