10-701: Introduction to Machine Learning

Lecture 4 – Linear Regression

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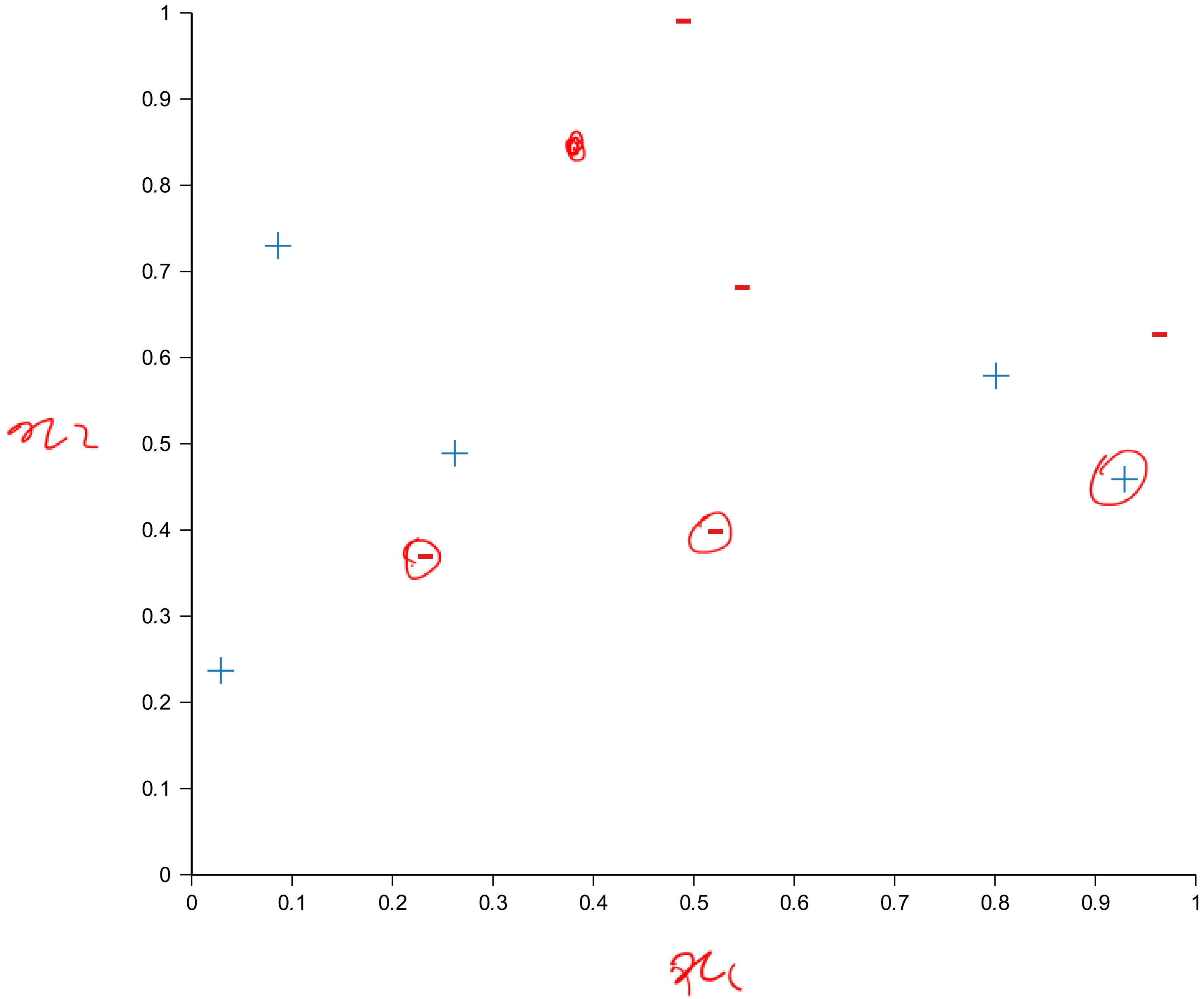
* Slides adopted from F24 offering of 10701 by Henry Chai.

Nearest Neighbor: Example



Generalization of Nearest Neighbor (Cover and Hart, 1967)

- Claim: under certain conditions, as $n \rightarrow \infty$, with high probability, the true error rate of the nearest neighbor model $\leq 2 \ *$ the Bayes error rate (the optimal classifier)
- Proof (cont.):
- $err(h) = \mathbb{E}_{x'}[\mathbb{1}(h(\boldsymbol{x}') \neq y')] = P\{h(\boldsymbol{x}') \neq y'\}$

$$= P\{h(\boldsymbol{x}') = 1, y' = 0\} + P\{h(\boldsymbol{x}') = 0, y' = 1\}$$

$$= \pi\left(\boldsymbol{x}^{\left(\hat{\imath}(\boldsymbol{x}')\right)}\right)(1 - \pi(\boldsymbol{x}')) + \left(1 - \pi\left(\boldsymbol{x}^{\left(\hat{\imath}(\boldsymbol{x}')\right)}\right)\right)\pi(\boldsymbol{x}')$$

$$\rightarrow \pi(\boldsymbol{x}')(1 - \pi(\boldsymbol{x}')) + (1 - \pi(\boldsymbol{x}'))\pi(\boldsymbol{x}')$$

$$= 2\pi(\boldsymbol{x}')(1 - \pi(\boldsymbol{x}'))$$

$$\leq 2\min\Big(\pi(\boldsymbol{x}'), (1 - \pi(\boldsymbol{x}'))\Big) = 2err(h^*) \ \blacksquare$$

Source: https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=1053964

k-Nearest Neighbors (kNN)

- Why limit ourselves to just one neighbor?
- 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)

k-Nearest Neighbors (kNN)

- Why limit ourselves to just one neighbor?
- 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

