RICE

Rice Data Science Bootcamp

Instructor: Natalie Berestovsky, PhD

Occidental Petroleum/

Anadarko Petroleum

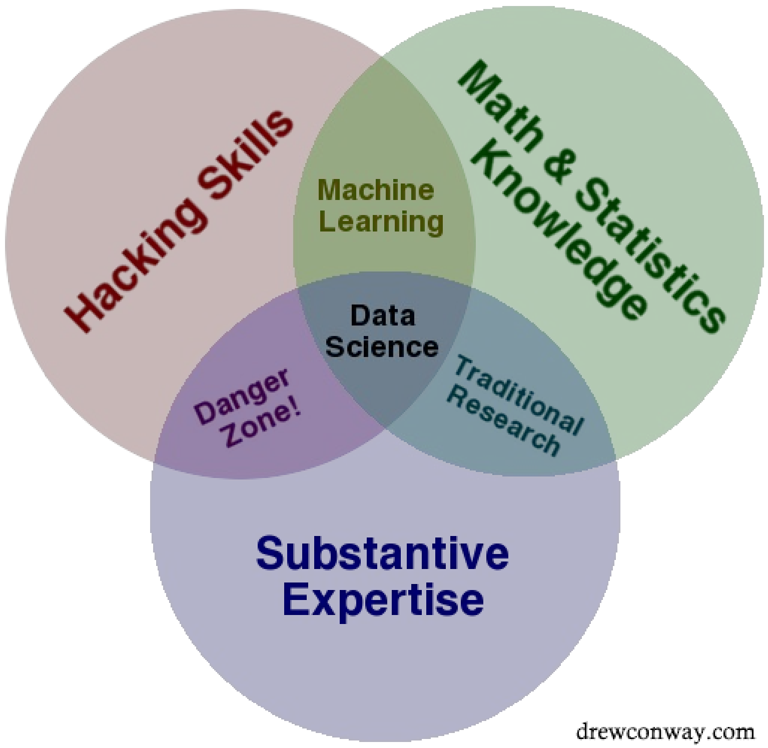
Your instructor

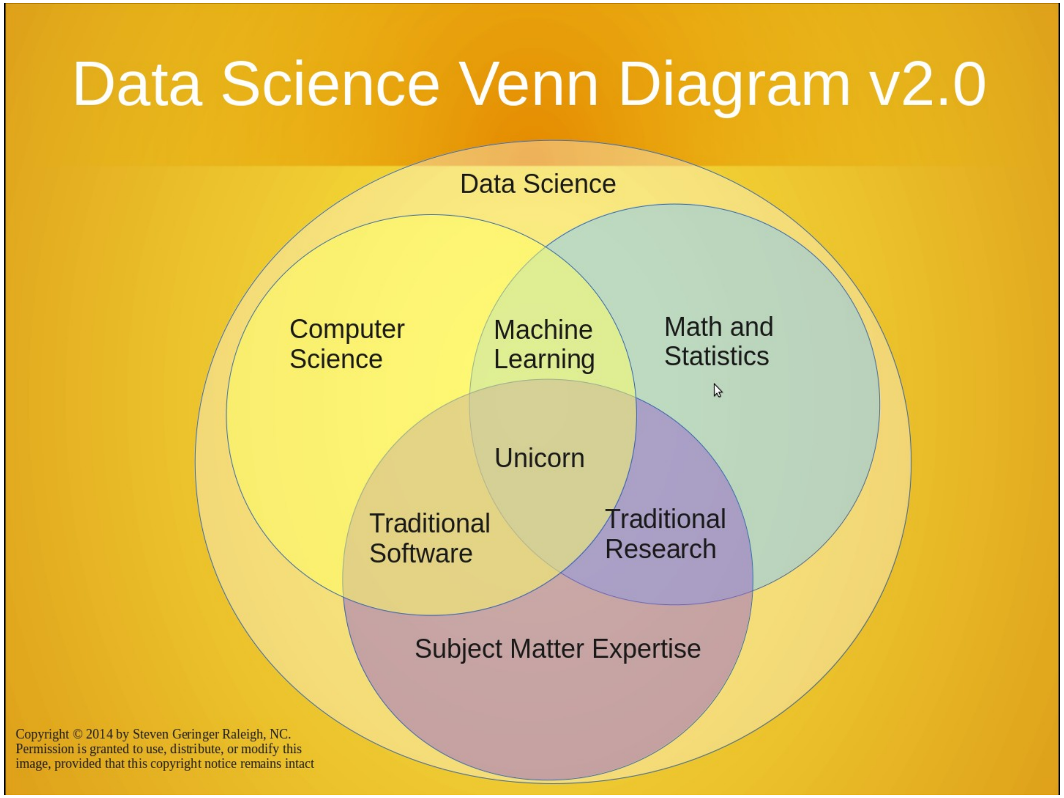
- Education
  - BS in Computer Science from UT-Austin
  - MS and PhD in Computer Science from Rice

- Professional Experience:
  - Worked in Chevron for 6 years ~~in Chevron~~
  - Data Scientist in Anadarko for 2.5 years
  - Next: Oxy?

