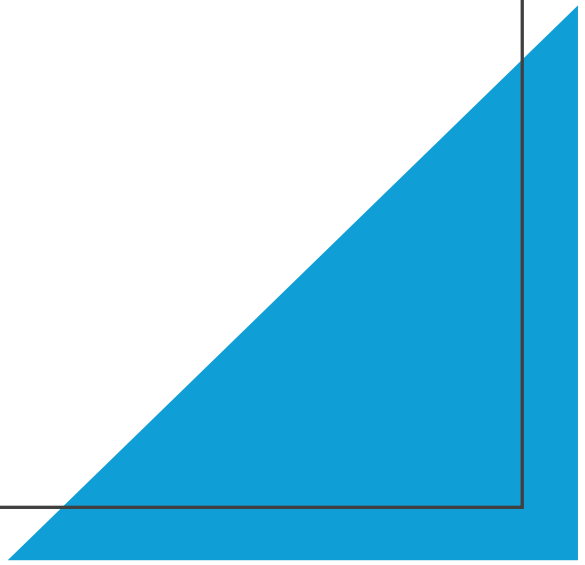
Week 2 Discussion

CSCI 567 Fall 2025



1. MULTIPLE-CHOICE QUESTIONS: One or more correct choice(s) for each question.

1.1. Which one of these is a sign of overfitting?

a. Low training error, low test error

b. Low training error, high test error

c. High training error, low test error

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1.1. Which one of these is a sign of overfitting?

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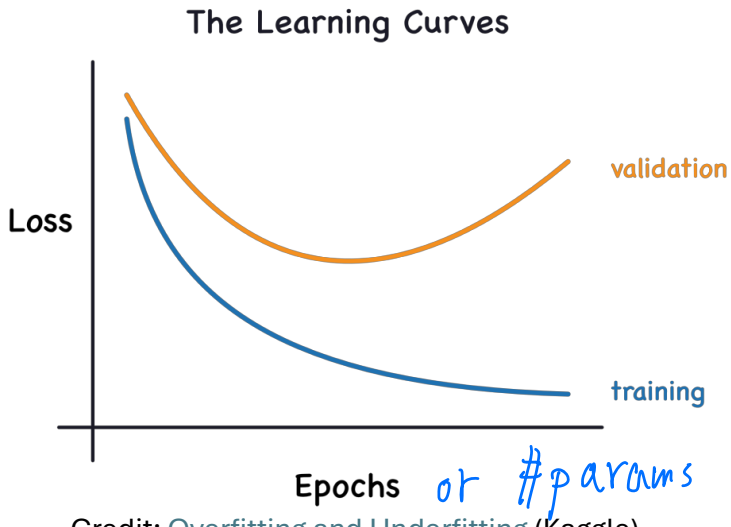
This is like the "definition" of overfitting



Credit: Overfitting and Underfitting (Kaggle)

1.2. Which of the following can help prevent overfitting?

a. Using more training data

b. Training until you get the smallest training error

c. Including a regularization term in the loss function

d. All of the above

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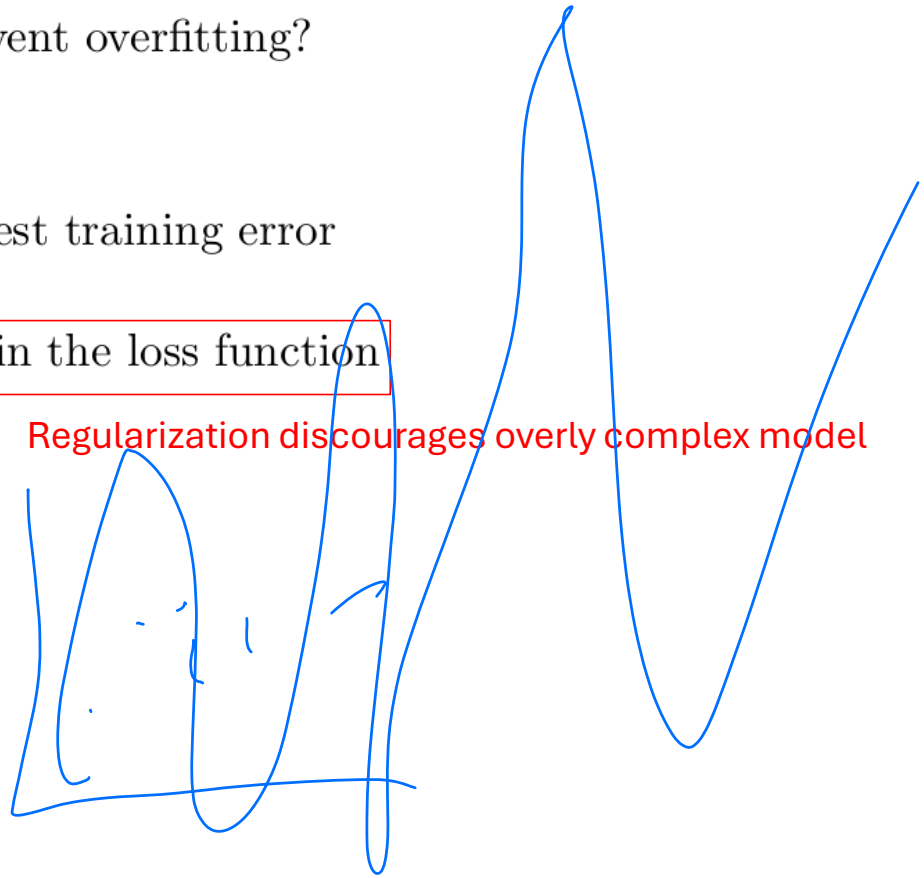