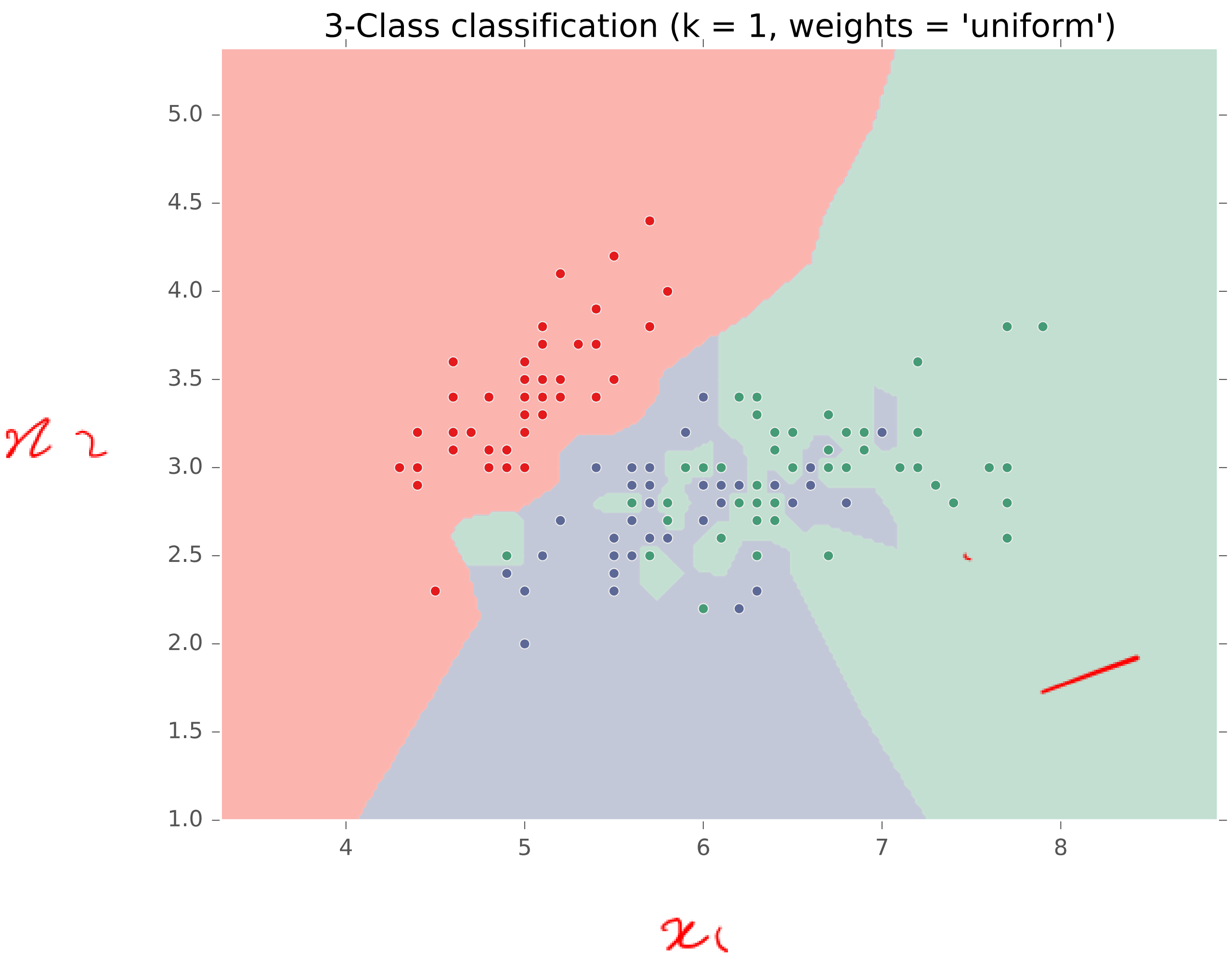


Figure courtesy of Matt Gormley

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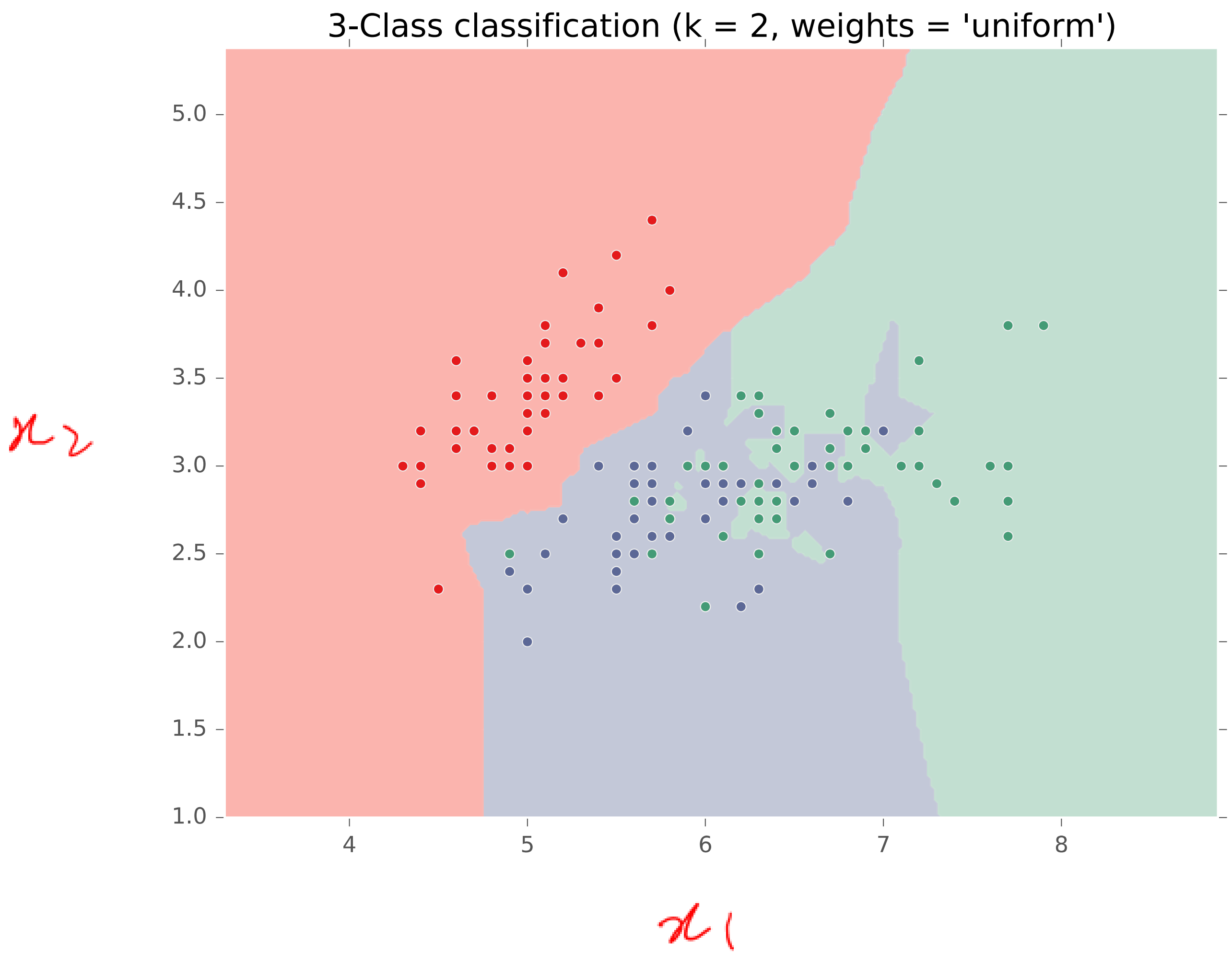

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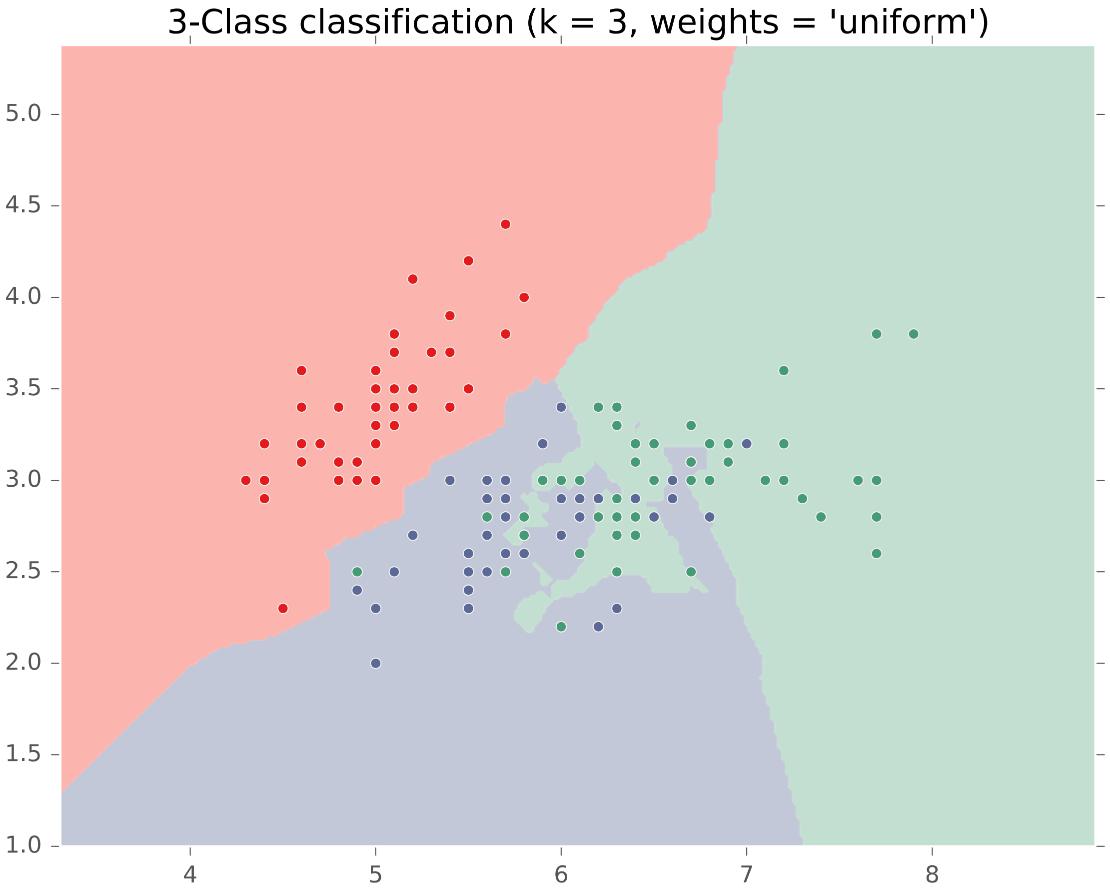

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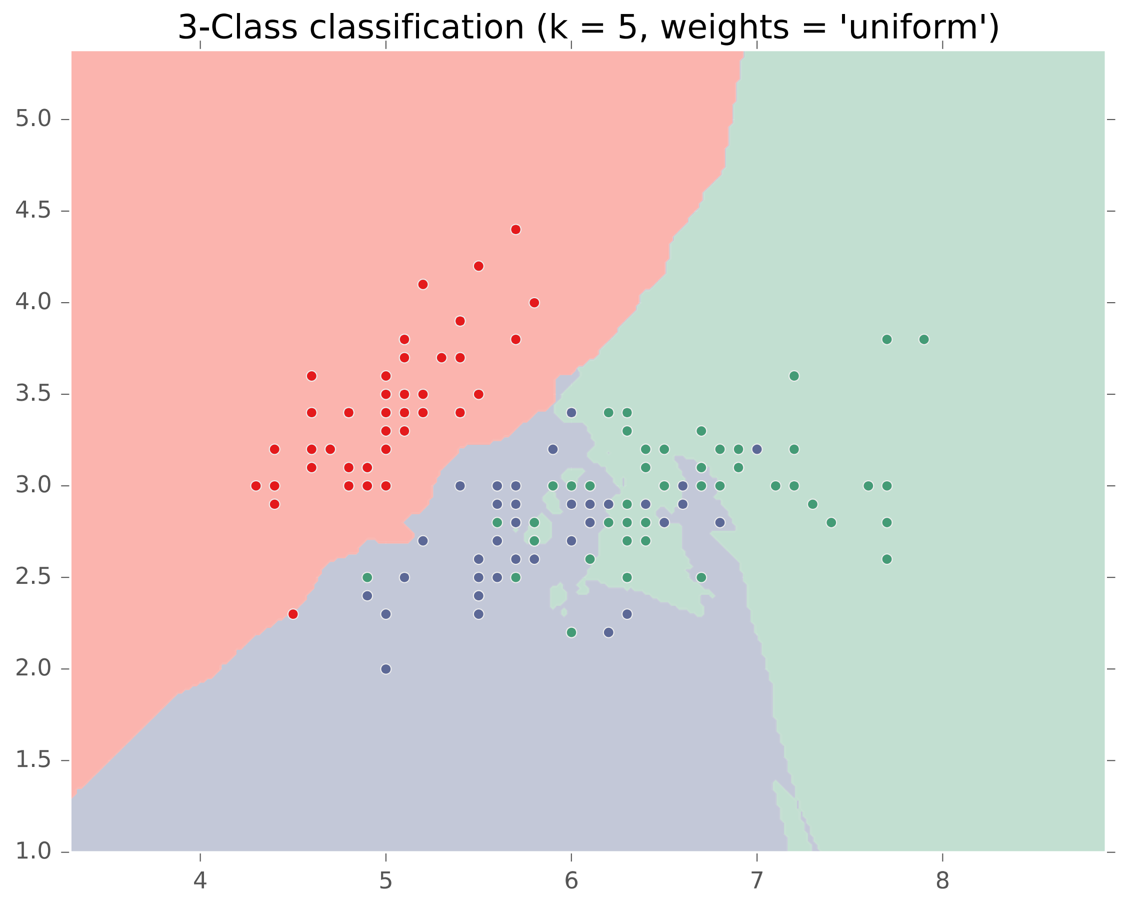