- AI experience:
  - ML techniques, deep learning
  - Google Cloud Platform

Data Science





RICE

Supervised vs unsupervised

- *Supervised / Unsupervised / Both*
  - Recognizing digits in the images (S)
  - Gene clustering (U)
  - Identifying alerts in your streaming data (B)
  - Predicting stock prices (B)
  - Anomaly / fraud detection (B)
  - Ranking public speech impact from recordings (U)
  - Face recognition (S)
  - Automated text completion (Gmail) (S)
  - Voice recognition (S)

Supervised vs unsupervised

Unsupervised vs. Supervised Learning

Data Matrix:

$$\mathbf{X}_{n \times p} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ \vdots & & \ddots & \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{pmatrix}$$

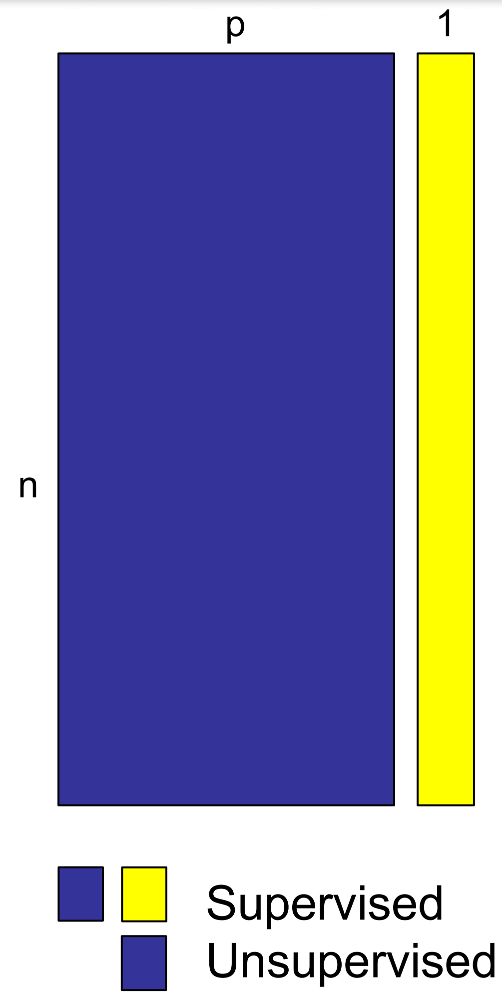
- Rows: n observations / samples / subjects.
- Columns: p features / variables.

Supervised Learning:

$$Y = (y_1, y_2, \ldots y_n)^T$$

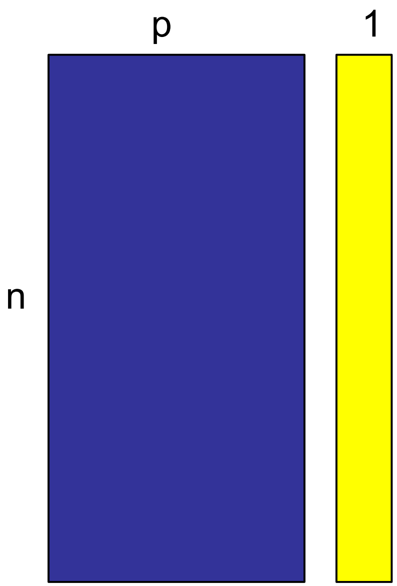
- Classification: Y - n labels.
- Regression: Y - n continuous outcomes.

Unsupervised Learning: No outcomes / labels!

