10-701: Introduction to Machine Learning Lecture 4 – Linear Regression

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1/29/24

Front Matter

- Announcements:
  - HW1 released 1/24, due 2/2 at 11:59 PM
- Recommended Readings:
  - Murphy, [Sections 7.1-7.3]

Recall: k-Nearest Neighbors (kNN)

- Classify a point as the most common label among the labels of the k nearest training points
- Tie-breaking (in case of even k and/or more than 2 classes)
  - Weight votes by distance
  - Remove furthest neighbor
  - Add next closest neighbor
  - Use a different distance metric

kNN on Fisher Iris Data

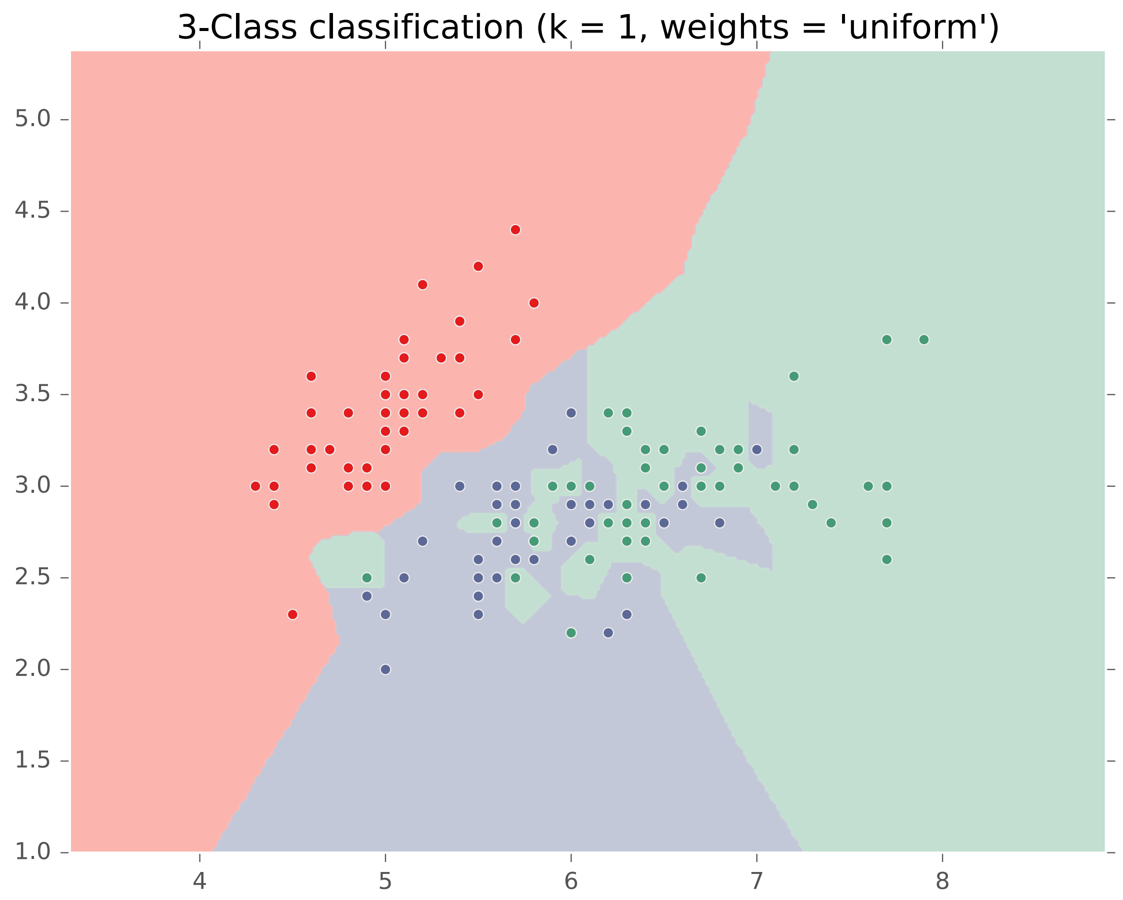

Figure courtesy of Matt Gormley

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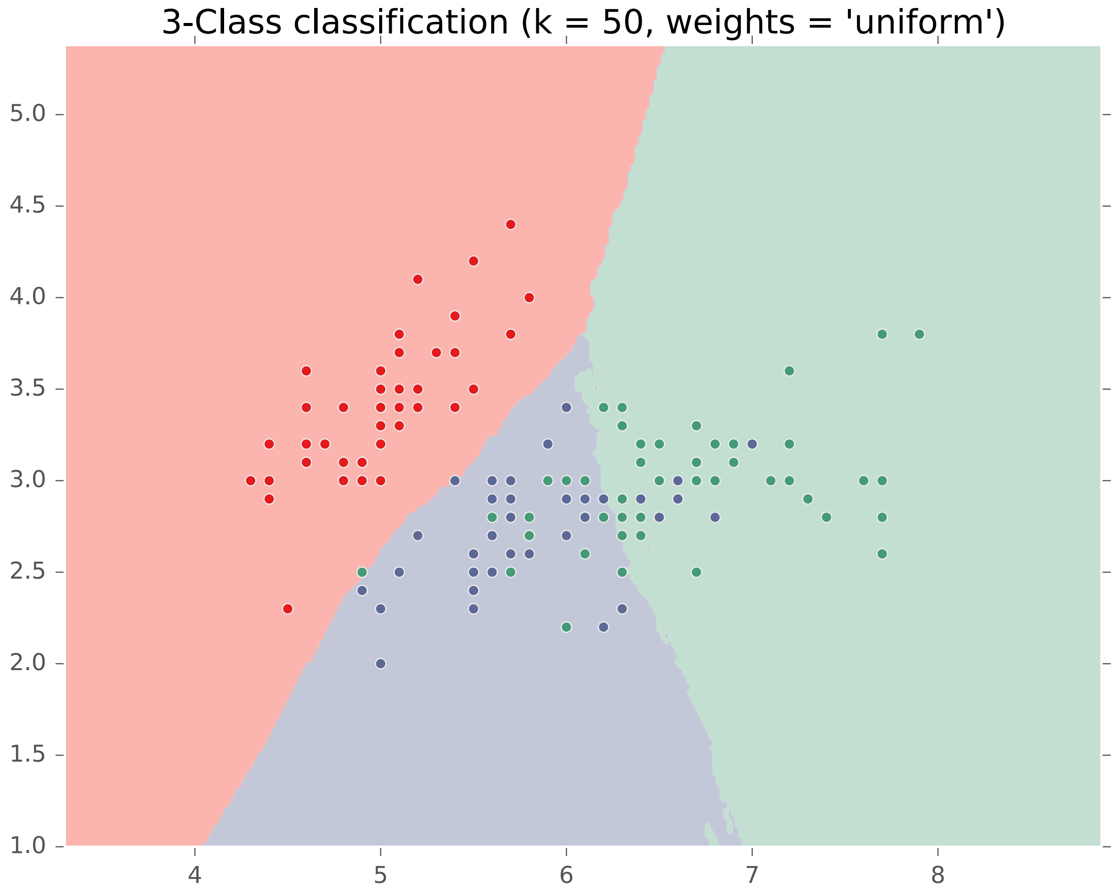