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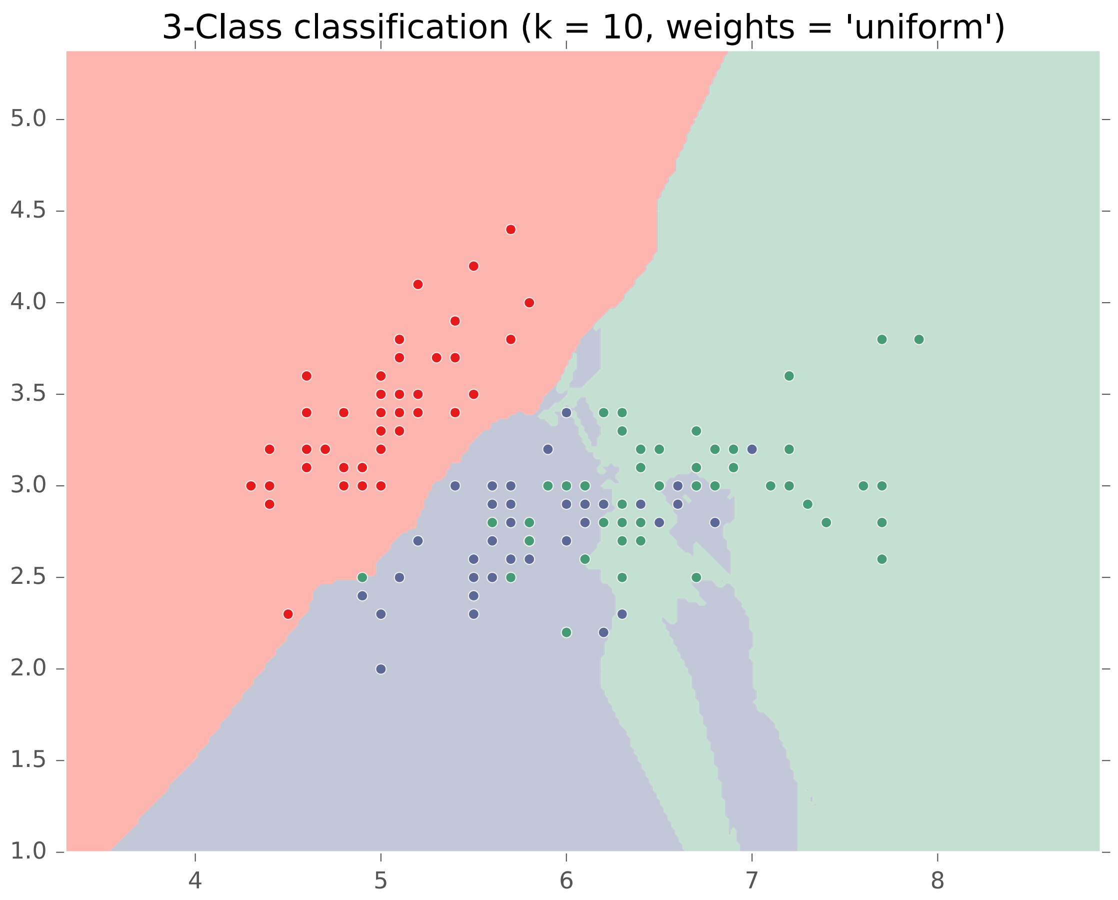

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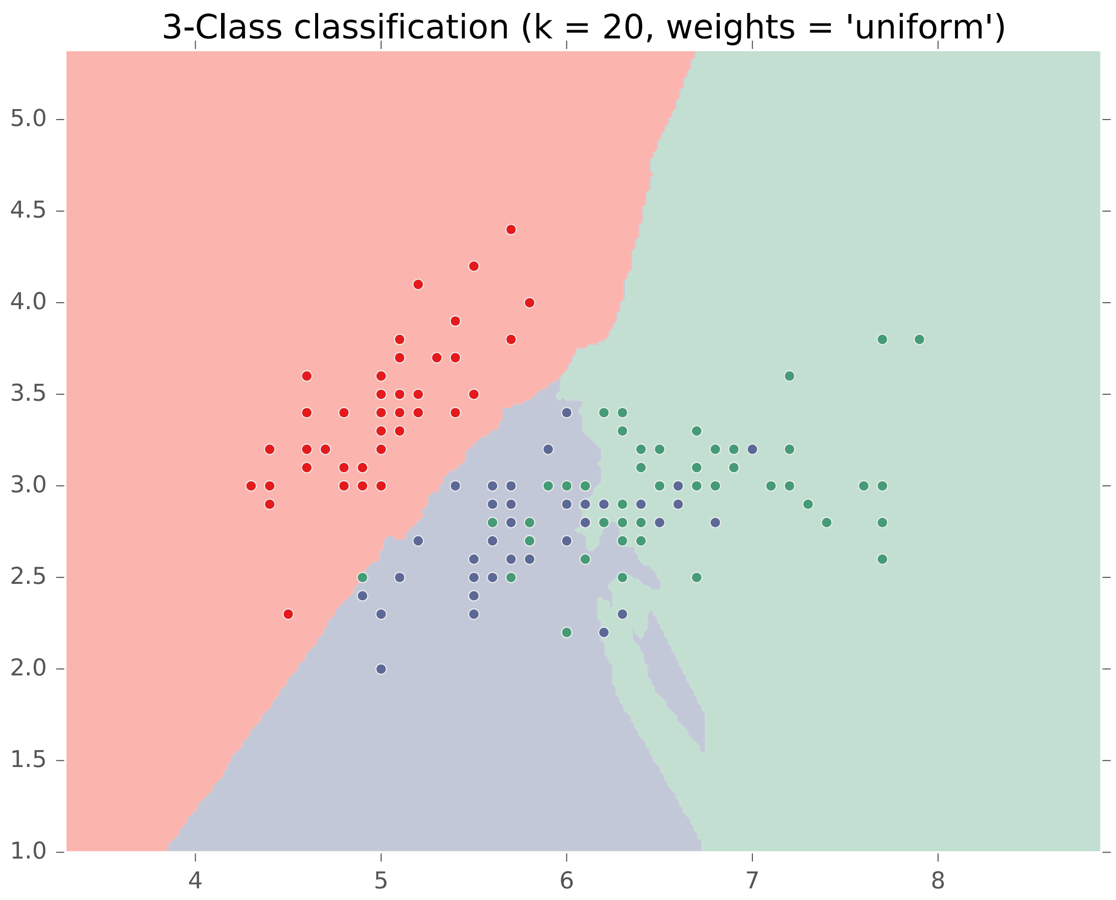

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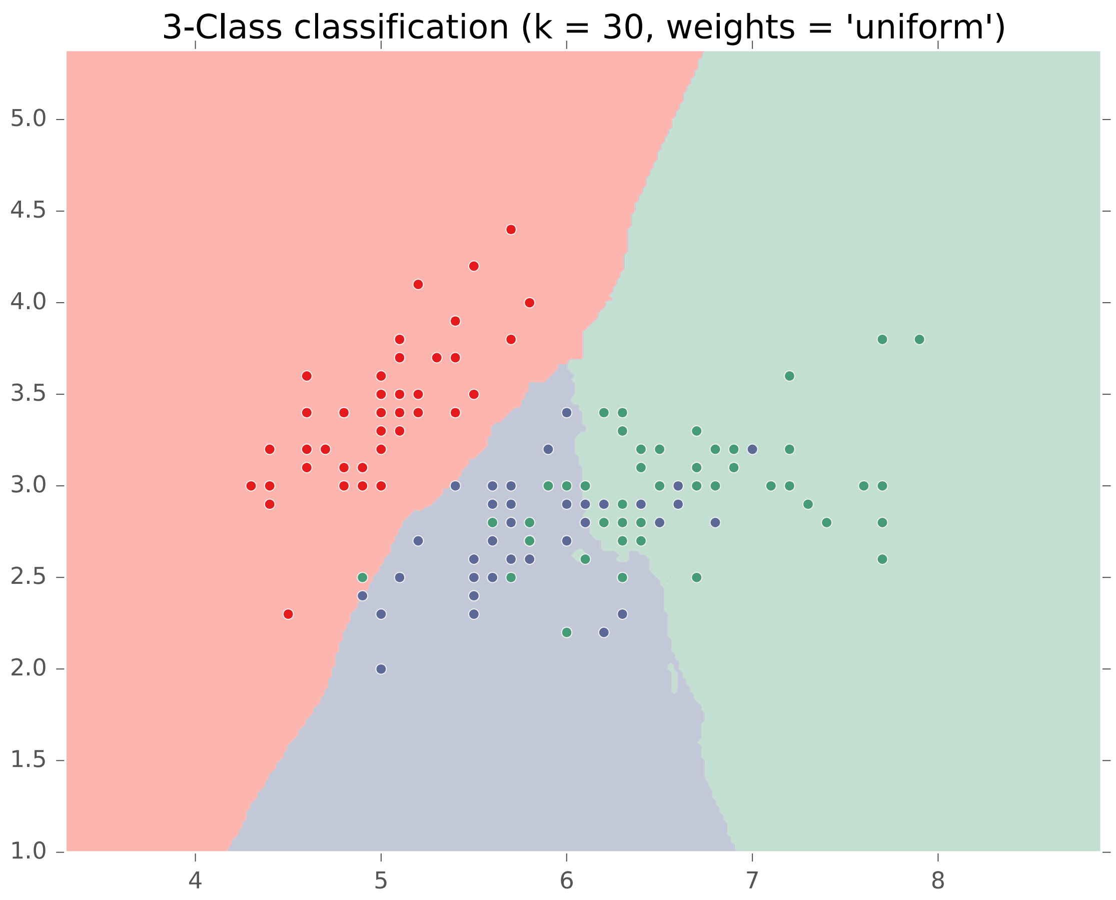