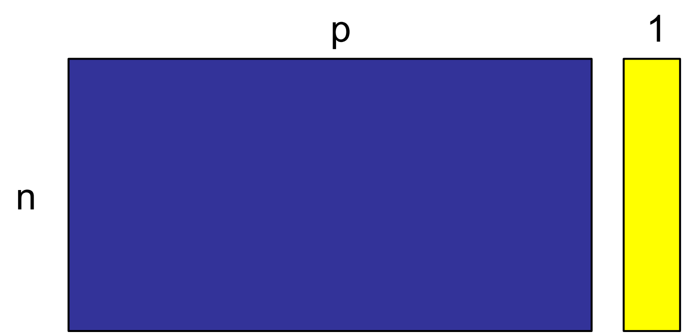


Data Dimensions

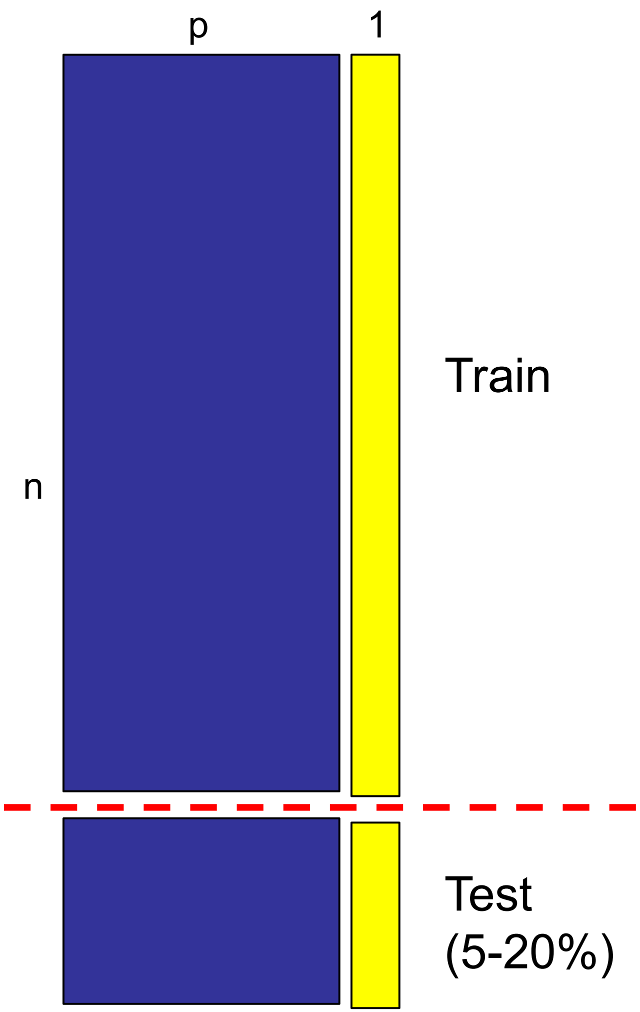
- n >> p
- More samples than features
- Examples?



- n << p
- Fewer samples than features
- Examples?

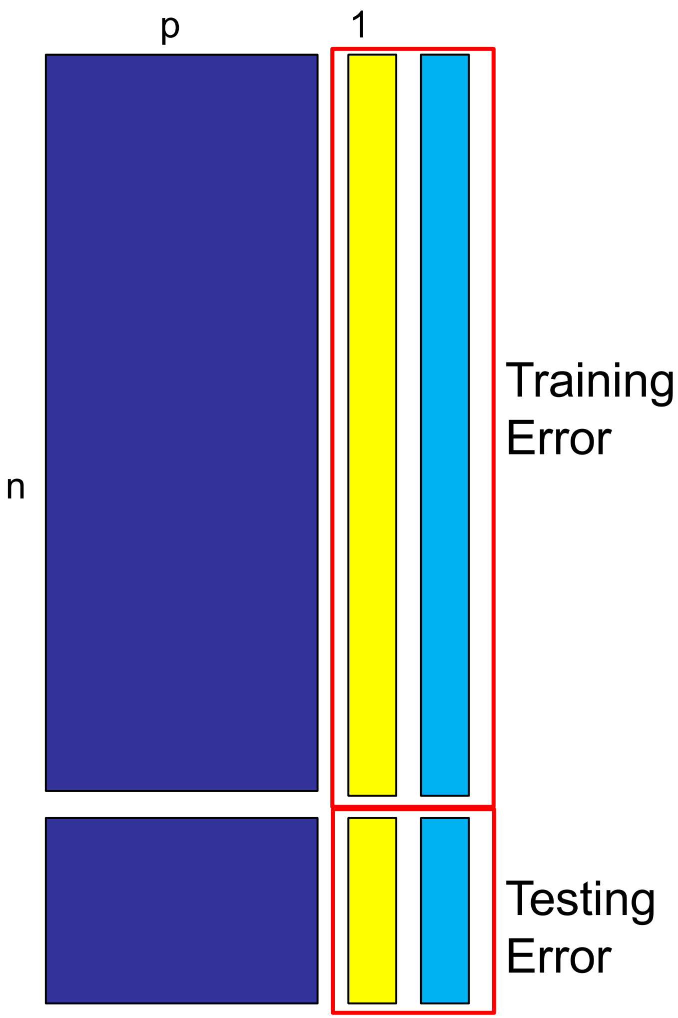


Modeling methodology



- Train / test split
  - Hold out validation
    - Selects x% of data randomly
  - K-fold cross validation
    - Shuffles that data (or not)
    - Split the data into k equal sets
    - For each split, use k-1 set for training and test on the k^{th}

Assessing your model



- Training error
  - Error of how well the model generates the data that it has seen
- Testing error
  - Error on unseen data (prediction)
- Generally $E_{train} <= E_{test}$
- What if $E_{train} << E_{test}$?
- What if $E_{train} > E_{test}$?