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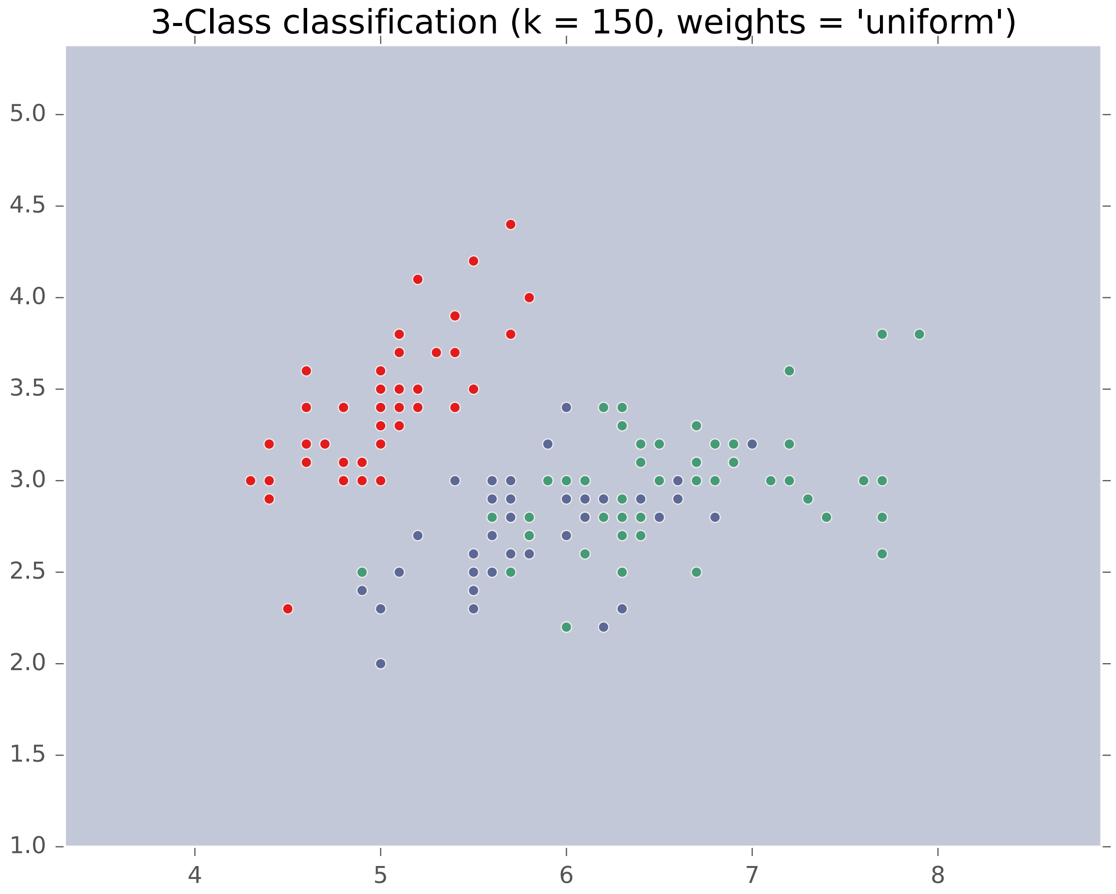

Figure courtesy of Matt Gormley

Setting k

- When $k = 1$:
  - many, complicated decision boundaries
  - may ***overfit***
- When $k = N$:
  - no decision boundaries; always predicts the most common label in the training data
  - may ***underfit***
- k controls the complexity of the hypothesis set $\Longrightarrow$ k affects how well the learned hypothesis will generalize

Setting k

- Theorem:
  - If k is some function of N s.t. $k(N) \rightarrow \infty$ and $\frac{k(N)}{N} \rightarrow 0$ as $N \rightarrow \infty$ …
  - … then (under certain assumptions) the true error of a kNN model $\rightarrow$ the Bayes error rate
- Heuristics:
  - $k = \lfloor \sqrt{N} \rfloor$
  - $k = 3$
- This is fundamentally a question of **model selection**: each value of k corresponds to a different "model"

Model Selection

- A **model** is a (typically infinite) set of classifiers that a learning algorithm searches through to find the best one (the ”hypothesis space”)
- **Model parameters** are the numeric values or structure that are selected by the learning algorithm
- **Hyperparameters** are the tunable aspects of the model that are not selected by the learning algorithm

Example: Decision Trees

- Model = set of all possible trees, potentially narrowed down according to the hyperparameters (see below)
- Model parameters = structure of a specific tree e.g., splits, split order, predictions at leaf nodes,
- Hyperparameters = splitting criterion, max-depth, tie-breaking procedures, etc…

Model Selection

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Example: kNN

- Model = set of all possible nearest neighbors classifiers
- Model parameters = none! kNN is a “non-parametric model”
- Hyperparameters = k

Model Selection with Test Sets

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{test}$, suppose we have multiple candidate models:

$$\mathcal{H}_1, \mathcal{H}_2, \dots, \mathcal{H}_M$$

- Learn a classifier from each model using only $\mathcal{D}_{train}$:

$$h_1 \in \mathcal{H}_1, h_2 \in \mathcal{H}_2, \dots, h_M \in \mathcal{H}_M$$

- Evaluate each one using $\mathcal{D}_{test}$ and choose the one with lowest test error:

$$\hat{m} = \underset{m \in \{1,\dots,M\}}{\operatorname{argmin}} \; err(h_m, \mathcal{D}_{test})$$

Model Selection with Test Sets?

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$$\hat{m} = \underset{m \in \{1,\ldots,M\}}{\operatorname{argmin}}\ err(h_m, \mathcal{D}_{test})$$

- Is $err(h_{\hat{m}}, \mathcal{D}_{test})$ a good estimate of $err(h_{\hat{m}})$?

Model Selection with Validation Sets

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{val} \cup \mathcal{D}_{test}$, suppose we have multiple candidate models:

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- Learn a classifier from each model using only $\mathcal{D}_{train}$:

$$h_1 \in \mathcal{H}_1, h_2 \in \mathcal{H}_2, \dots, h_M \in \mathcal{H}_M$$

- Evaluate each one using $\mathcal{D}_{val}$ and choose the one with lowest *validation* error:

$$\hat{m} = \underset{m \in \{1,\dots,M\}}{\operatorname{argmin}} \; err(h_m, \mathcal{D}_{val})$$

- Now $err(h_{\hat{m}}, \mathcal{D}_{test})$ is a good estimate of $err(h_{\hat{m}})$!

Hyperparameter Optimization with Validation Sets

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{val} \cup \mathcal{D}_{test}$, suppose we have multiple candidate hyperparameter settings:

$$\theta_1, \theta_2, \dots, \theta_M$$

- Learn a classifier for each setting using only $\mathcal{D}_{train}$:

$$h_1, h_2, \dots, h_M$$

- Evaluate each one using $\mathcal{D}_{val}$ and choose the one with lowest *validation* error:

$$\hat{m} = \underset{m \in \{1,\dots,M\}}{\operatorname{argmin}} \; err(h_m, \mathcal{D}_{val})$$

- Now $err(h_{\hat{m}}, \mathcal{D}_{test})$ is a good estimate of $err(h_{\hat{m}})$!