1.3. Let $\mathbf{X} \in \mathbb{R}^{N \times D}$ be a data matrix with each row corresponding to the feature of an example and $\mathbf{y} \in \mathbb{R}^{N}$ be a vector of all the outcomes. The least square solution is $(\mathbf{X}^\intercal \mathbf{X})^{-1}\mathbf{X}^\intercal \mathbf{y}$. Which of the following is the least square solution if we scale each data point by a factor of 4 (i.e. the new dataset is $4\mathbf{X}$)?

a. $4(\mathbf{X}^\intercal \mathbf{X})^{-1}\mathbf{X}^\intercal \mathbf{y}$

b. $\frac{1}{4}(\mathbf{X}^\intercal \mathbf{X})^{-1}\mathbf{X}^\intercal \mathbf{y}$

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d. None of the above

$$(cX)^T = c \cdot X^T$$

$$(cX)^{-1} = \frac{1}{c} \cdot X^{-1}$$

$$= \left((4X)^T (4X) \right)^{-1}$$

$$= (16 X^T X)^{-1}$$

$$= \frac{1}{16} X^{-1} X^{-T} \cdot 4 X^T$$

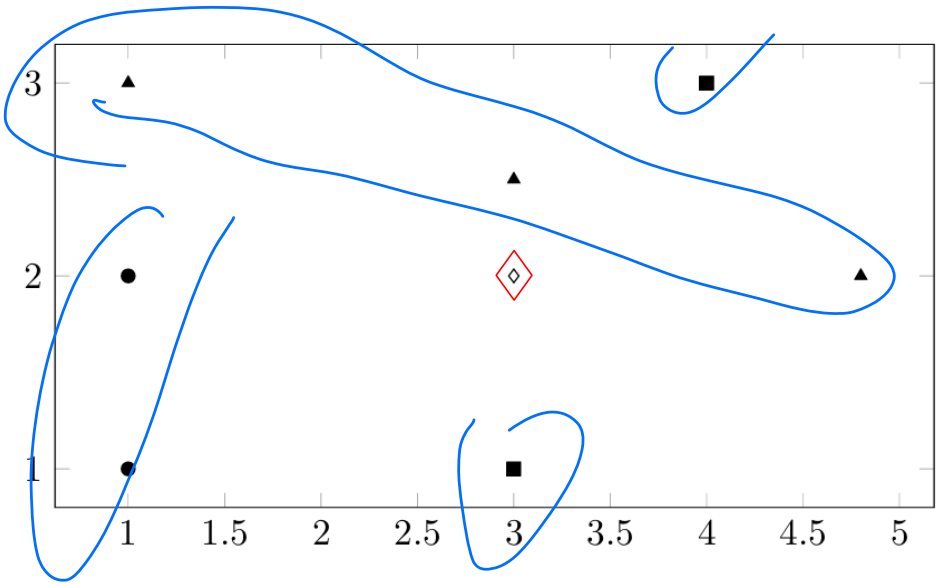
1.4. Consider the following two-dimensional dataset with $N = 7$ training points of three classes (triangle, square, and circle), and additionally one test point denoted by the diamond. Which of the following configuration of the K-nearest neighbor algorithm will predict triangle for the test point?