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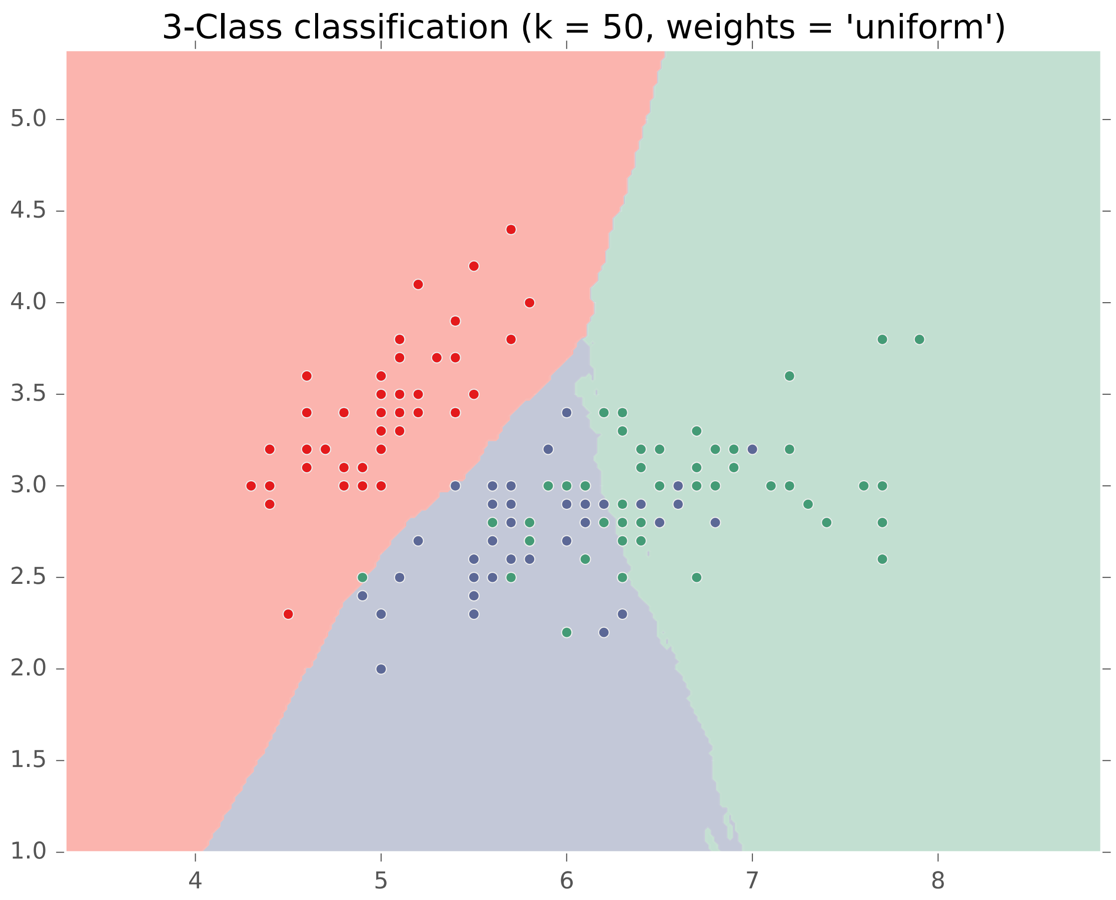

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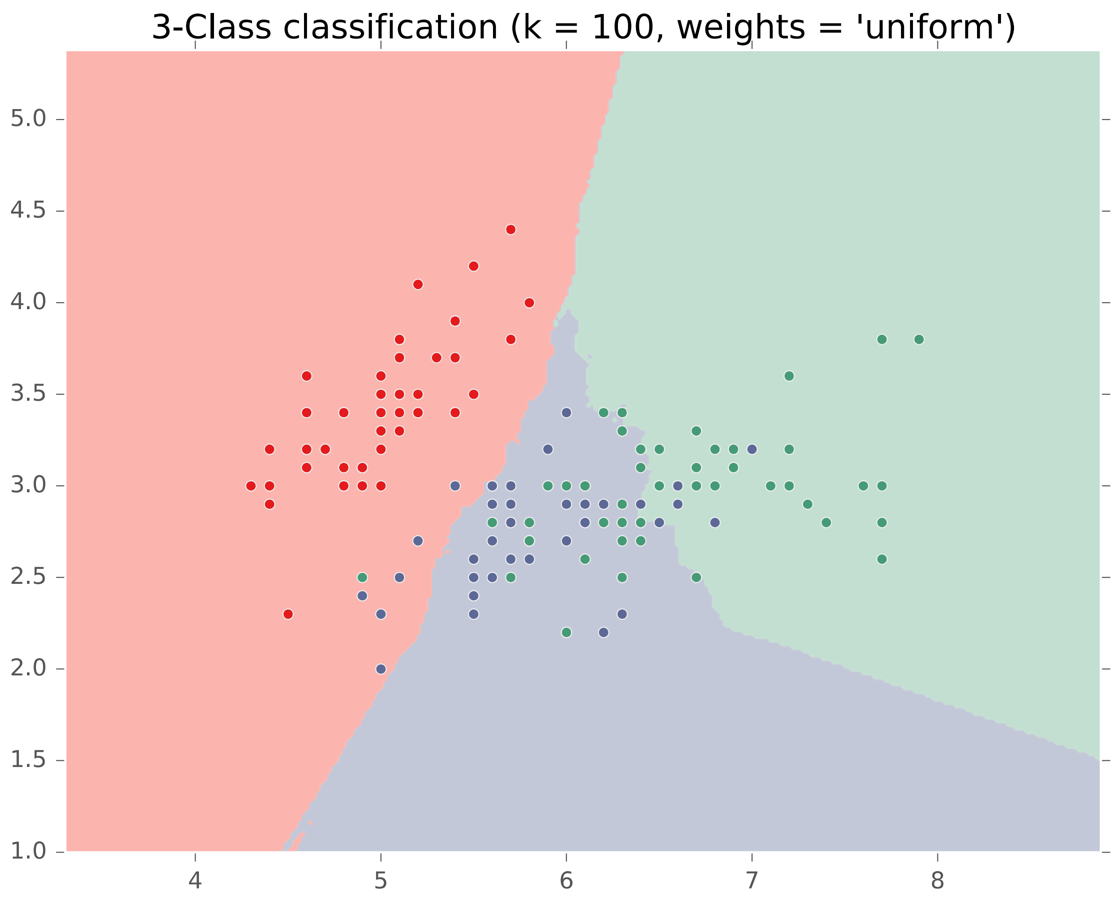

Figure courtesy of Matt Gormley

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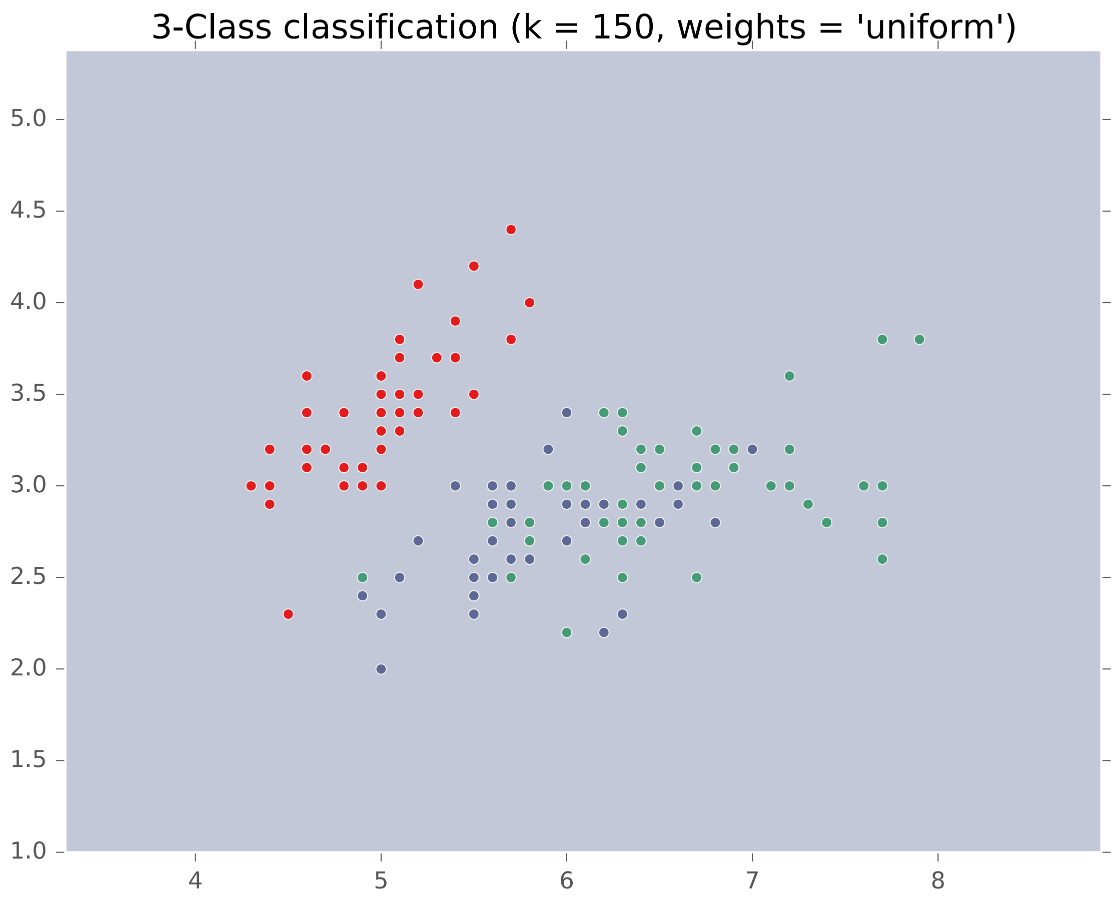


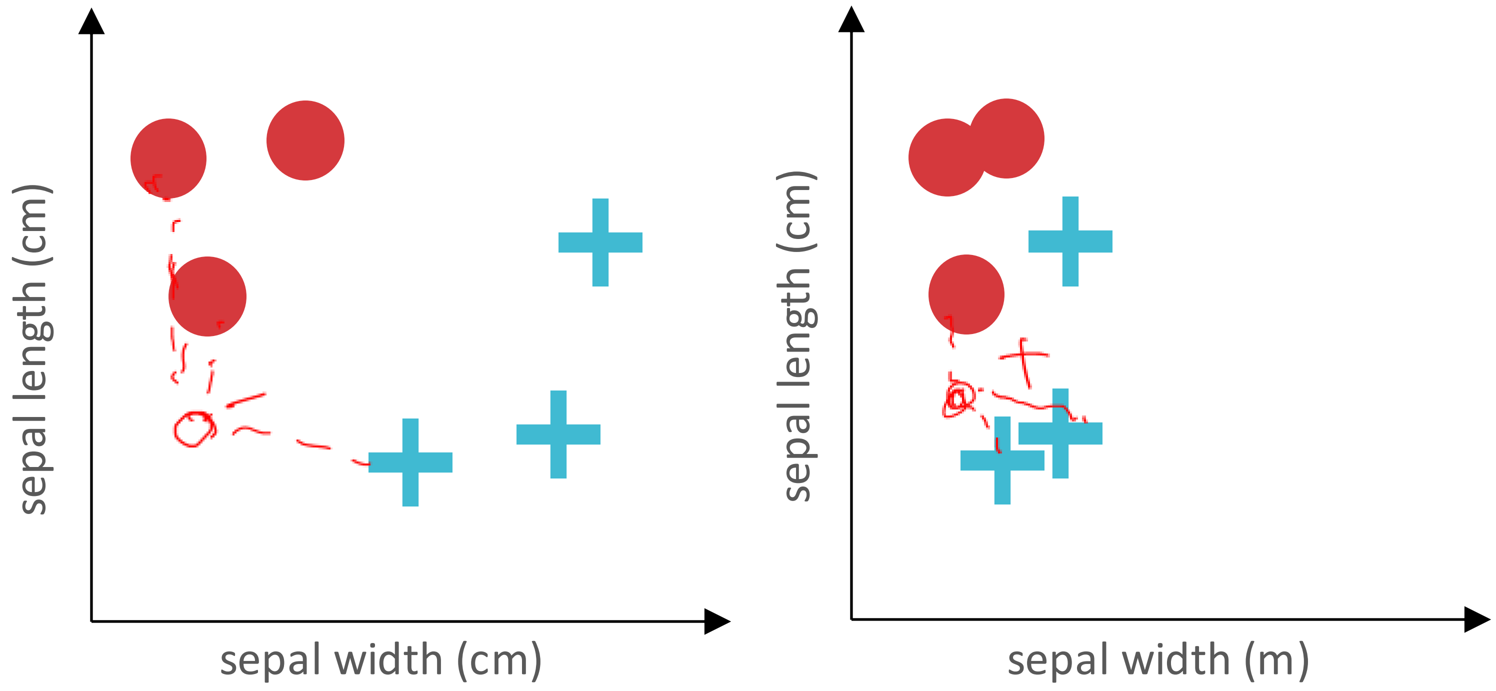
Figure courtesy of Matt Gormley

kNN: Inductive Bias

- What is the inductive bias of a kNN model that uses the Euclidean distance metric?

kNN: Inductive Bias

- What is the inductive bias of a kNN model that uses the Euclidean distance metric?
- Similar points should have similar labels and *all features are equivalently important for determining similarity*



- Feature scale can dramatically influence results!