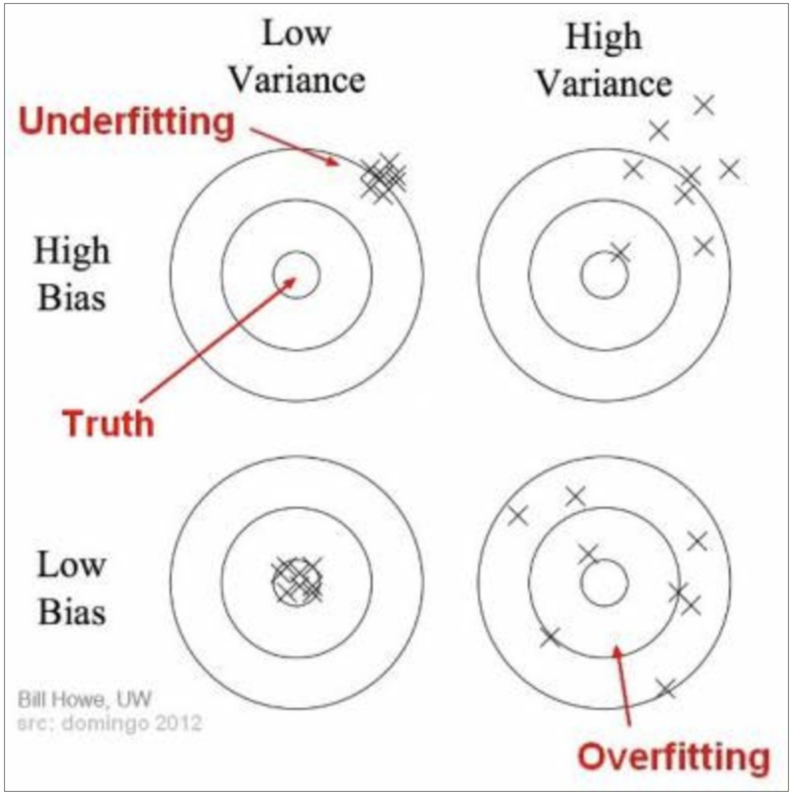
Overfitting and underfitting

$$Err(x) = E\left[(Y - \hat{f}(x))^2\right]$$

$$Err(x) = \left(E[\hat{f}(x)] - f(x)\right)^2 + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] + \sigma_e^2$$

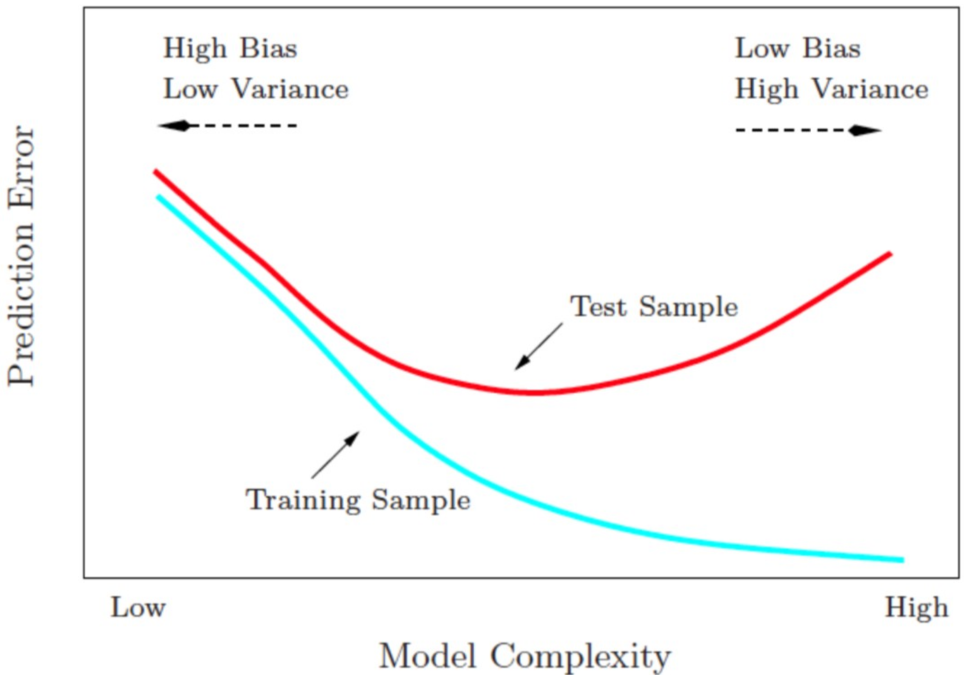
$$Err(x) = \mathrm{Bias}^2 + \mathrm{Variance} + \mathrm{Irreducible\ Error}$$

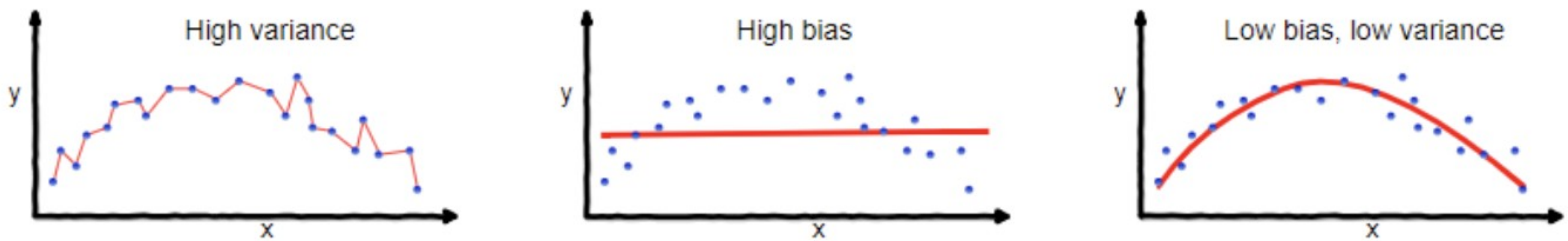
- **Bias** – difference between predicted and true value
  - *High bias* – generalized model, high error
  - *Low bias* – fits well to the training set, low training error
- **Variance** – variability of prediction for a given data point
  - *High variance* – sensitive to training data set
  - *Low variance* – not sensitive to changes in training set
- **Irreducible error** – noise in the data