Pro tip: train your final model using *both* training and validation datasets

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{val} \cup \mathcal{D}_{test}$, suppose we have multiple candidate hyperparameter settings:

$$\theta_1, \theta_2, \dots, \theta_M$$

- Learn a classifier for each setting using only $\mathcal{D}_{train}$:

$$h_1, h_2, \dots, h_M$$

- Evaluate each one using $\mathcal{D}_{val}$ and choose the one with lowest *validation* error:

$$\hat{m} = \underset{m \in \{1,\dots,M\}}{\operatorname{argmin}} \; err(h_m, \mathcal{D}_{val})$$

- Train a new model on $\mathcal{D}_{train} \cup \mathcal{D}_{val}$ using $\theta_{\hat{m}}$, $h_{\hat{m}}^{+}$
- $err(h_{\hat{m}}^{+}, \mathcal{D}_{test})$ is still a good estimate of $err(h_{\hat{m}}^{+})$!

Setting k for kNN with Validation Sets

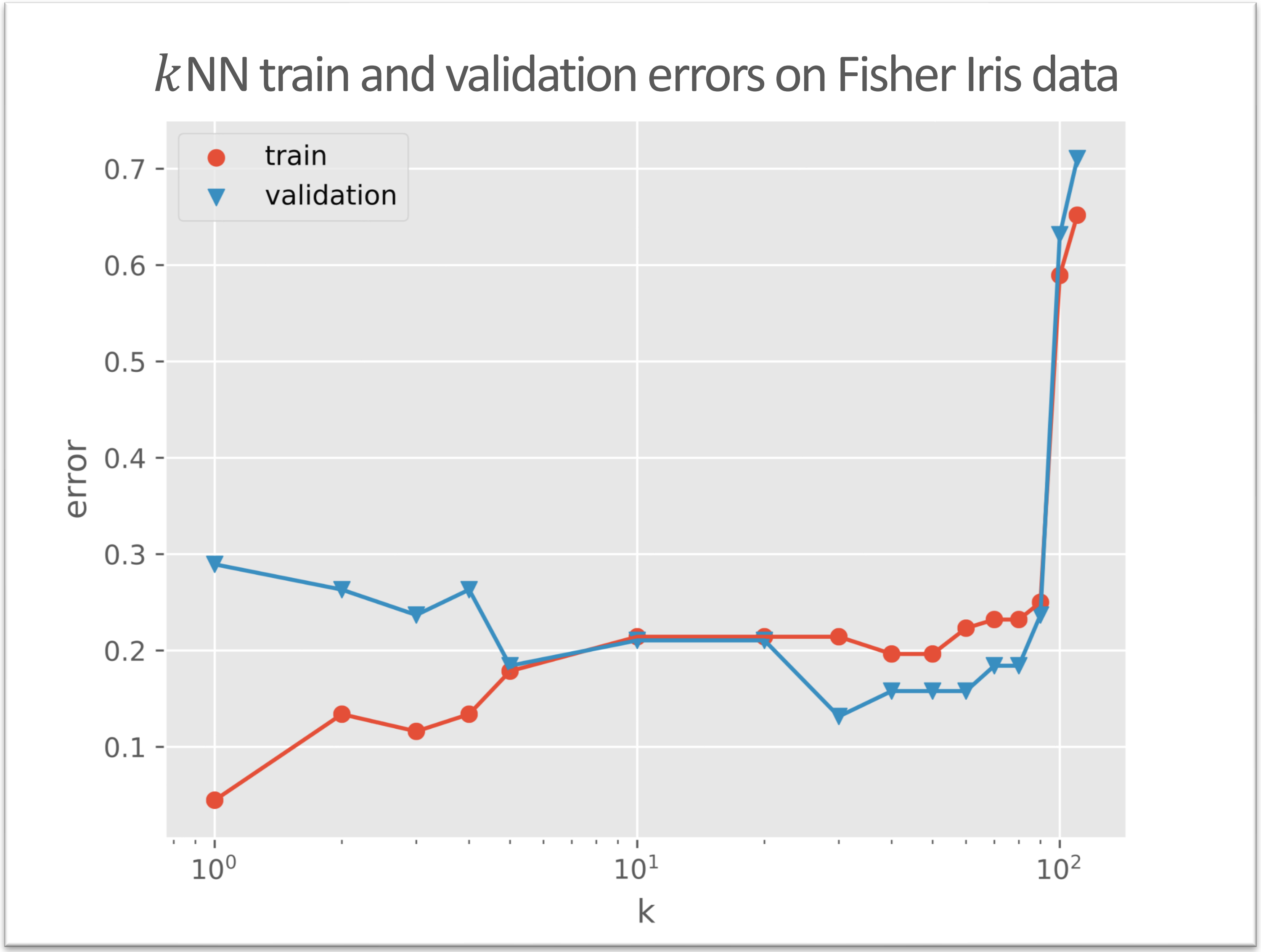
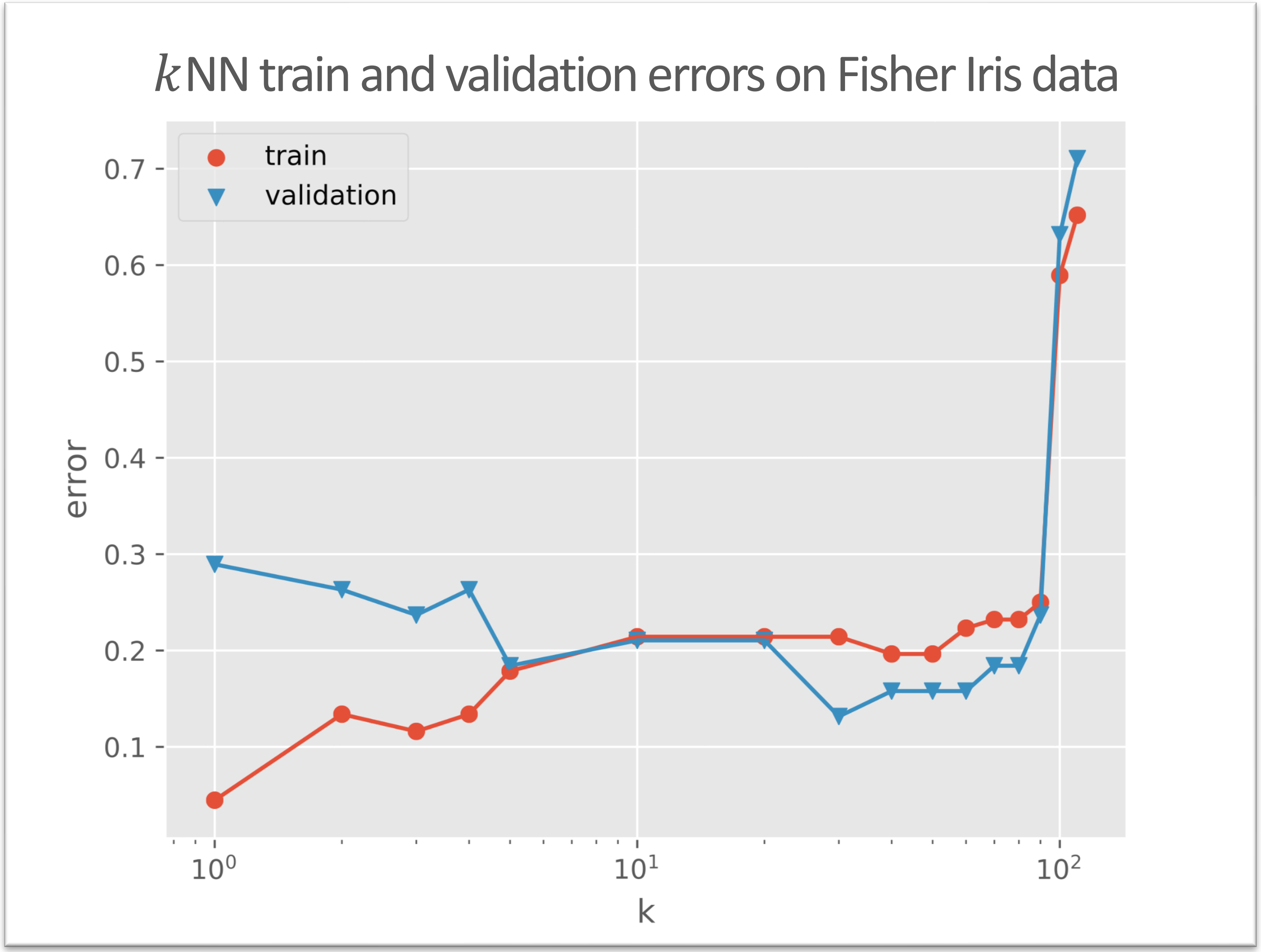