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 space $\Longrightarrow k$ affects how well the learned model will generalize

Setting k

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

Model Selection

- A **model or hypothesis class** is a (typically infinite) set of classifiers that a learning algorithm searches through to find the best one
- **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/hypothesis class** = set of all possible trees, potentially narrowed down according to the hyperparameters (e.g., max depth)
- **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/hypothesis class** = 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 model/hypothesis spaces:

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

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

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

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

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

Model Selection with Test Sets?

- Given $\mathcal{D} = \mathcal{D}_{train} \cup \mathcal{D}_{test}$, suppose we have multiple candidate <u>model/hypothesis spaces</u>:

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

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

- 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 model/hypothesis spaces: :

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

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

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

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

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

- 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 <u>hyperparameter settings</u>:

$$\theta_1, \theta_2, \ldots, \theta_M$$

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

$$h_1, h_2, \ldots, h_M$$

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

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

- Train a new model on $\boxed{\mathcal{D}_{train} \cup \mathcal{D}_{val}}$ 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

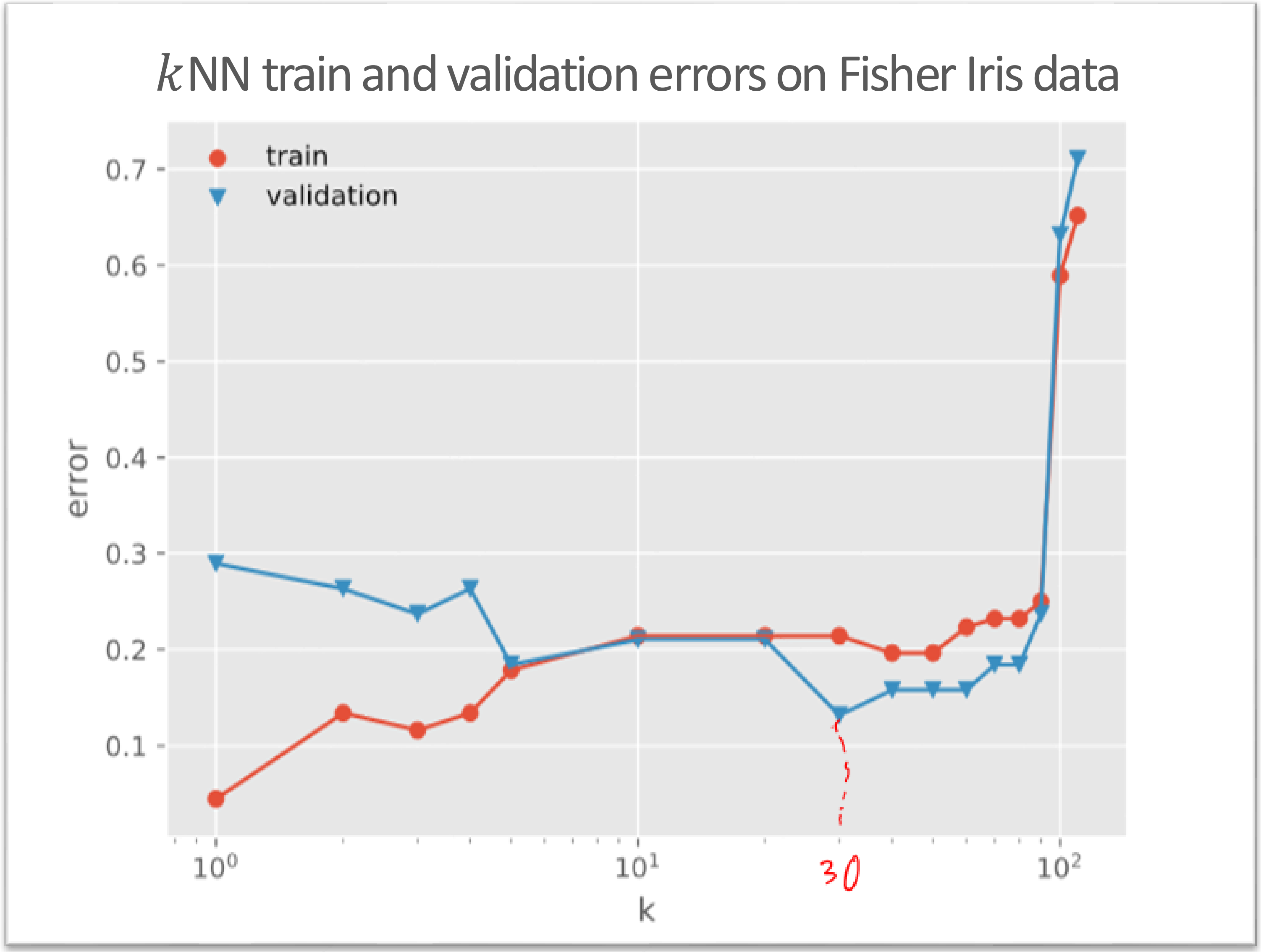


Figure courtesy of Matt Gormley

How should we partition our dataset?

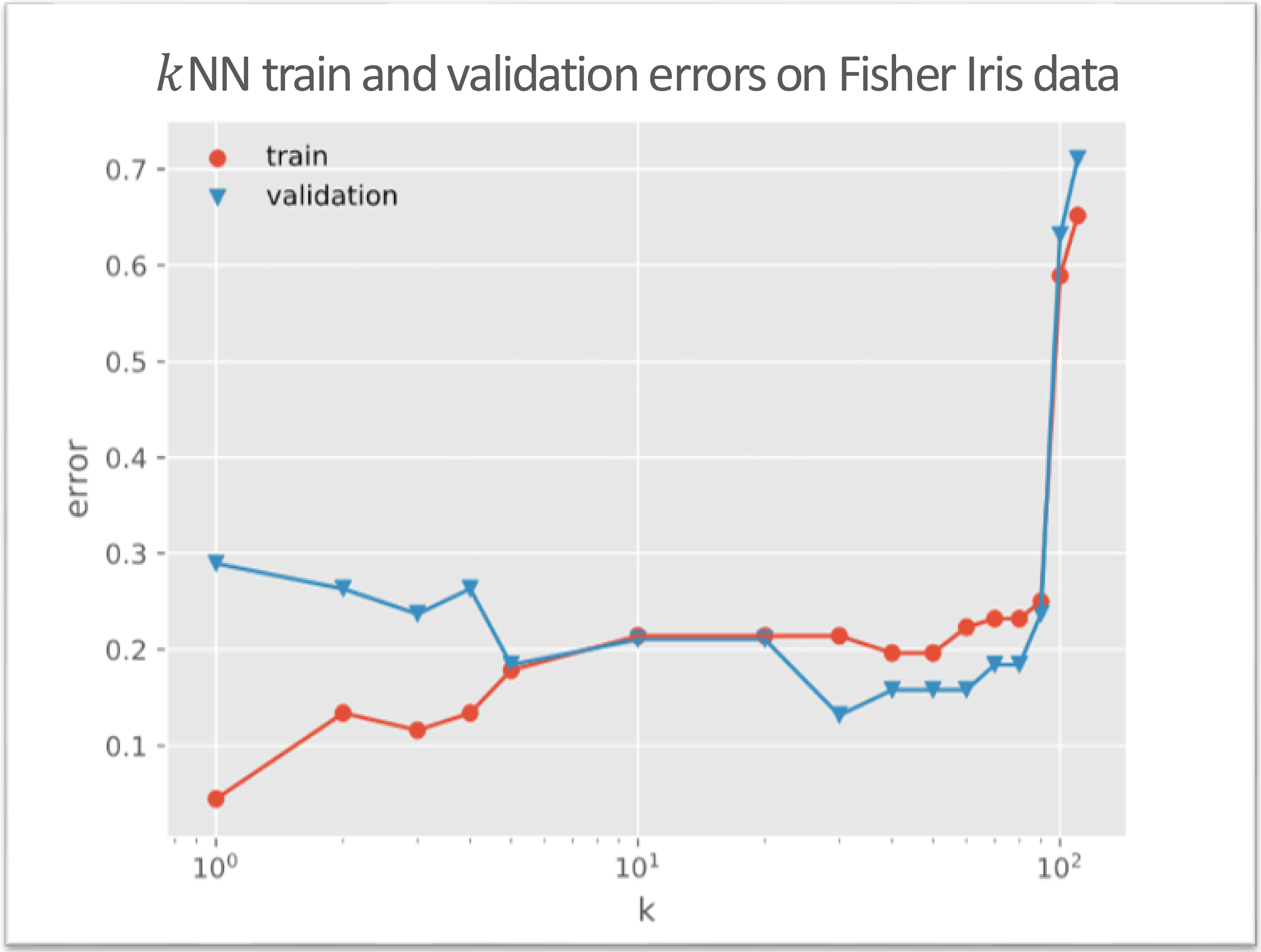
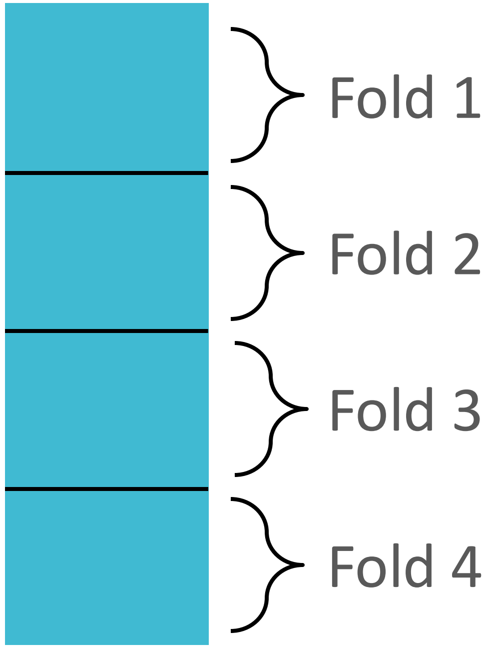


Figure courtesy of Matt Gormley

remaining data when D_{test} is set aside.