Overfitting and underfitting

- Bias-variance tradeoff
  - Complex, many parameters
    - overfitting
  - Simple, few parameters
    - underfitting





overfitting **underfitting** **Good balance**

Supervised vs unsupervised

	Supervised	Unsupervised
Discrete	***Classification***	***Clustering***
	KNN **Datasets:** *Wine dataset*	K-Means Hierarchical clustering (Biclustering) **Datasets:** Synthetic data NCI60
Continuous	***Regression***	***Dimensionality reduction***
	Multilinear regression Ridge regression Lasso regression **Datasets:** *Boston housing dataset* *Synthetic data*	Principle Component Analysis (PCA) **Datasets:** Art data NCI60

K Nearest Neighbors

sklearn.neighbors.KNeighborsClassifier

class `sklearn.neighbors.` **`KNeighborsClassifier`** (*n_neighbors=5*, *weights='uniform'*, *algorithm='auto'*, *leaf_size=30*, *p=2*, *metric='minkowski'*, *metric_params=None*, *n_jobs=None*, ***kwargs*) [source]

Classifier implementing the k-nearest neighbors vote.

Read more in the User Guide.

Parameters:

n_neighbors : *int, optional (default = 5)*

Number of neighbors to use by default for `kneighbors` queries.

weights : *str or callable, optional (default = 'uniform')*

weight function used in prediction. Possible values:

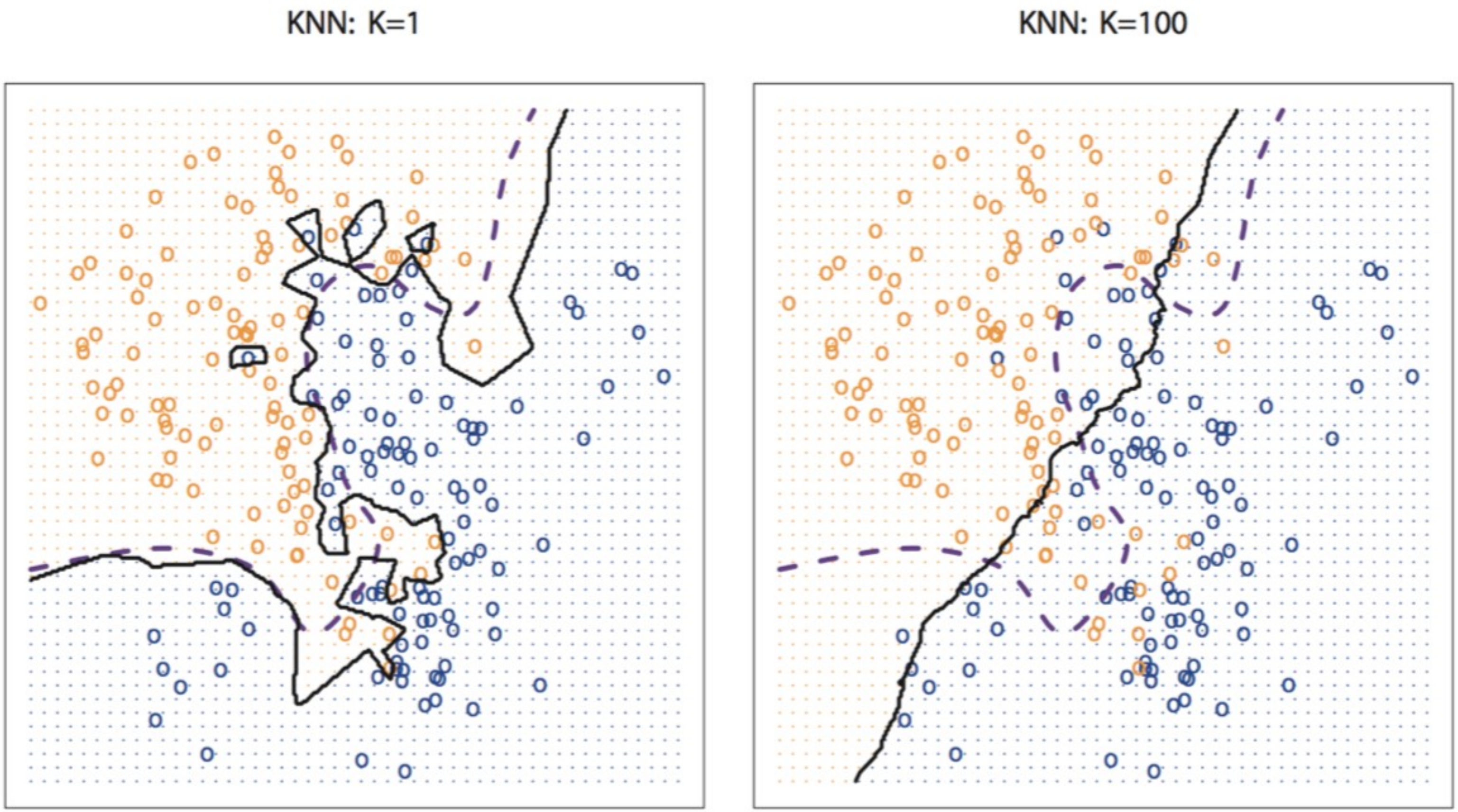
- 'uniform' : uniform weights. All points in each neighborhood are weighted equally.
- 'distance' : weight points by the inverse of their distance. in this case, closer neighbors of a query point will have a greater influence than neighbors which are further away.
- [callable] : a user-defined function which accepts an array of distances, and returns an array of the same shape containing the weights.