Figure courtesy of Matt Gormley

How should we partition our dataset?



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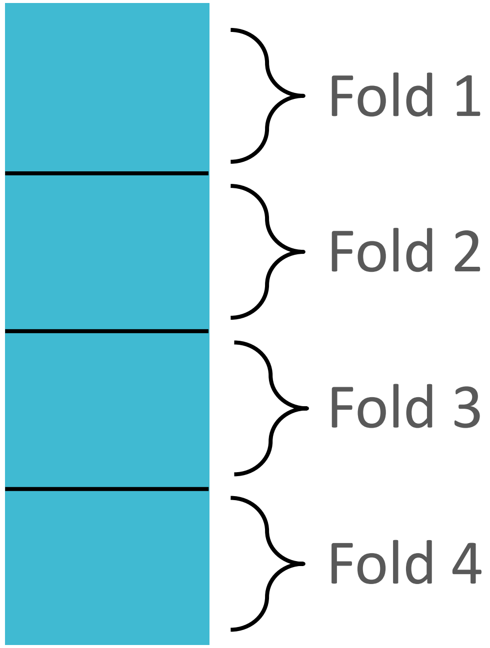
K-fold cross-validation

- Given $\mathcal{D}$, split $\mathcal{D}$ into K equally sized datasets or folds: $\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_K$
- Use each one as a validation set once:



- Let h_{-i} be the classifier learned using $\mathcal{D}_{-i} = \mathcal{D} \backslash \mathcal{D}_i$ (all folds other than $\mathcal{D}_i$) and let $e_i = err(h_{-i}, \mathcal{D}_i)$
- The K-fold cross validation error is

$$err_{cv_K} = \frac{1}{K} \sum_{i=1}^{K} e_i$$

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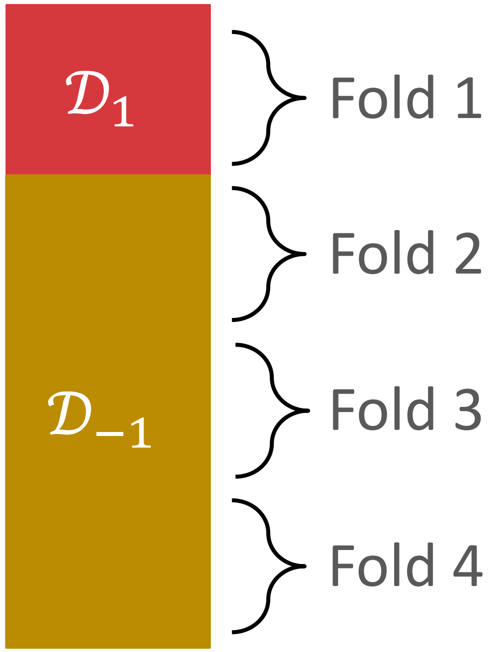

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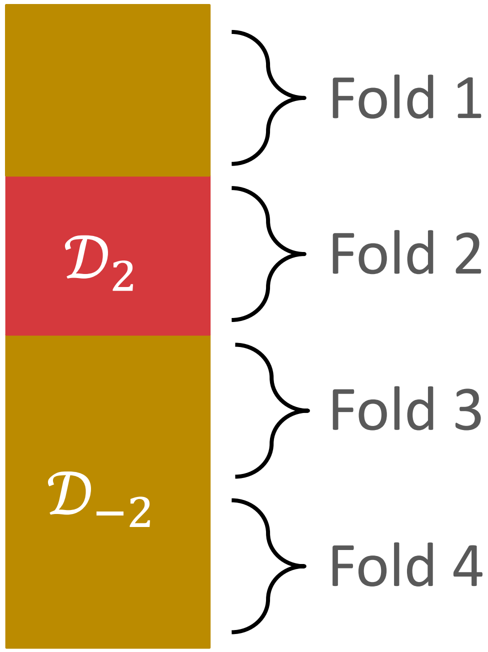

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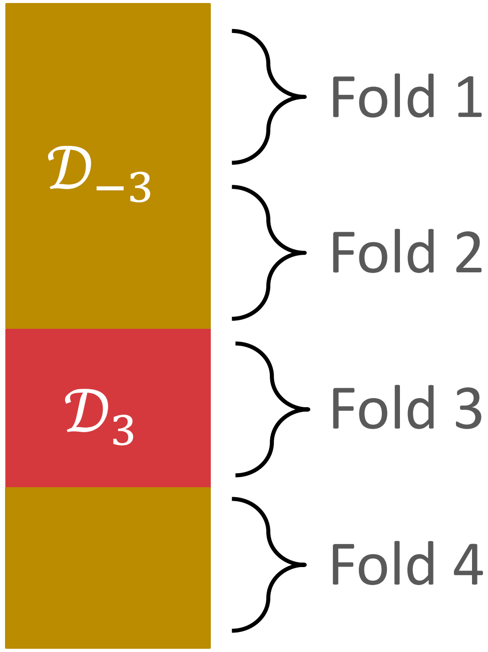