a. $K = 1$, L2 distance

b. $K = 3$, L1 distance

c. $K = 3$, L2 distance

d. $K = 7$, any distance



$\bar{x} \in \mathbb{R}^D$, $x_i \in \mathbb{R}^D$, $i = 1, \ldots, N$

$\|\bar{x} - x_i\|_1 = \sum_d |\bar{x}_d - x_{id}|$

$\|\bar{x} - x_i\|_2 = \sqrt{\sum_d (\bar{x}_d - x_{id})^2}$

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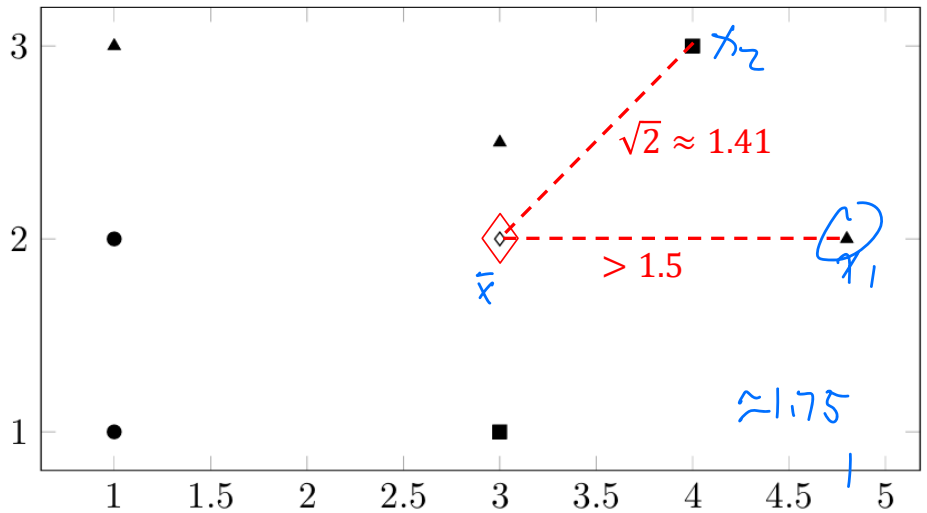

$\|\bar{x} - x_2\|_1 = 2$ $\|\bar{x} - x_1\|_1 \simeq 1.75$

1.5. Which of the following on linear regression is correct?

a. The least square solution has a closed-form formula, even if L2 regularization is applied.

b. The covariance matrix $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ is not invertible if and only if the number of data points N is smaller than the dimension D.

c. When the covariance matrix $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ is not invertible, the Residual Sum of Squares (RSS) objective has no minimizers.

d. Linear regression is a parametric method.

1.5. Which of the following on linear regression is correct?

a. The least square solution has a closed-form formula, even if L2 regularization is applied.

$w^* = (X^T X + \lambda \Sigma)^{-1} X^T y$.

b. The covariance matrix $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ is not invertible if and only if the number of data points N is smaller than the dimension D.

Even if $N \geq D$, $X^T X$ can still be **not** invertible , e.g., due to "collinearity"

c. When the covariance matrix $\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X}$ is not invertible, the Residual Sum of Squares (RSS) objective has no minimizers.

Infinitely many solutions

d. Linear regression is a parametric method.

2. Nearest Neighbor Classification

We mentioned that the Euclidean/L2 distance is often used as the *default* distance for nearest neighbor classification. It is defined as

$$E(\mathbf{x}, \mathbf{x}') = ||\mathbf{x} - \mathbf{x}'||_2 = \sqrt{\sum_{d=1}^{D} (x_d - x'_d)^2} \tag{1}$$

In some applications such as information retrieval, the cosine distance is widely used too. It is defined as

$$C(\mathbf{x}, \mathbf{x}') = 1 - \frac{\mathbf{x}^\intercal \mathbf{x}'}{||\mathbf{x}||_2 ||\mathbf{x}'||_2} = 1 - \frac{\sum_{d=1}^{D} (x_d \cdot x'_d)}{||\mathbf{x}||_2 ||\mathbf{x}'||_2} \tag{2}$$

where the L2 norm of $\mathbf{x}$ is defined as

$$||\mathbf{x}||_2 = \sqrt{\sum_{d=1}^{D} x_d^2}. \tag{3}$$

Show that, if data is normalized with unit L2 norm, that is, $||\mathbf{x}||_2 = 1$ for all $\mathbf{x}$ in the training and test sets, changing the distance function from the Euclidean distance to the cosine distance will NOT affect the nearest neighbor classification results.

$x^T x = \|x\|_2^2$

When $\|x\| = \|x'\| = 1$,

$C(x, x') = 1 - x^T x'$

$E(x, x')^2 = (x - x')^T (x - x') = \|x\|^2 + \|x'\|^2 - 2 x^T x' = 2\, C(x, x')$.

