Linear Regression

Thursday, January 16, 2020 13:34

Linear Regression

Real-value target function

(instead of yes/no, we estimate a real value)

Approximate some function $y_n = f(\underline{x}_n)$ by a linear function

MODEL SETUP

$\mathcal{D} = \{(\underline{x}_1, y_1) \dots\}$ same as before

$\underline{x}_i \in \mathbb{R}^{d+1}$ $y_i \in \mathbb{R}$ $\underline{w} \in \mathbb{R}^{d+1}$

Regression: $\hat{y}_n = \underline{w}^T \underline{x}_n$

(predict by $\underline{w}^T \cdot \underline{x}_n$)

COMPACT REPRESENTATION

Data matrix

$$X = \begin{bmatrix} x_{10} = 1, & x_{11}, & \dots & x_{1d} \\ x_{20} = 1, & x_{21} & \dots & x_{2d} \\ x_{30} = 1, & x_{31} & \dots & x_{3d} \\ x_{N0} = 1, & x_{N1} & \dots & x_{Nd} \end{bmatrix} \in \mathbb{R}^{N \times (d+1)}$$

$$X = \begin{bmatrix} \underline{x}_1^T \\ \underline{x}_2^T \\ \vdots \\ \underline{x}_N^T \end{bmatrix}$$

we represent input data as a matrix for compact computation

Observation Vector

$$\underline{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix} \in \mathbb{R}^N$$

$$\Rightarrow \underbrace{\hat{\underline{y}}}_{N \text{ size}} = \begin{bmatrix} \underline{x}_1^T \underline{w} \\ \underline{x}_2^T \underline{w} \\ \vdots \\ \underline{x}_N^T \cdot \underline{w} \end{bmatrix} = \underbrace{X}_{N \times (d+1) \text{ size}} \underbrace{\underline{w}}_{(d+1) \text{ size}}$$

ideally $\hat{\underline{y}} = \underline{y}$ after training.

case ① $N < d+1$:

Many Solutions (# of unknowns > # of equations)

case ② $N = d+1$: (overfitting)

Single/Unique solution: $\hat{y} = y$

case ③ $N > d+1$:

No solution for $\hat{y} = y$

$\Rightarrow \hat{y} \neq y$ (but approximation is good enough)

$\Rightarrow$ Typically we want $N \gg d+1$ so we do not suffer from overfitting

Loss Function

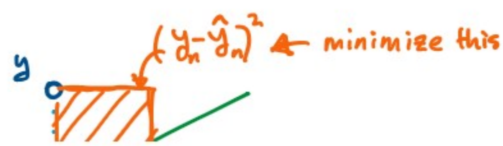
intuition: we can measu distance:

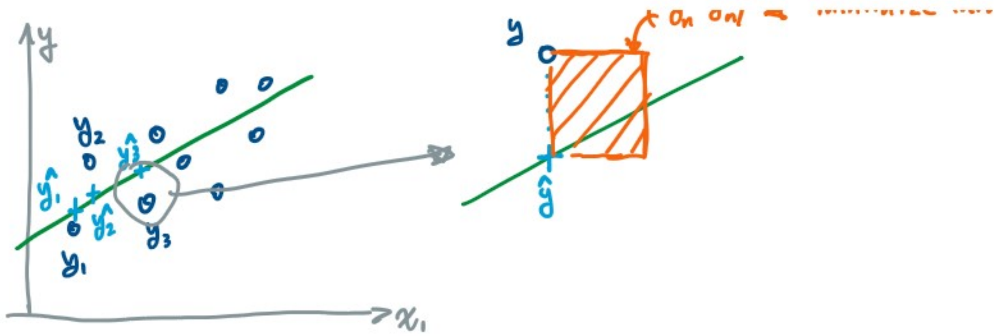
$$\boxed{E_{in}(\underline{w}) = \frac{1}{N} \|\underline{y} - \hat{\underline{y}}\|_2 = \frac{1}{N} \sum_{n=1}^{N} (y_n - \hat{y}_n)^2}$$

$$= \frac{1}{N} \|\underline{y} - X\underline{w}\|^2 = \frac{1}{N} \sum_{n=1}^{N} \underbrace{(y_n - \underline{x}_n^T \underline{w})^2}_{\text{error of each data : } e_n}$$

VISUAL EXAMPLE:

Conside 1-dimensional input





we want optimised weights

$$\underline{w}^* = \arg\min(E_{in}(\underline{w})) \qquad \underline{w} \in \mathbb{R}^{d+1}$$

$$= \arg\min\left(\frac{1}{N}\|\underline{y} - X\underline{w}\|^2\right)$$

How do we minimize this ?

