Function Approximation I

- Given data points $(x_i, y_i), i = 1, \ldots, n$
  Find a function to approximate these points
- We can do interpolation

$$y_i = f(x_i), i = 1, \ldots, n.$$

- However, data may have noise.
- Thus in some situations for the given points we get an approximation function that has the "trend" of these points

Function Approximation II

- Minimizing the error:

$$\min_f \sum_{i=1}^{n} (y_i - f(x_i))^2 \tag{1}$$

or

$$\min_f \sum_{i=1}^{n} |y_i - f(x_i)|$$

with

$$f(x) = ax + b$$

Assume $x \in R^1, y \in R^1$

Function Approximation III

- (1): least square approximation
  why (1): easier calculation

Least Square Approximation I

- Now we would like to find a and b. Let

$$E = \sum_{i=1}^{n} (y_i - (ax_i + b))^2$$

Least Square Approximation II

Then

$$
\begin{aligned}
& \min_{a,b} \sum_{i=1}^{n} (y_i - (ax_i + b))^2 \\
\equiv \; & \min_{a,b} \sum_{i=1}^{n} y_i^2 - 2y_i(ax_i + b) + (ax_i + b)^2 \\
\equiv \; & \min_{a,b} \sum_{i=1}^{n} -2y_i(ax_i + b) + a^2x_i^2 + 2abx_i + b^2
\end{aligned}
$$

Least Square Approximation III

$$
\begin{aligned}
\equiv \; & \min_{a,b} \Bigg((\sum_{i=1}^{n} -2y_i x_i)a + (\sum_{i=1}^{n} -2y_i)b + (\sum_{i=1}^{n} x_i^2)a^2 \\
& +(\sum_{i=1}^{n} 2x_i)ab + nb^2 \Bigg)
\end{aligned}
$$

Least Square Approximation IV

- First derivative

$$\frac{\partial E}{\partial a} = 0 \Rightarrow$$

$$(\sum_{i=1}^{n} -2y_i x_i) + 2(\sum_{i=1}^{n} x_i^2)a + (\sum_{i=1}^{n} 2x_i)b = 0$$

$$\frac{\partial E}{\partial b} = 0 \Rightarrow$$

$$(\sum_{i=1}^{n} -2y_i) + (\sum_{i=1}^{n} 2x_i)a + 2nb = 0$$

Least Square Approximation V

- Rearrange terms:
  Define

$$S_{xx} = \sum_{i=1}^{n} x_i^2, S_x = \sum_{i=1}^{n} x_i$$

$$S_{xy} = \sum_{i=1}^{n} x_i y_i, S_y = \sum_{i=1}^{n} y_i$$

Least Square Approximation VI

Now

$$S_{xx}a + S_x b = S_{xy}$$
$$S_x a + nb = S_y$$

Then

$$a = \frac{nS_{xy} - S_x S_y}{nS_{xx} - S_x^2}$$
$$b = \frac{S_{xx}S_y - S_x S_{xy}}{nS_{xx} - S_x^2}$$

Least Square Approximation VII

- Issues:

  Does $\nabla E = 0$ imply optimality ?
- We need secondary derivative (i.e. $\nabla^2 E$) to be positive semi-definite

$$
\begin{aligned}
\nabla^2 E &= \begin{bmatrix} \frac{\partial E}{\partial a \partial a} & \frac{\partial E}{\partial a \partial b} \\ \frac{\partial E}{\partial b \partial a} & \frac{\partial E}{\partial b \partial b} \end{bmatrix} \\
&= \begin{bmatrix} 2S_{xx} & 2S_x \\ 2S_x & 2n \end{bmatrix}
\end{aligned}
$$

Least Square Approximation VIII

$S_{xx} > 0, n > 0$, and determinant:

$$\begin{aligned} & S_{xx} n - S_x^2 \\ = \; & \sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} 1^2 - (\sum_{i=1}^{n} x_i)^2 \geq 0 \end{aligned}$$

Remember

$$(a_1 b_1 + \cdots + a_n b_n)^2 \leq (a_1^2 + \cdots + a_n^2)(b_1^2 + \cdots + b_n^2)$$

Least Square Approximation IX

- Nonlinear least-square

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

with

$$f(x) = ax^2 + bx + c$$

Quadratic least square

- Now we have three variables and three equations
- The situation is similar to standard least square, so we do not get into details