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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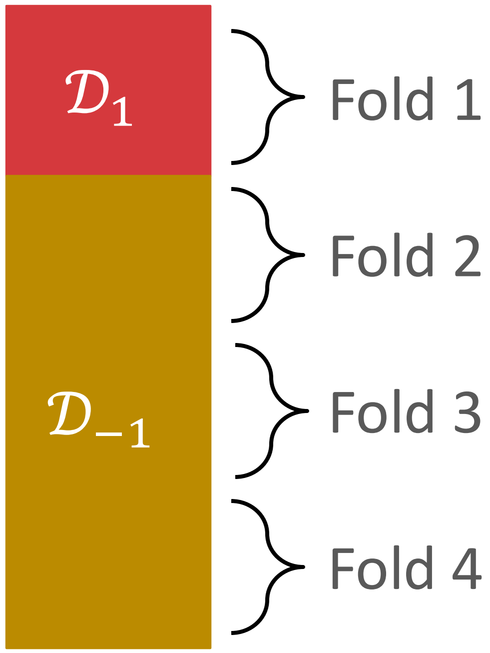

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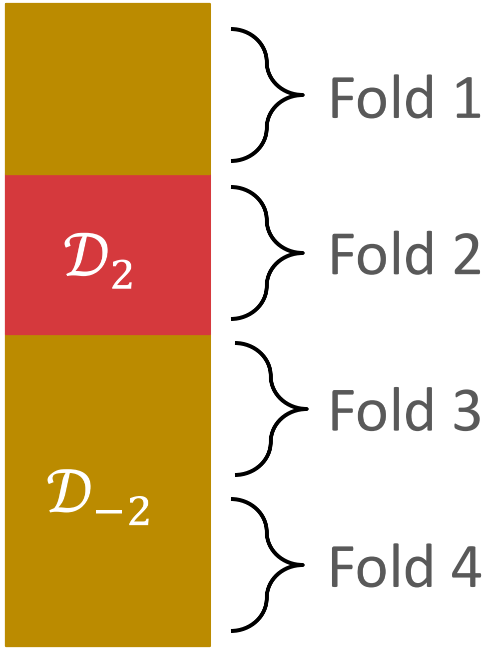

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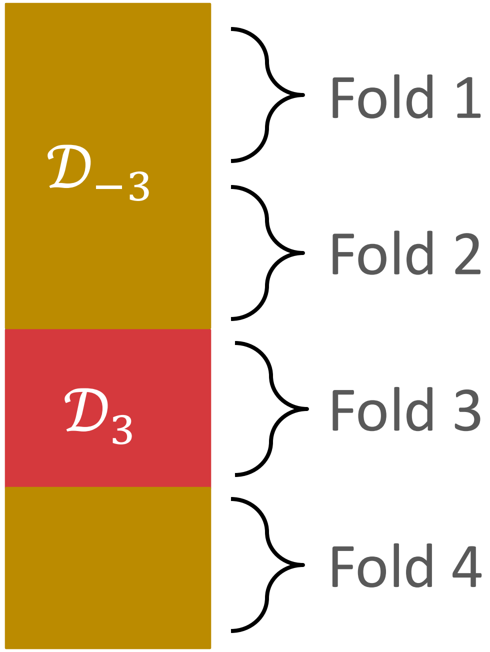

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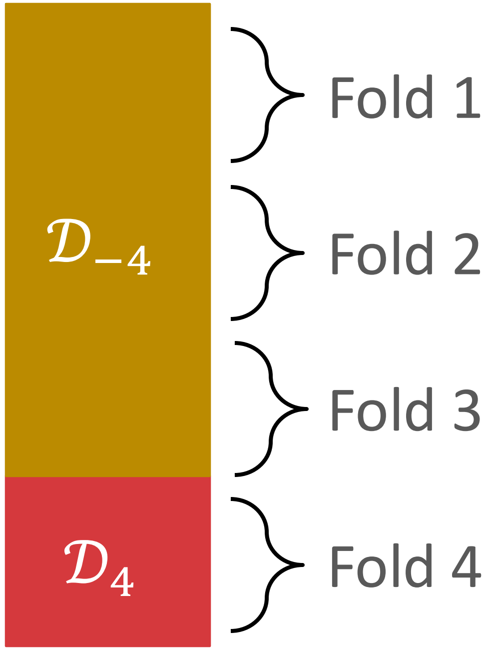

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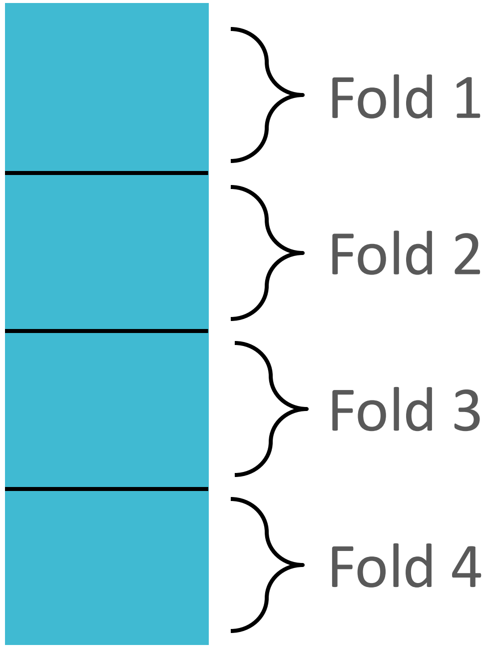

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$$err_{cv_K} = \frac{1}{K} \sum_{i=1}^{K} e_i$$

- Special case when $K = N$: Leave-one-out cross-validation.

K-fold cross-validation

- Given $\mathcal{D}$, split $\mathcal{D}$ into K equally sized datasets or folds: $\mathcal{D}_1, \mathcal{D}_2, \dots, \mathcal{D}_K$
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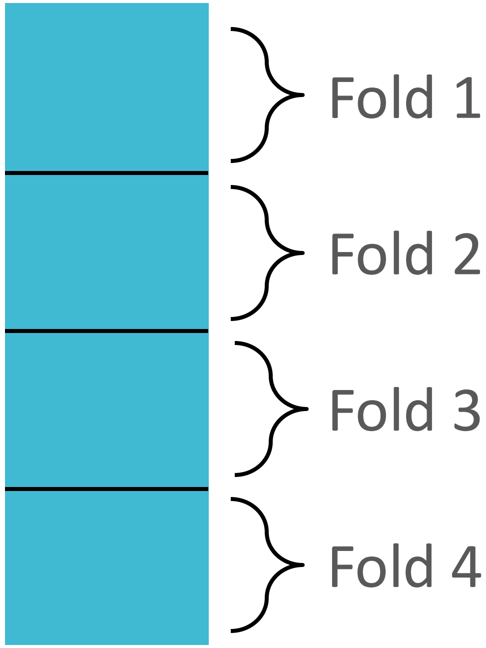

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- The K-fold cross validation error is

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

- Choosing between m candidates requires training $\cancel{K}$ times.

mK

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)** **regression task**

features / targets

data points

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

Decision Tree 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
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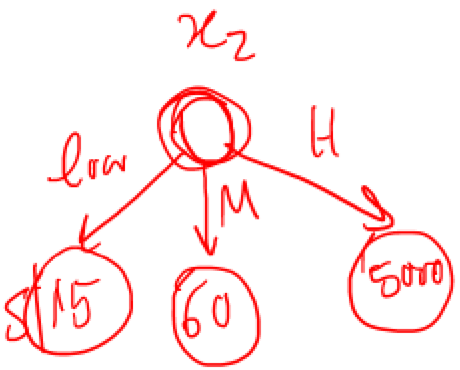
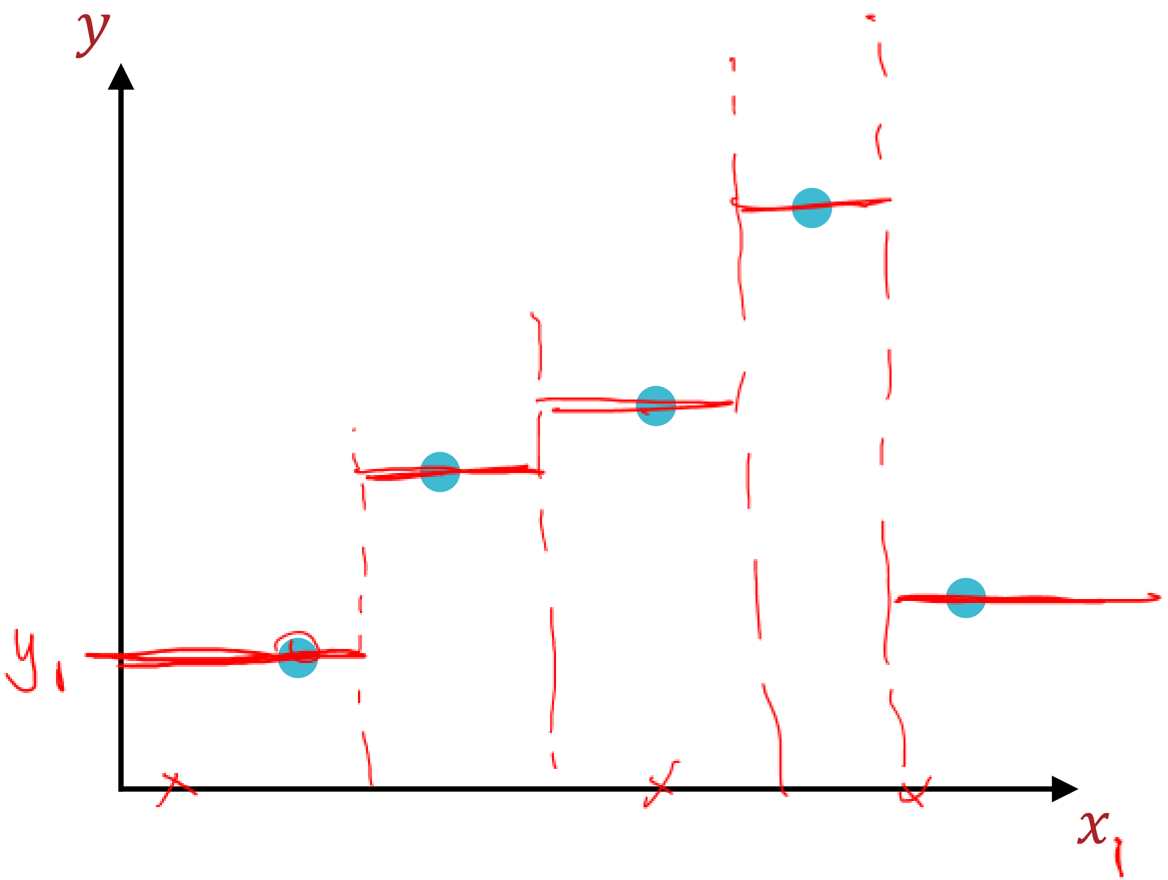
Yes	Medium	Normal	$100
Yes	High	Abnormal	$5000