Recall $\|\underline{a}\|^2 = \underline{a}^T\underline{a}$

$$E_{in}(\underline{w}) = \frac{1}{N}(\underline{y} - X\underline{w})^T(\underline{y} - X\underline{w})$$

$$= \frac{1}{N}\left(\underline{y}^T\underline{y} - \underbrace{\underline{w}^T X \underline{y} - \underline{y}^T X \underline{w}}_{-2\underline{y}^T X \underline{w}} + \underline{w}^T X^T X \underline{w}\right)$$

$$= \frac{1}{N}\left(\underline{y}^T\underline{y} - 2\underline{y}^T X \underline{w} + \underline{w}^T X^T X \underline{w}\right)$$

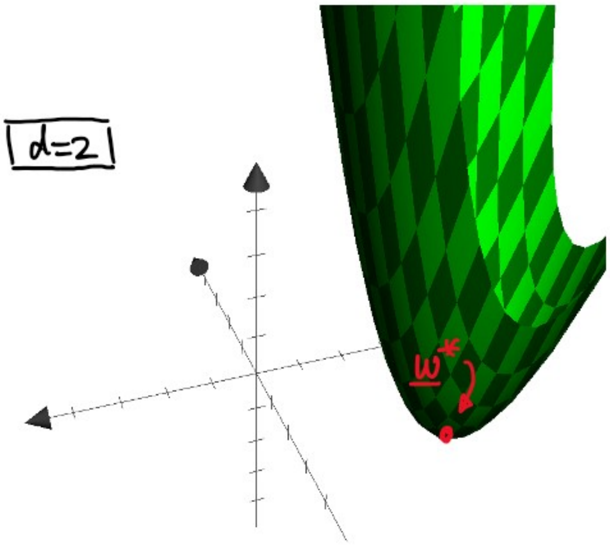
concavity determined by X^TX
↳ if all eigenvalues are ⊕/⊖/mix of ⊕ and ⊖

this looks like quadratic. ∩ ∪

Quadratic form in $\underline{w}$ is convex

⇒ there exists a local minimum.

$\boxed{d=2}$



To get to w^*, find global minimum.

$$\nabla\left(E_{in}(\underline{w})\right) = 0$$

LINEAR ALG RULES

- $f(\underline{w}) = \underline{w}^T \underline{v} = \underline{v}^T \underline{w}$

  $\nabla f(\underline{w}) = \underline{v}$

- $\nabla(\underline{w}^T A \underline{w}) = (A + A^T)\underline{w} = 2A\underline{w}$

$$\nabla\left(E_{in}(\underline{w})\right) = \frac{1}{N}\left(0 - 2\underline{y}^T \underline{x} + 2X^T X \underline{w}^*\right) = 0$$

$$\Rightarrow \quad \cancel{2}\,\underline{y}^T \underline{x} = \cancel{2}\,X^T X \underline{w}^*$$

$$\Rightarrow \quad \boxed{\underline{w}^* = (X^T X)^{-1} X \underline{y}}$$

Least square solution.

Finally, we can use w^* to predict:

$$\hat{y} = X\underline{w}^* = \underbrace{X(X^T X)^{-1} X^T}_{\substack{H \\ \text{matrix}}} \cdot \underline{y}$$

H

matrix

Special: This is a closed form solution.

Geometric Intepretation

$$X\underline{w} = \sum_{i=0}^{d} w_i \cdot \underline{q}_i$$ ← $\underline{q}$ are columns of X