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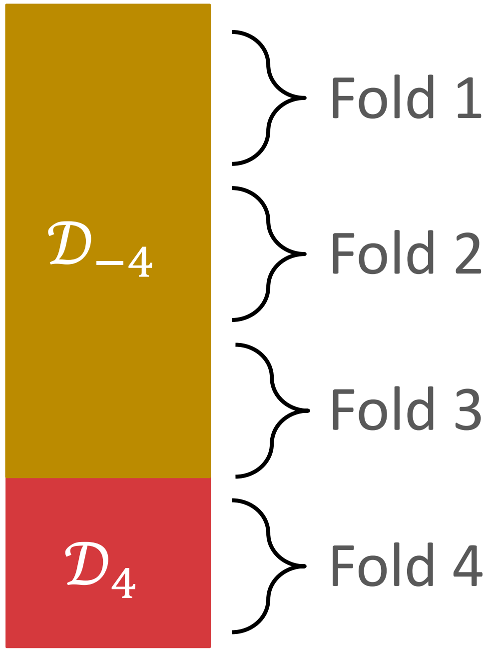

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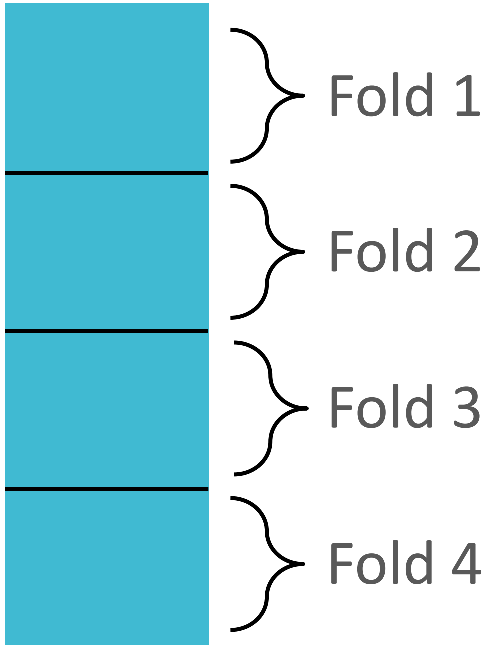

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- The K-fold cross validation error is

$$err_{cv_K} = \frac{1}{K} \sum_{i=1}^{K} e_i$$

- Special case when $K = N$: Leave-one-out cross-validation
- Choosing between m candidates requires training mK times

Summary

	Input	Output
Training	• training dataset • hyperparameters	• best model parameters
Hyperparameter Optimization	• training dataset • validation dataset	• best hyperparameters
Cross-Validation	• training dataset • validation dataset	• cross-validation error
Testing	• test dataset • classifier	• test error

Key Takeaways

- Real-valued features and decision boundaries
- Nearest neighbor model and generalization guarantees
- kNN "training" and prediction
- Effect of k on model complexity
- kNN inductive bias
- Differences between training, validation and test datasets in the model selection process
- Cross-validation for model selection
- Relationship between training, hyperparameter optimization and model selection

Recall: Regression

- Learning to diagnose heart disease

  as a **(supervised)** **<u>regression</u> task**

features | targets

x_1 Family History	x_2 Resting Blood Pressure	x_3 Cholesterol	y Heart Disease?
Yes	Low	Normal	$\$0$
No	Medium	Normal	$\$20$
No	Low	Abnormal	$\$30$
Yes	Medium	Normal	$\$100$
Yes	High	Abnormal	$\$5000$

data points

Decision Tree Regression

- Learning to diagnose heart disease

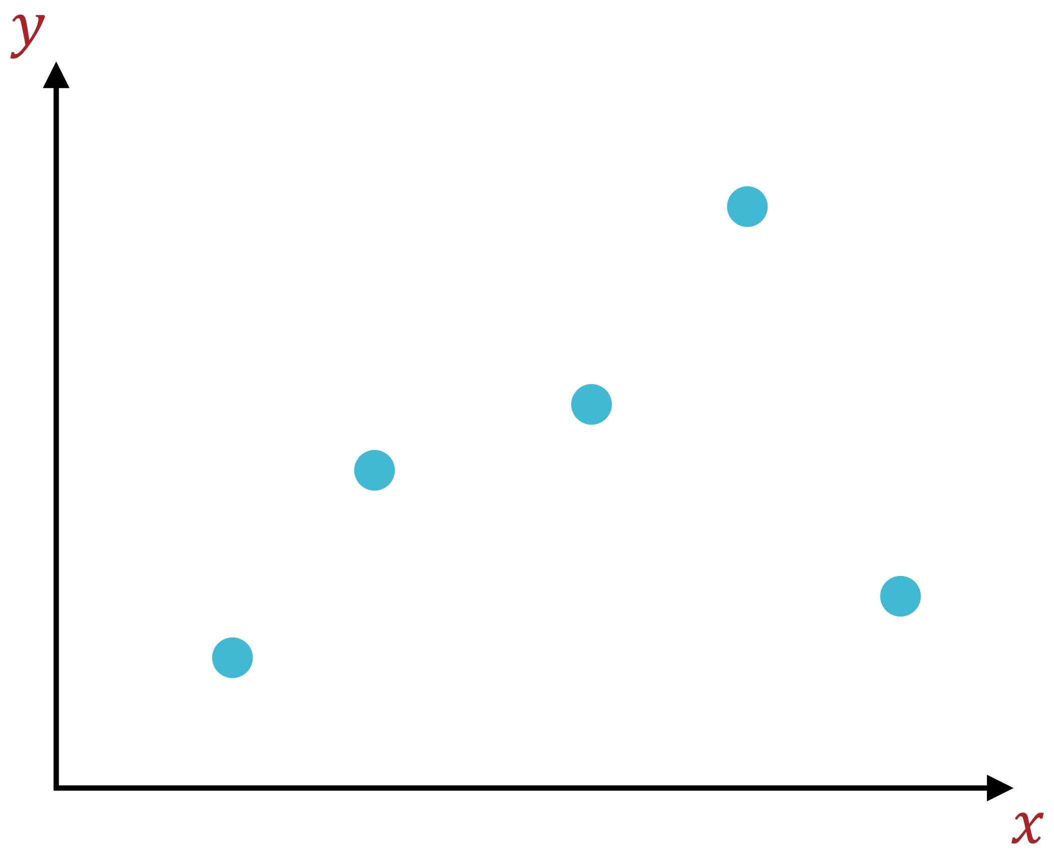
as a **(supervised)** **regression task**

x_1 Family History	x_2 Resting Blood Pressure	x_3 Cholesterol	y Heart Disease?
Yes	Low	Normal	\$0
No	Medium	Normal	\$20
No	Low	Abnormal	\$30
Yes	Medium	Normal	\$100
Yes	High	Abnormal	\$5000

features: x_1, x_2, x_3; targets: y; data points: rows

1-NN Regression

- Suppose we have real-valued targets $y \in \mathbb{R}$ and one-dimensional inputs $x \in \mathbb{R}$