data points



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 $\boldsymbol{x} = [1, x_1, \dots, x_D]^T \in \mathbb{R}^D$
- **Assume**

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

$$y = w^T x \qquad x \in \mathbb{R}^{D+1}$$

General Recipe for Machine Learning

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

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

Matrix Notation

- 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**

$$y = \boldsymbol{w}^T\boldsymbol{x} \rightarrow \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_D \end{bmatrix}$$

- Notation: given training data $\mathcal{D} = \left\{\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)\right\}_{n=1}^{N}$

- $$X = \begin{bmatrix} 1 & \boldsymbol{x}^{(1)^T} \\ 1 & \boldsymbol{x}^{(2)^T} \\ \vdots & \vdots \\ 1 & \boldsymbol{x}^{(N)^T} \end{bmatrix} = \begin{bmatrix} \boxed{1 \quad x_1^{(1)} \quad \cdots \quad x_D^{(1)}} \\ 1 \quad x_1^{(2)} \quad \cdots \quad x_D^{(2)} \\ \vdots \quad \vdots \quad \ddots \quad \vdots \\ 1 \quad x_1^{(N)} \quad \cdots \quad x_D^{(N)} \end{bmatrix} \in \mathbb{R}^{N \times D+1}$$

feature vector for i=1

⋮

i=N

is the *design matrix*

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

Minimizing the Squared Error

$$\ell_D(\boldsymbol{w}) = \frac{1}{N}\sum_{n=1}^{N}\left(\underbrace{\boldsymbol{w}^T\boldsymbol{x}^{(n)}} - y^{(n)}\right)^2 = \underbrace{\frac{1}{N}\sum_{n=1}^{N}\left(x^{(n)T}\omega - y^{(n)}\right)^2}$$

verify

$$= \frac{1}{N}(X\omega - Y)^T(X\omega - Y) \quad \left[= \frac{1}{N}\|X\omega - Y\|_2^2\right]$$

$$= \frac{1}{N}\Big(\omega^T X^T X \omega - \underbrace{\underbrace{Y^T X \omega} - \underbrace{\omega^T X^T Y}}_{2\omega^T X^T Y} + \underbrace{Y^T Y}\Big)$$

$$\nabla_\omega \ell_D(\omega) = 2X^TX\omega - 2X^TY \cancel{+0}$$

$$= 0 \Rightarrow \cancel{2}X^TX\hat{\omega} = \cancel{2}X^TY$$

$$\Rightarrow \boxed{\hat{\omega} = (X^TX)^{-1}X^TY}$$

$$H_\omega \ell_D(\omega) = 2X^TX \succeq 0$$

$\hookrightarrow$ p.s.d

Minimizing the Squared Error

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

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

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

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

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

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

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

Minimizing the Squared Error

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

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

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

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

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

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

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

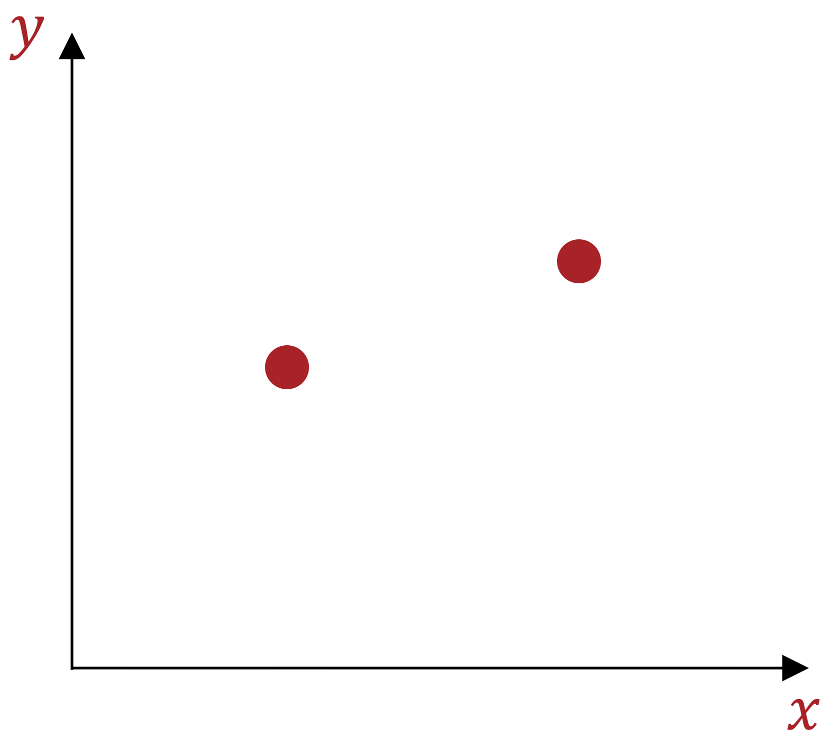
Closed Form Solution

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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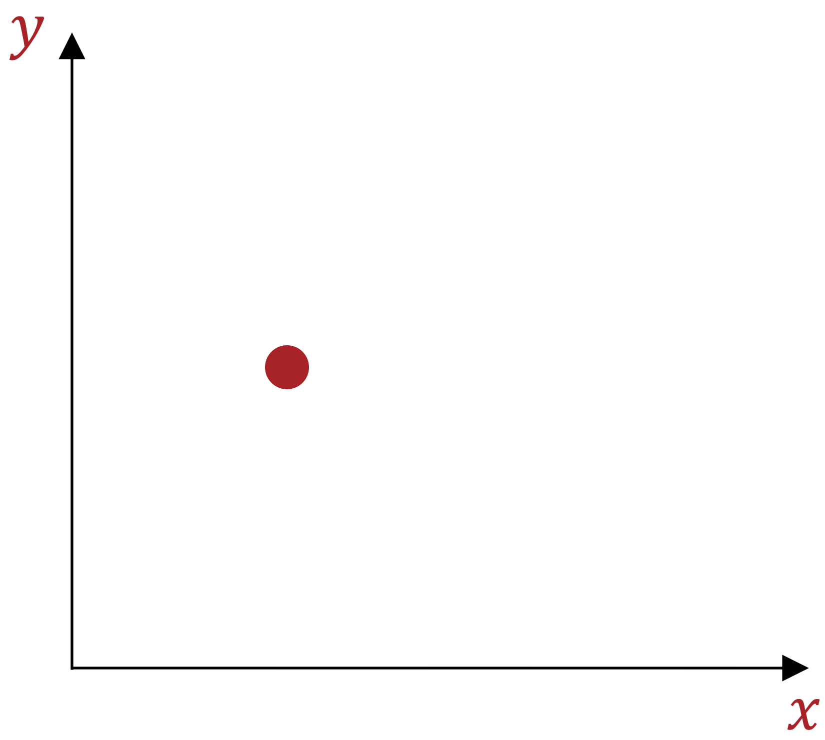