($\|x\| = 1$, $\|x'\| = 1$)

3. Linear Regression

In the lectures, we have described the least mean square solution for linear regression as

$$\boldsymbol{w}^* = (\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}})^{-1}\tilde{\boldsymbol{X}}^{\mathrm{T}}\boldsymbol{y}$$

where $\tilde{\boldsymbol{X}}$ is the design matrix (N rows, $D+1$ columns) and $\boldsymbol{y}$ is the N-dimensional column vector of the true values in the training data $\mathcal{D} = \{(\boldsymbol{x}_n, y_n)\}_{n=1}^{N}$.

Question 3.1 We mentioned a practical challenge for linear regression: when $\tilde{\boldsymbol{X}}^{\mathrm{T}}\tilde{\boldsymbol{X}}$ is not invertible. Please use a concise mathematical statement (*in one sentence*) to summarize the relationship between the training data $\tilde{\boldsymbol{X}}$ and the dimensionality of $\boldsymbol{w}$ when this scenario happens. Then use this statement to explain why this scenario must happen when $N < D+1$.

Why? If $N < D+1$, then $\tilde{X}^T\tilde{X}$ not invertible.

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$N < D + 1 \Rightarrow \operatorname{rank}(\tilde{X}^T\tilde{X}) < D + 1$

$\Leftrightarrow \tilde{X}^T\tilde{X}$ not invertible

Why?

- $\tilde{X}^T\tilde{X}$ is $(D+1) \times (D+1)$ matrix
- $\operatorname{rank}(\tilde{X}^T\tilde{X}) = \operatorname{rank}(\tilde{X}) \leq \min\{N, D+1\}$

In general, invertible $\Leftrightarrow$ full rank

Question 3.2 In this problem we use the notation $w_0 + \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}$ for the linear model, that is, we do not append the constant feature 1 to x. In the lecture we saw that when $D = 0$, the bias w_0^* is simply the mean of the sample responses

$$w_0^* = \frac{1}{N}\mathbf{1}_N^{\mathrm{T}}\boldsymbol{y} = \frac{1}{N}\sum_n y_n, \tag{4}$$

where $\mathbf{1}_N = [1, 1, \ldots, 1]^{\mathrm{T}}$ is an N-dimensional column vector whose entries are all ones. Now, we would like you to generalize this to arbitrary D and arrive at a more general condition where Eqn. (4) holds.

Design matrix *(without bias)*

$$X = \begin{pmatrix} - & x_1^T & - \\ - & x_2^T & - \\ & \vdots & \\ - & x_N^T & - \end{pmatrix} \in \mathbb{R}^{N\times D}$$

Prediction

$\hat{y}_i = x_i^T w + w_0$ $\quad \hat{y} = Xw + w_0 1_N$

"Residual" error

$\epsilon_i = y_i - \hat{y}_i = y_i - x_i^T w - w_0$ $\quad \epsilon = y - \hat{y} = y - Xw - w_0 1_N$

objective minimize $(w_0, w) \in \mathbb{R}^{D+1}$ RSS.

1) write down the residual sum of squares objective w.r.t. the variable of interest;

Fix any w^*,

$$w_0^* = \operatorname*{argmin}_{w_0} \|y - Xw^* - w_0 1_N\|_2^2$$

2) take derivative with respect to w_0 and set it to 0;

$$0 = -2\, 1_N^T (y - Xw^* - w_0^* 1_N) \Rightarrow N w_0 = 1_N^T y - (1_N^T X) w^*$$

$(1_N^T X) = 0_D^T$

$$\sum_{i=1}^N \epsilon_i^2 = \|\epsilon\|_2^2 = \epsilon^T \epsilon.$$

$$RSS = \|y - Xw - w_0 1_N\|_2^2$$

3) solve the obtained equation and conclude that Eqn. (4) holds if

$$\frac{1}{N}\sum_n x_{nd} = 0, \quad \forall d = 1, 2, \ldots, D, \tag{5}$$

(5) $\Rightarrow \sum_n x_{nd} = 0 \Rightarrow [X^T 1_N]_d = 0$

that is, each feature has zero mean.

$$w_0 = \frac{1}{N} 1_N^T y = \frac{1}{N}\sum_i y_i.$$

$$\frac{\partial \epsilon_i}{\partial w_0} = -1.$$

$$\frac{\partial \|\epsilon\|_2^2}{\partial w_0} = \frac{\partial \epsilon_i}{\partial w_0} = -2\epsilon_i$$

$$\frac{\partial \|\epsilon\|^2}{\partial w_0} = -2\sum_i \epsilon_i = -2 \cdot 1_N^T \epsilon = 0$$