Linear Regression

- Suppose we have real-valued targets $y \in \mathbb{R}$ and D-dimensional inputs $\boldsymbol{x} = [\quad x_1, \dots, x_D]^T \in \mathbb{R}^D$
- **Assume**

$$y = \boldsymbol{w}^T \boldsymbol{x} + w_0$$

Linear Regression

- Suppose we have real-valued targets $y \in \mathbb{R}$ and D-dimensional inputs $\boldsymbol{x} = [1, x_1, \dots, x_D]^T \in \mathbb{R}^{D+1}$
- **Assume**

$$y = \boldsymbol{w}^T \boldsymbol{x}$$

- Notation: given training data $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$
  - $$X = \begin{bmatrix} 1 & \boldsymbol{x}^{(1)^T} \\ 1 & \boldsymbol{x}^{(2)^T} \\ \vdots & \vdots \\ 1 & \boldsymbol{x}^{(N)^T} \end{bmatrix} = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_D^{(1)} \\ 1 & x_1^{(2)} & \cdots & x_D^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(N)} & \cdots & x_D^{(N)} \end{bmatrix} \in \mathbb{R}^{N \times D+1}$$

    is the *design matrix*
  - $\boldsymbol{y} = \left[y^{(1)}, \dots, y^{(N)}\right]^T \in \mathbb{R}^N$ is the *target vector*

General Recipe for Machine Learning

1. Define a model and model parameters

2. Write down an objective function

3. Optimize the objective w.r.t. the model parameters

Recipe for Linear Regression

1. Define a model and model parameters
   1. Assume $y = \boldsymbol{w}^T \boldsymbol{x}$
   2. Parameters: $\boldsymbol{w} = [w_0, w_1, \dots, w_D]$

2. Write down an objective function
   1. Minimize the mean squared error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \frac{1}{N} \sum_{n=1}^{N} \left(\boldsymbol{w}^T \boldsymbol{x}^{(n)} - y^{(n)} \right)^2$$

3. Optimize the objective w.r.t. the model parameters
   1. Solve in *closed form*: take partial derivatives, set to 0 and solve

Minimizing the Squared Error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} - y^{(n)}\right)^2 = \frac{1}{N}\sum_{n=1}^{N}\left({\boldsymbol{x}^{(n)}}^T\boldsymbol{w} - y^{(n)}\right)^2$$

$$= \frac{1}{N}\|X\boldsymbol{w} - \boldsymbol{y}\|_2^2 \text{ where } \|\boldsymbol{z}\|_2 = \sqrt{\sum_{d=1}^{D} z_d^2} = \sqrt{\boldsymbol{z}^T\boldsymbol{z}}$$

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

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

$$\nabla_{\boldsymbol{w}}\ell_{\mathcal{D}}(\widehat{\boldsymbol{w}}) = \frac{1}{N}(2X^T X\widehat{\boldsymbol{w}} - 2X^T\boldsymbol{y}) = 0$$

$$\to X^T X\widehat{\boldsymbol{w}} = X^T\boldsymbol{y}$$

$$\to \widehat{\boldsymbol{w}} = (X^T X)^{-1}X^T\boldsymbol{y}$$

Minimizing the Squared Error

$$\ell_{\mathcal{D}}(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(\boldsymbol{w}^T\boldsymbol{x}^{(n)} - y^{(n)}\right)^2 = \frac{1}{N}\sum_{n=1}^{N}\left(\boldsymbol{x}^{(n)^T}\boldsymbol{w} - y^{(n)}\right)^2$$

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$$\nabla_{\boldsymbol{w}}\ell_{\mathcal{D}}(\widehat{\boldsymbol{w}}) = \frac{1}{N}(2X^T X\widehat{\boldsymbol{w}} - 2X^T\boldsymbol{y}) = 0$$

$$H_{\boldsymbol{w}}\ell_{\mathcal{D}}(\boldsymbol{w}) = \frac{2}{N}X^T X \rightarrow H_{\boldsymbol{w}}\ell_{\mathcal{D}}(\boldsymbol{w}) \text{ is positive semi-definite}$$

$$\hat{\boldsymbol{w}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

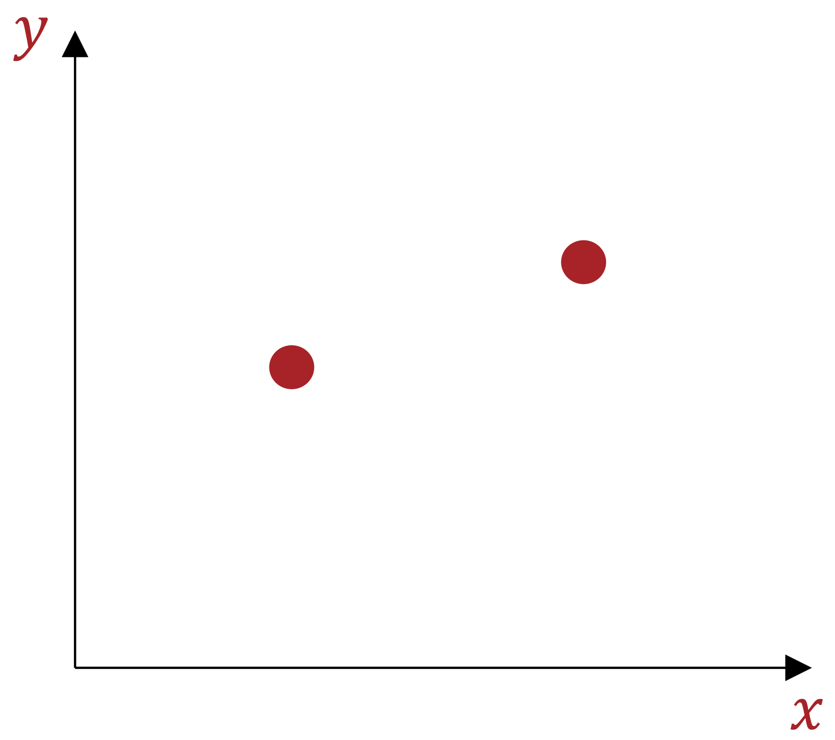
Closed Form Solution

1. Is $X^T X$ invertible?

2. If so, how computationally expensive is inverting $X^T X$?

Linear Regression: Uniqueness

- Consider a 1D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of weights $\boldsymbol{w}$) are there for the given dataset?



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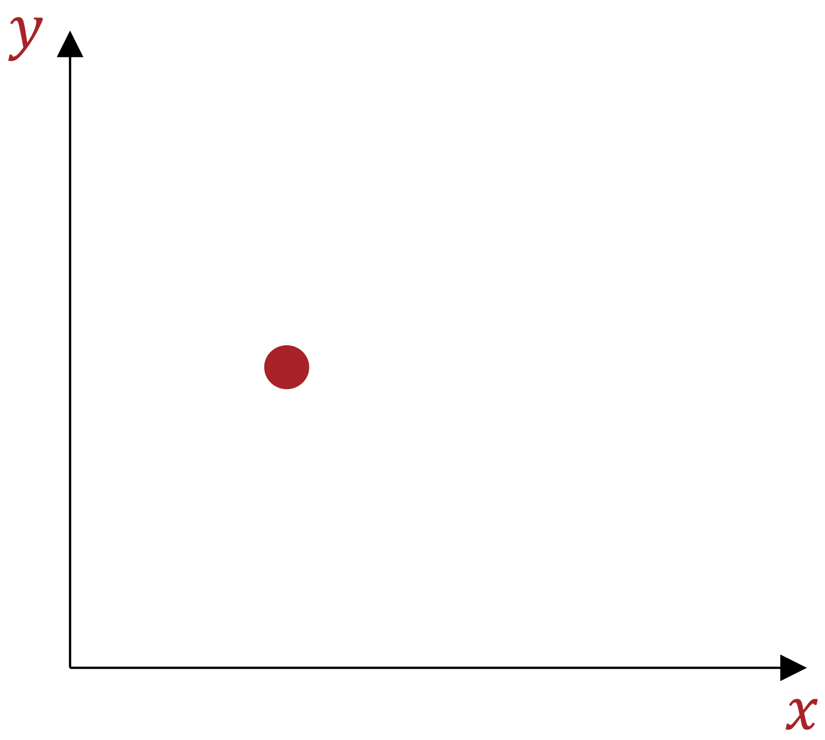