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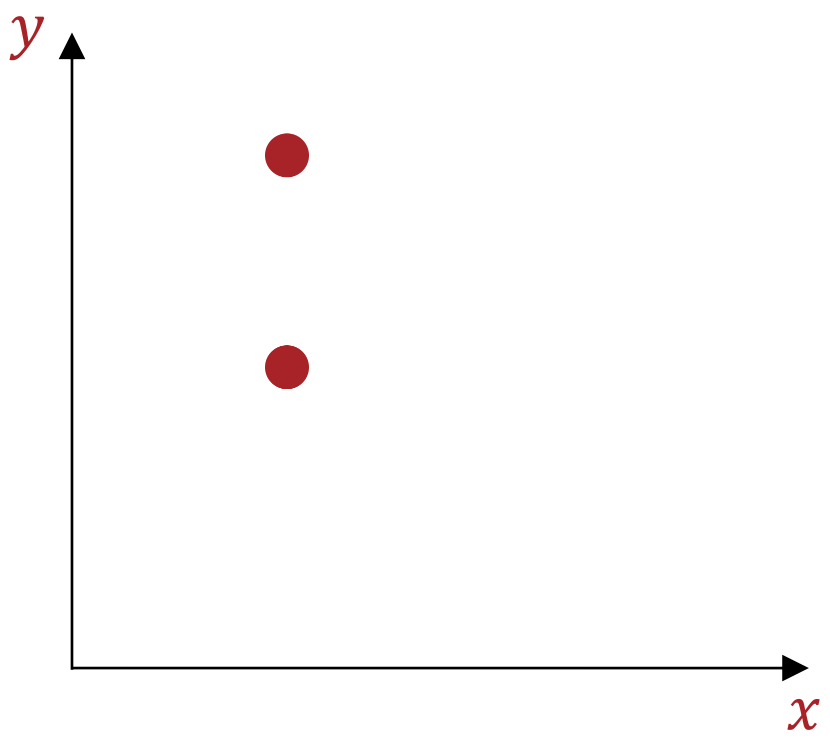
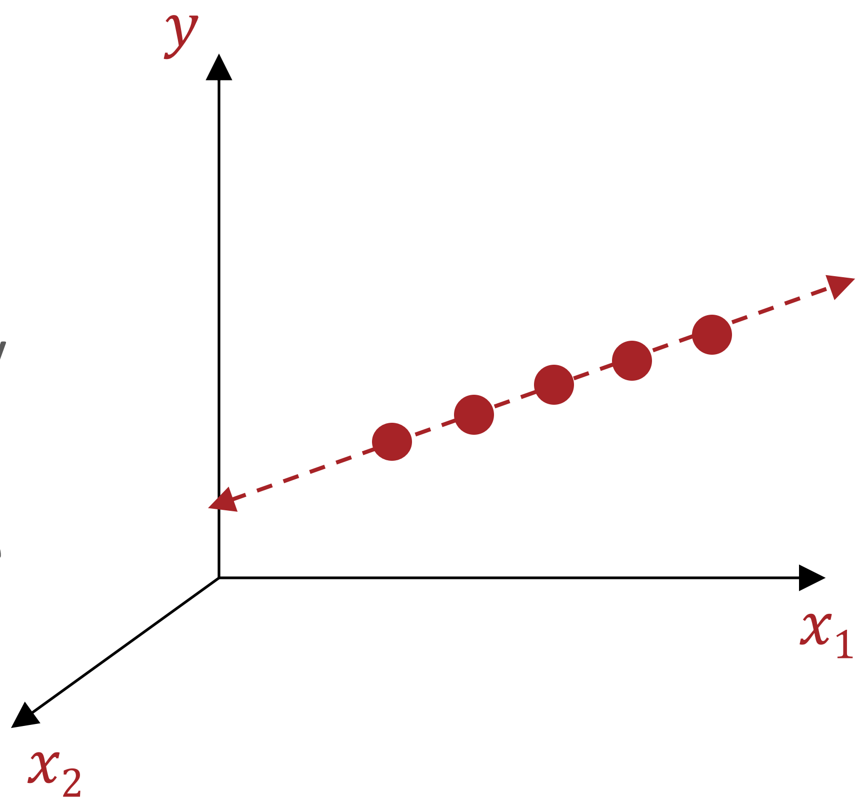


Linear Regression: Uniqueness

- 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?



Linear Regression: Uniqueness

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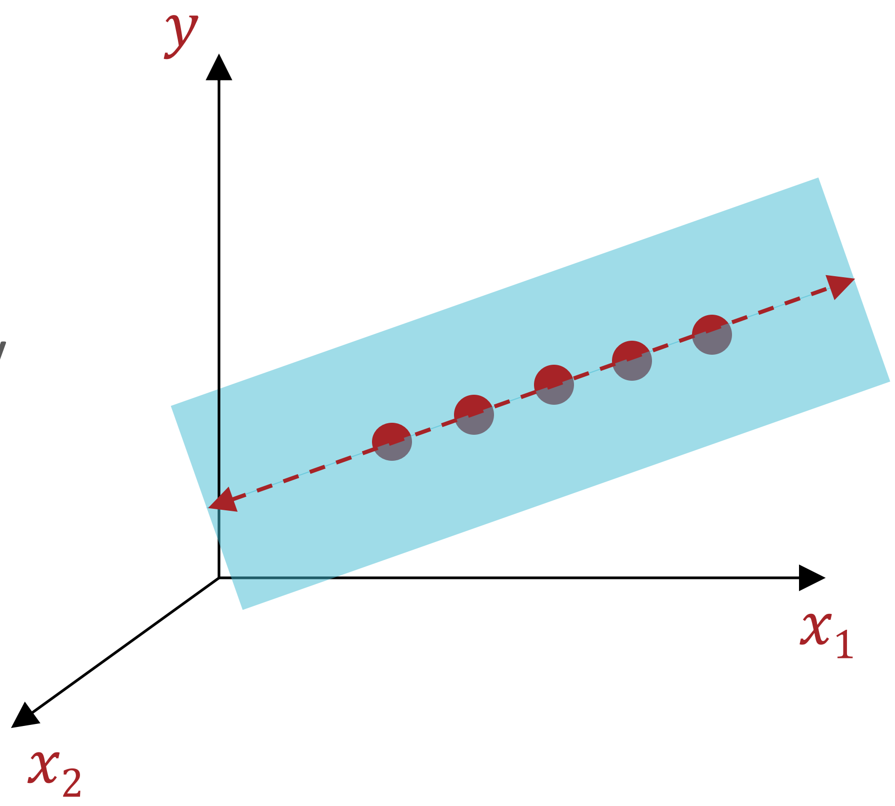

Linear Regression: Uniqueness

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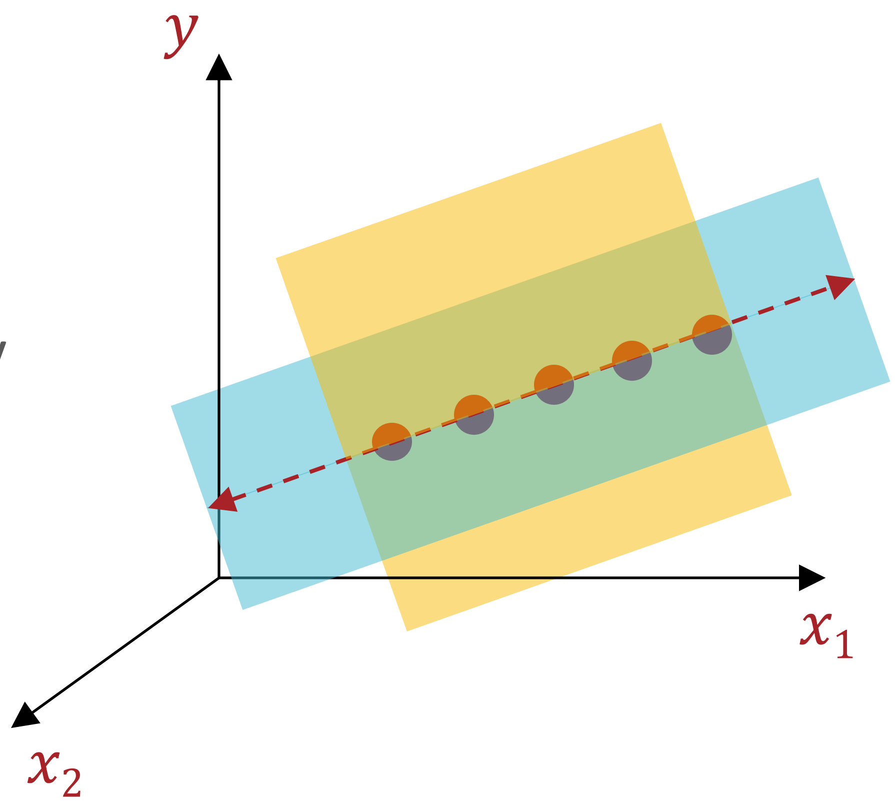


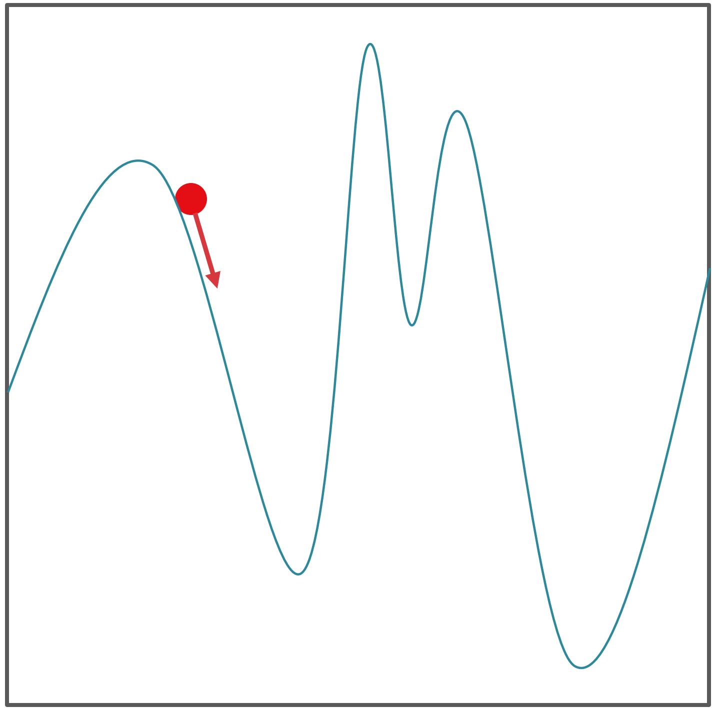
$$\hat{\boldsymbol{w}} = (X^T X)^{-1} X^T \boldsymbol{y}$$

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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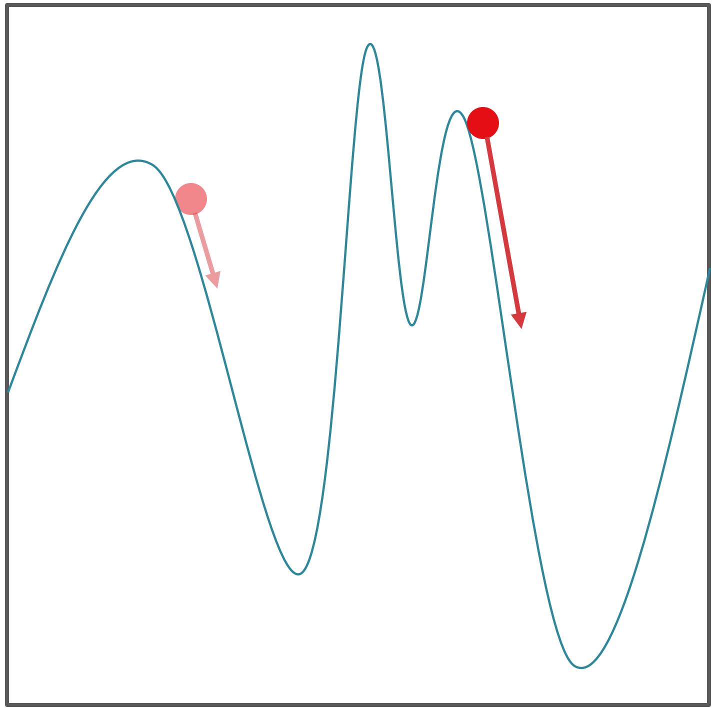

Gradient Descent: Intuition

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