algorithm : *{'auto', 'ball_tree', 'kd_tree', 'brute'}, optional*

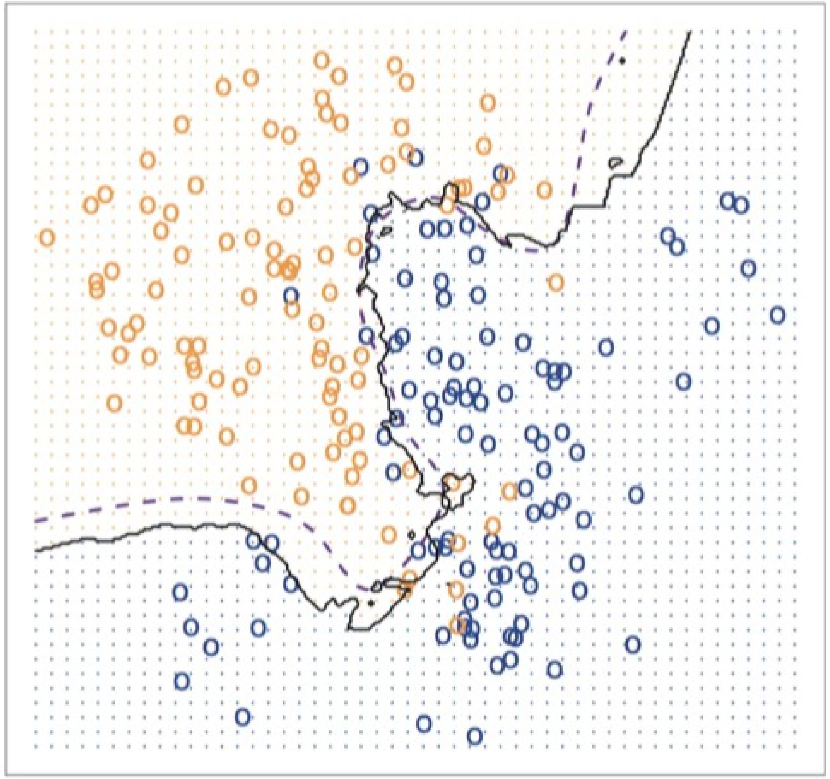
Algorithm used to compute the nearest neighbors:

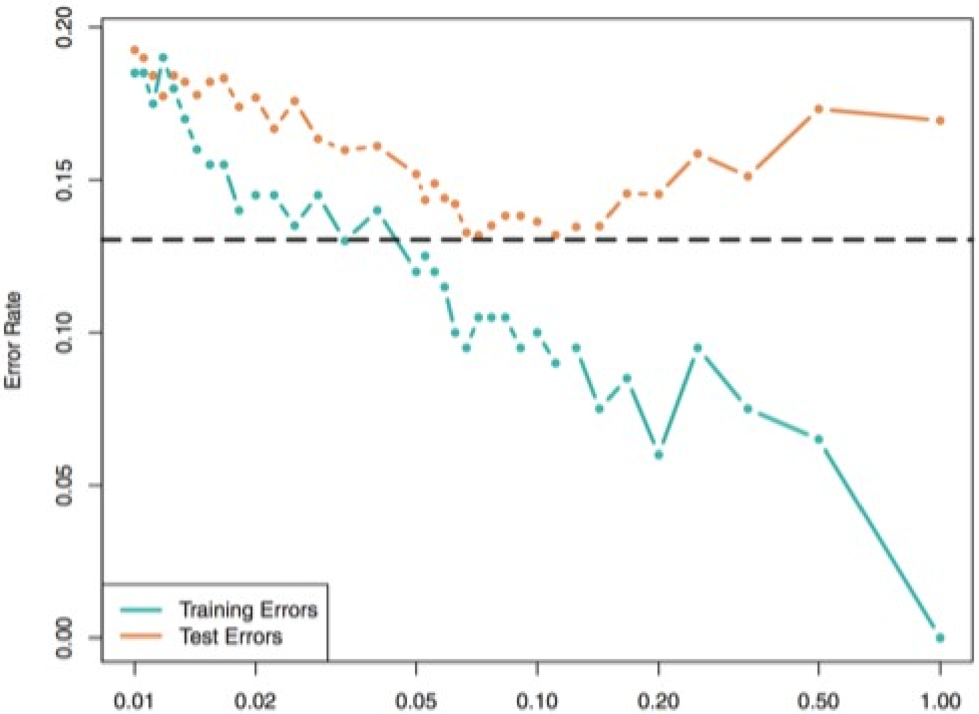
- 'ball_tree' will use `BallTree`
- 'kd_tree' will use `KDTree`