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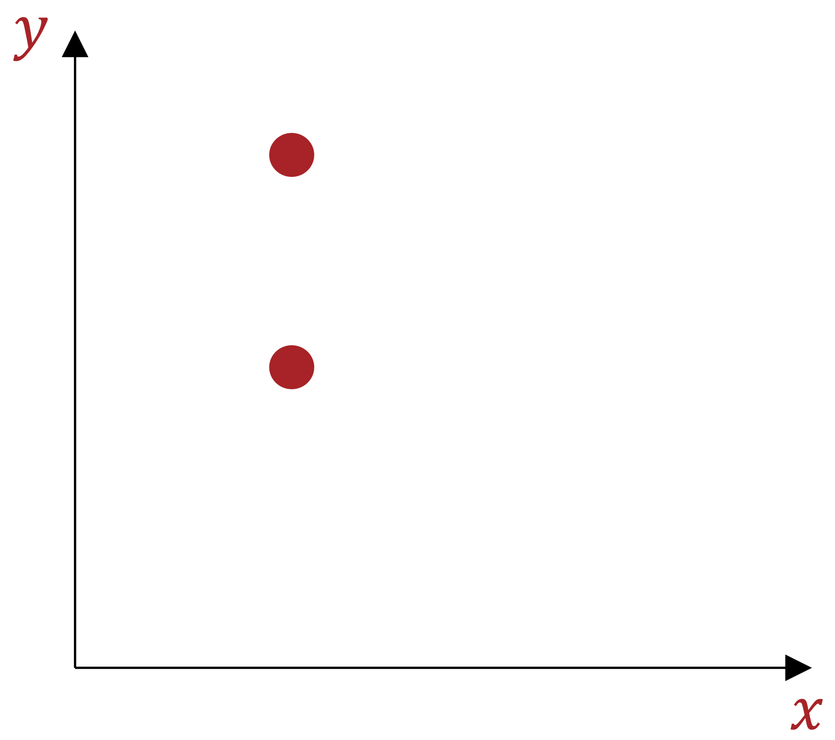
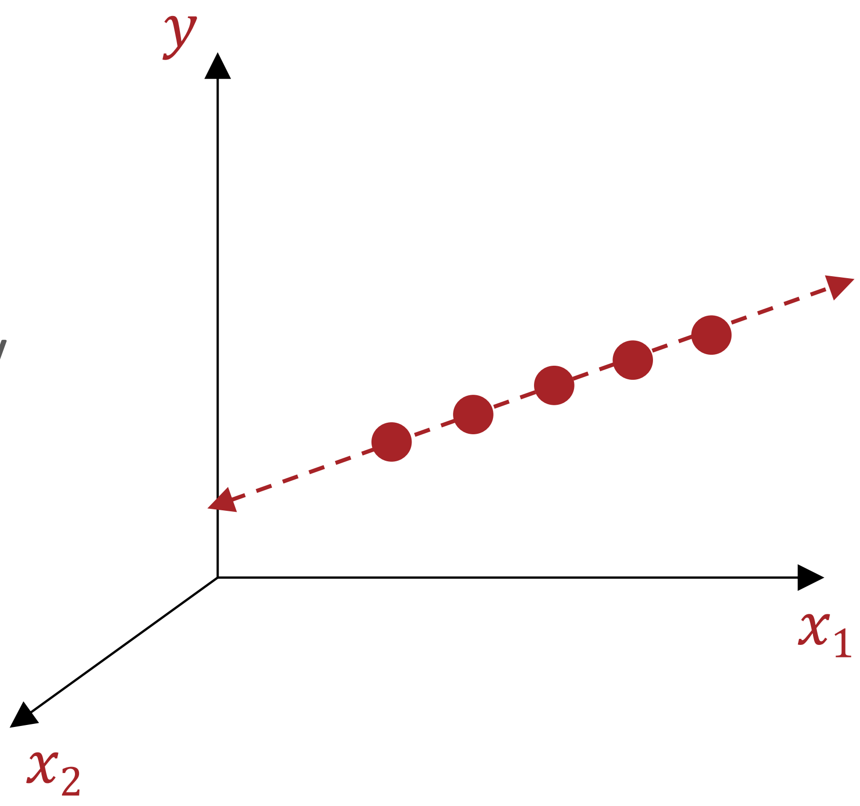


Linear Regression: Uniqueness

- Consider a 2D linear regression model trained to minimize the mean squared error: how many optimal solutions (i.e., sets of parameters θ) are there for the given dataset?



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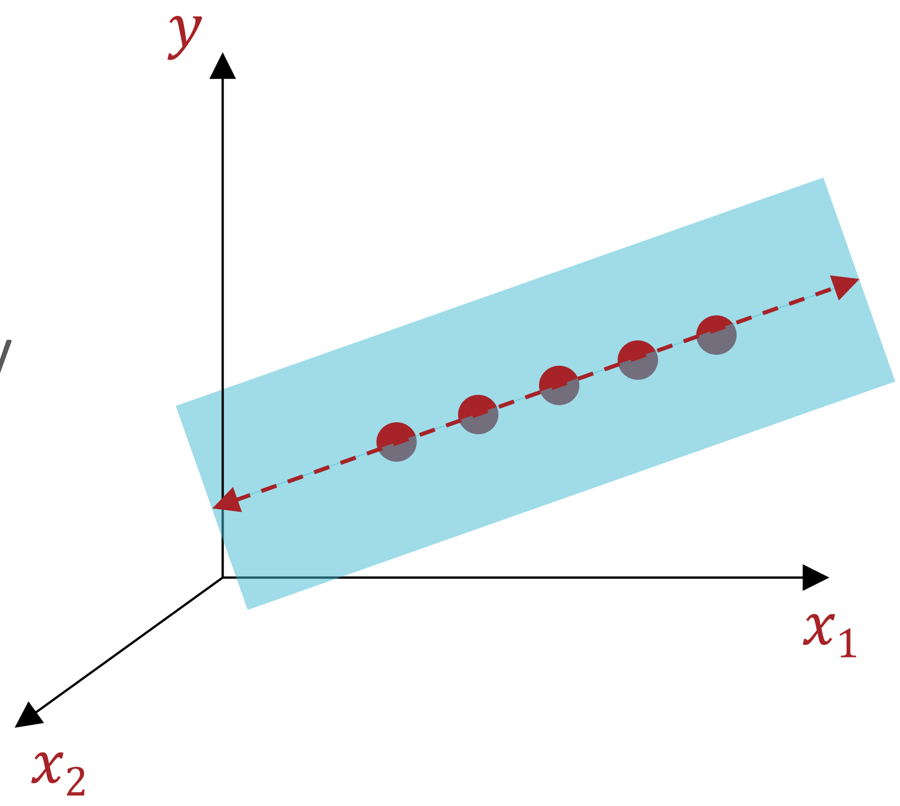

