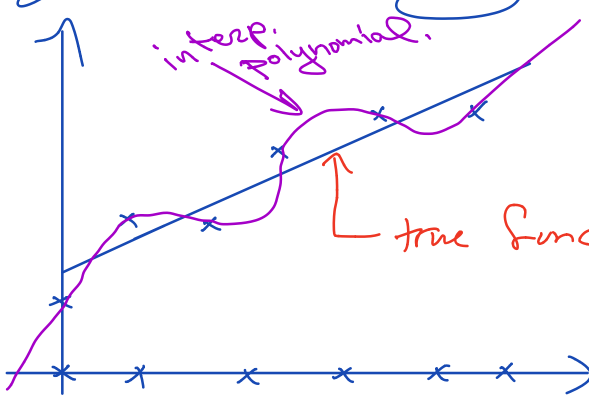
Least Squares Approximation

So far, we have been trying to fit data (x_i, y_i) exactly with functions
(e.g. polynomials, splines)

But often data is "noisy" and while it may originate from a simple function (e.g. $ax+b$), due to noise/error, no, e.g. straight line may fit the data



(x_i, y_i)
$i = 1, \ldots, m$

Can we do better; by trying, e.g. to find the best straight line fit?

Many possible notions of "better"

Example: want to pick a_0, a_1 to minimize

$$E_\infty(a_0, a_1) = \max_{1 \le i \le m} | y_i - (a_1 x_i + a_0) |$$

"minimax error"

$$E_1(a_0, a_1) = \sum_{i=1}^{m} | y_i - (a_1 x_i + a_0) |$$

absolute deviation

$$E_2(a_0, a_1) = \sum_{i=1}^{m} \left(y_i - (a_1 x_i + a_0) \right)^2$$

least squares

Each has pros & cons

(computational complexity, robustness to outliers, etc...)

(see book)

We will focus on Least Squares.

Warmup: Linear least squares (regression)

To minimize:

$$E(a_0, a_1) = \sum_{i=1}^{m} \left(y_i - (a_1 x_i + a_0) \right)^2$$

we solve

$$\frac{\partial E}{\partial a_0} = 0 \, , \quad \frac{\partial E}{\partial a_1} = 0$$

$$\Longleftrightarrow \begin{cases} 0 = \dfrac{\partial}{\partial a_0} \displaystyle\sum_{i=1}^{m} \left(y_i - (a_1 x_i + a_0) \right)^2 \\ 0 = \dfrac{\partial}{\partial a_1} \displaystyle\sum_{i=1}^{m} \left(y_i - (a x_i + a_0) \right)^2 \end{cases}$$

$$\Longleftrightarrow \begin{cases} 0 = \cancel{2} \displaystyle\sum_{i=1}^{m} \left(y_i - (a_1 x_i + a_0) \right)(-1) \\ 0 = \cancel{2} \displaystyle\sum_{i=1}^{m} \left(y_i - (a_1 x_i + a_0) \right)(-x_i) \end{cases}$$

normal equations

$$\begin{cases} a_0 m + a_1 \sum_{i=1}^{m} x_i = \sum_{i=1}^{m} y_i \\ a_0 \sum_{i=1}^{m} x_i + a_1 \sum_{i=1}^{m} x_i^2 = \sum_{i=1}^{m} x_i y_i \end{cases}$$

2 eq'ns, 2 unknowns

solve to get

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

$$a_1 = \frac{m \sum x_i y_i - \sum x_i \sum y_i}{m\left(\sum_{i=1}^{m} x_i^2\right) - \left(\sum_{i=1}^{m} x_i\right)^2}$$

(we have all the x_i's & y_i's so we can find a_0 & a_1)

Polynomial least squares

Same idea; if $P_n(x)$ is a polynomial of degree n, $P_n(x) = \sum_{i=0}^{n} a_i x^i$ and we have m data points (x_i, y_i), $i = 1, \dots, m$ with $n < m-1$, we can minimize

$$E = \sum_{i=1}^{m} (y_i - P_n(x_i))^2$$

$$= \sum_{i=1}^{m} y_i^2 - 2\sum_{i=1}^{m} \underbrace{P_n(x_i)}_{a_0 + a_1 x_i + a_2 x_i^2 + \cdots + a_n x_i^n} y_i + \sum_{i=1}^{m} (P_n(x_i))^2$$

Taking derivatives

$$\frac{\partial E}{\partial a_j} = 0 \quad , \quad j = 0, \dots, n$$

gives us $n+1$ normal equations
to solve for $a_0, \dots, a_n$
($n+1$ unknowns)

Normal Equations have a
unique solution when the
x_i are distinct.

Can use the same idea to
fit different functions.

e.g. $y = be^{ax}$ or $y = bx^a$

Procedure: (1) Write $E(a,b)$

(2) $\dfrac{\partial E}{\partial a} = 0$, $\dfrac{\partial E}{\partial b} = 0$

(3) Solve to find a, b