K Nearest Neighbors



K Nearest Neighbors





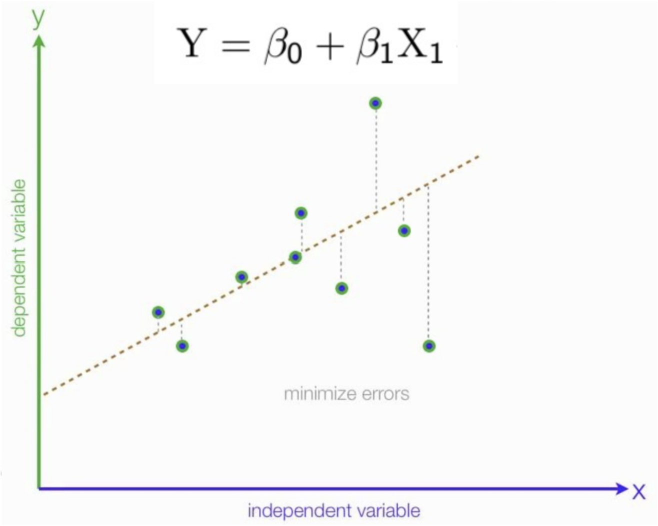
Linear regression

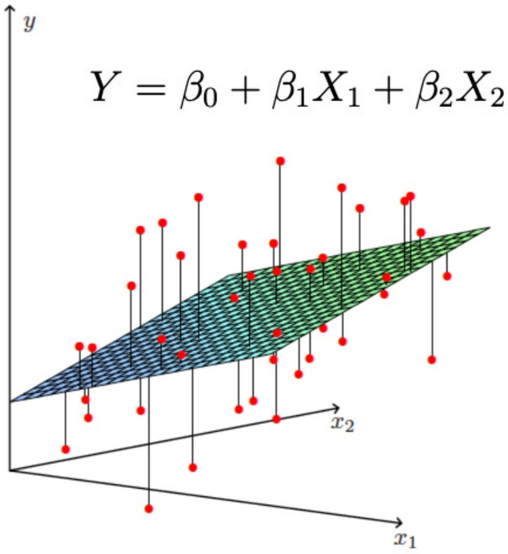
- Linear Model:

$$\mathrm{Y} = \beta_0 + \beta_1 \mathrm{X}_1 + \ldots + \beta_\mathrm{p} \mathrm{X}_\mathrm{p} + \epsilon.$$

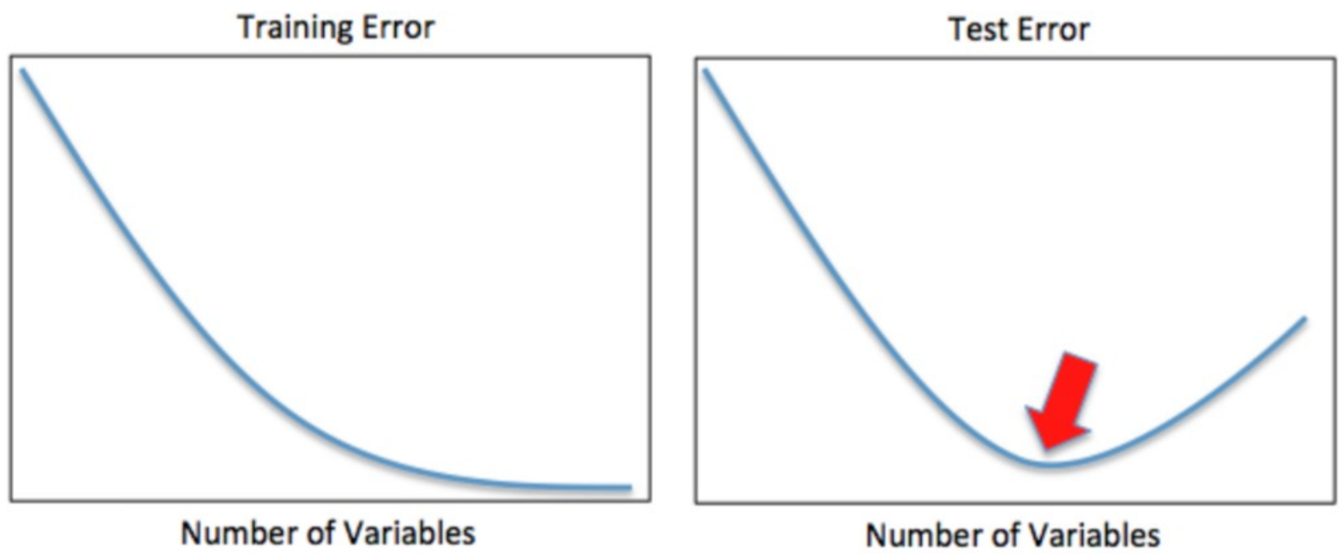
- Y - responses associated with n observations.
- $\mathrm{X_j}$ - $\mathrm{j^{th}}$ predictor measured for each of the n observations.
- ϵ measurement noise for the n observations.
- β_0 - Intercept.
- β_j - Coefficient of $\mathrm{j^{th}}$ predictor.