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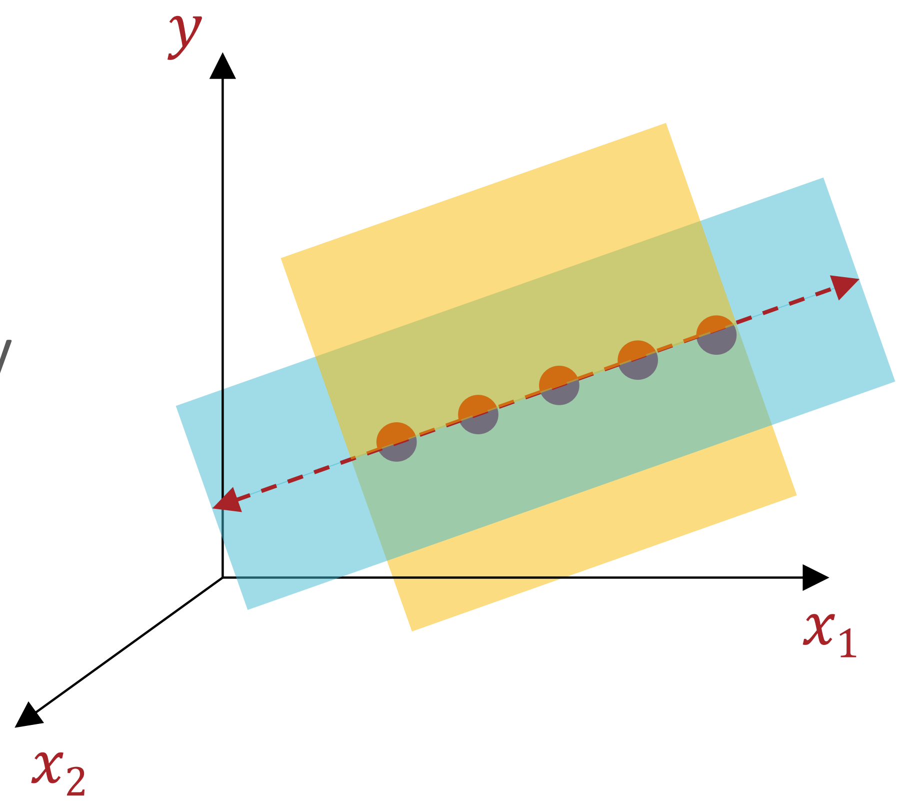


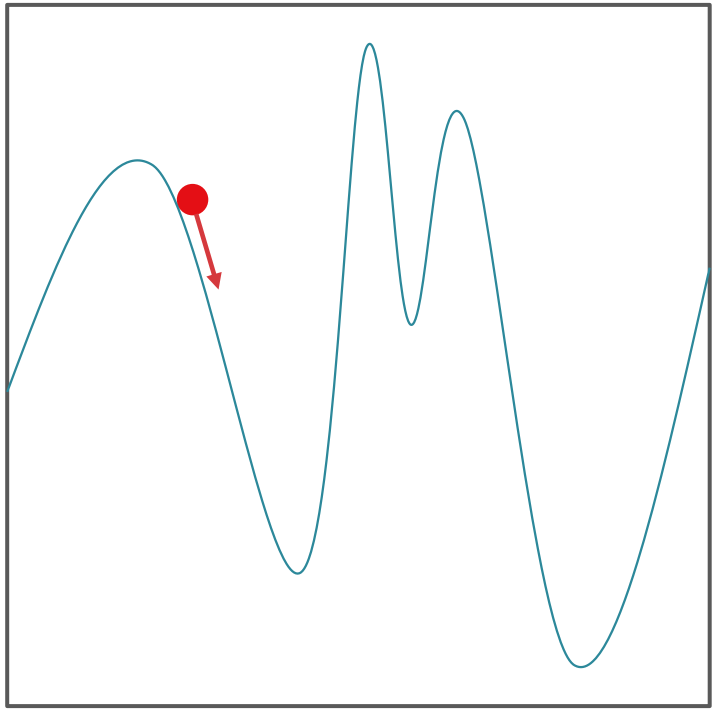
$$\hat{\boldsymbol{w}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

Closed Form Solution

1. Is $X^T X$ invertible?
   - When $N \gg D + 1$, $X^T X$ is (almost always) full rank and therefore, invertible
   - If $X^T X$ is not invertible (occurs when one of the features is a linear combination of the others) then there are infinitely many solutions.
2. If so, how computationally expensive is inverting $X^T X$?
   - $X^T X \in \mathbb{R}^{D+1 \times D+1}$ so inverting $X^T X$ takes $O(D^3)$ time…
     - Computing $X^T X$ takes $O(ND^2)$ time
   - What alternative optimization method can we use to minimize the mean squared error?

Gradient Descent: Intuition

- An iterative method for minimizing functions
- Requires the gradient to exist everywhere



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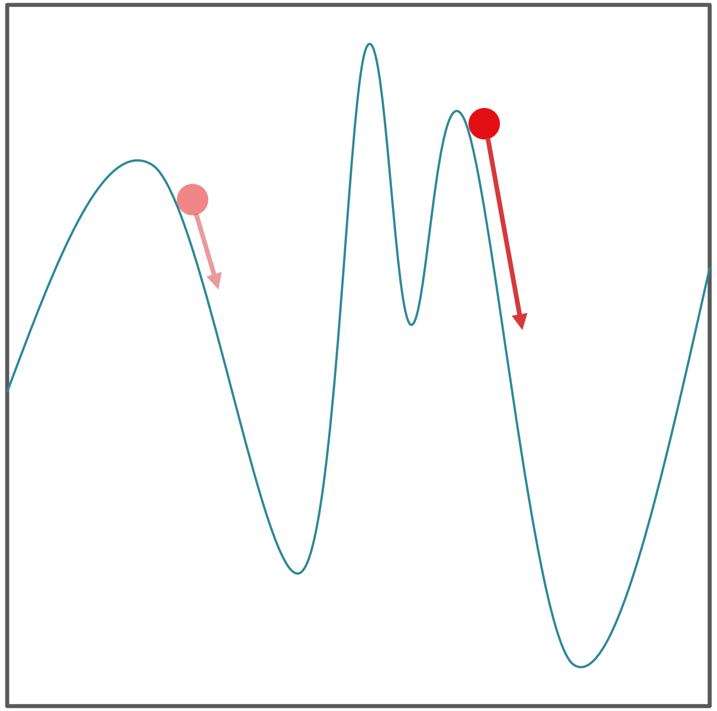

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