- Goal: Estimate β_0 and β_j's to fit linear model.





Remember overfitting?



- Solution:
  - Feature selection
    - Best subset regression, Forward and backward step-wise
  - Regularized linear regression
    - Ridge regression, Lasso regression

Ridge and Lasso regressions

- **Ridge**

$$\underset{\beta}{\text{minimize}} \quad ||\mathrm{Y} - \mathbf{X}\beta||_2^2 + \lambda||\beta||_2^2$$

  - It **shrinks the parameters,** therefore it is mostly used to prevent multicollinearity.
  - L2 makes weights small

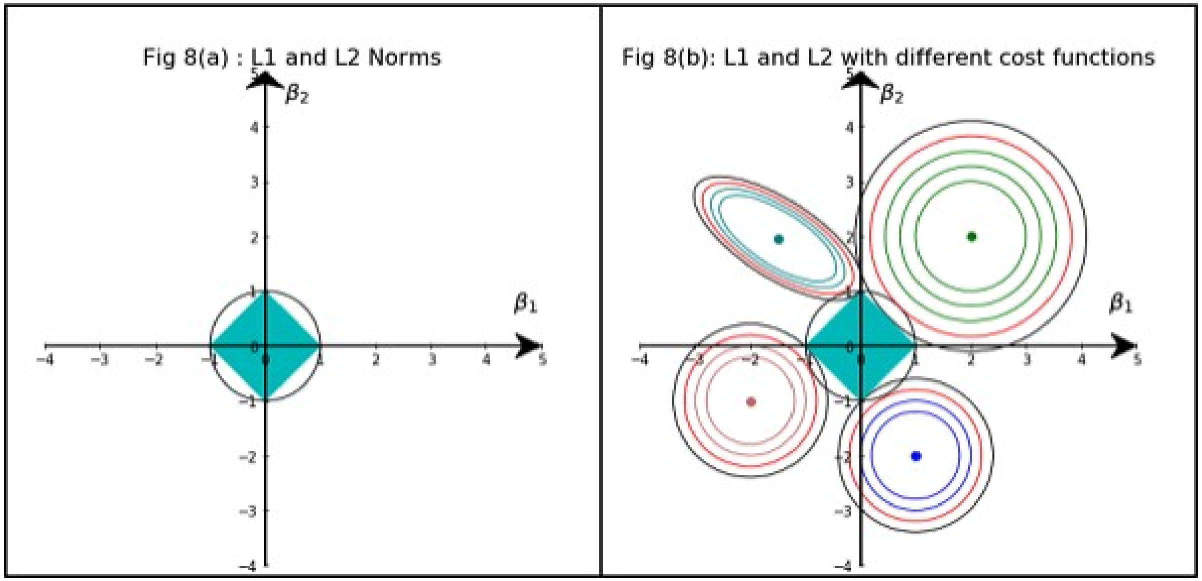
- **Lasso**

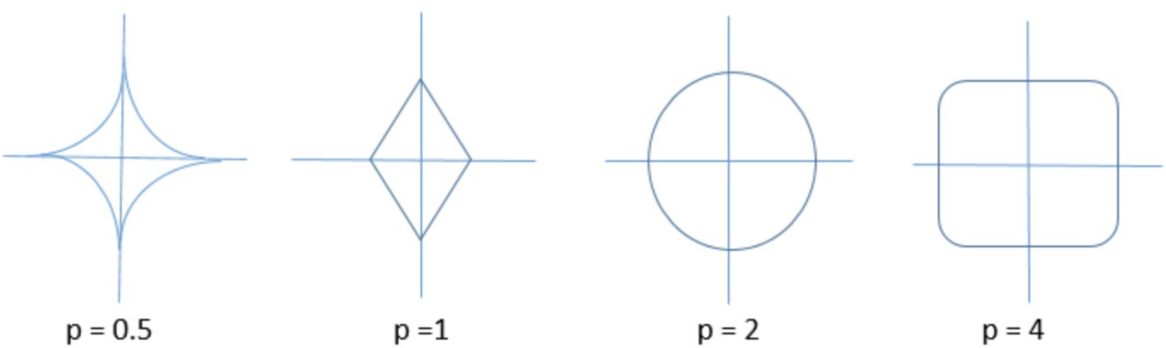
$$\underset{\beta}{\text{minimize}} \quad ||\mathrm{Y} - \mathbf{X}\beta||_2^2 + \lambda||\beta||_1$$

  - Used when we have more number of features, because it automatically does **feature selection**.
  - L1 removes weights

Regression			=	[Prediction]				
Regression	+	Ridge	=	[Prediction]	+	[Bias Variance Trade-off]		
Regression	+	Lasso	=	[Prediction]	+	[Bias Variance Trade-off]	+	[Feature Selection]

Ridge and Lasso regressions





- ***Force 1**: Bias term pulling β1 and β2 to lie somewhere on the black circle only.*
- ***Force 2**: Gradient Descent trying to travel to the global minimum indicated by the dots.*

- Each gradient descent contour corresponds to different LR
- The RED circle in each contour intersects the Ridge or L2 Norm.
- The BLACK circle in each contour intersects the Lasso or L1 Norm.