CDS Education

Introduction to Machine Learning for Python

Intro to Classification

Sanity Check

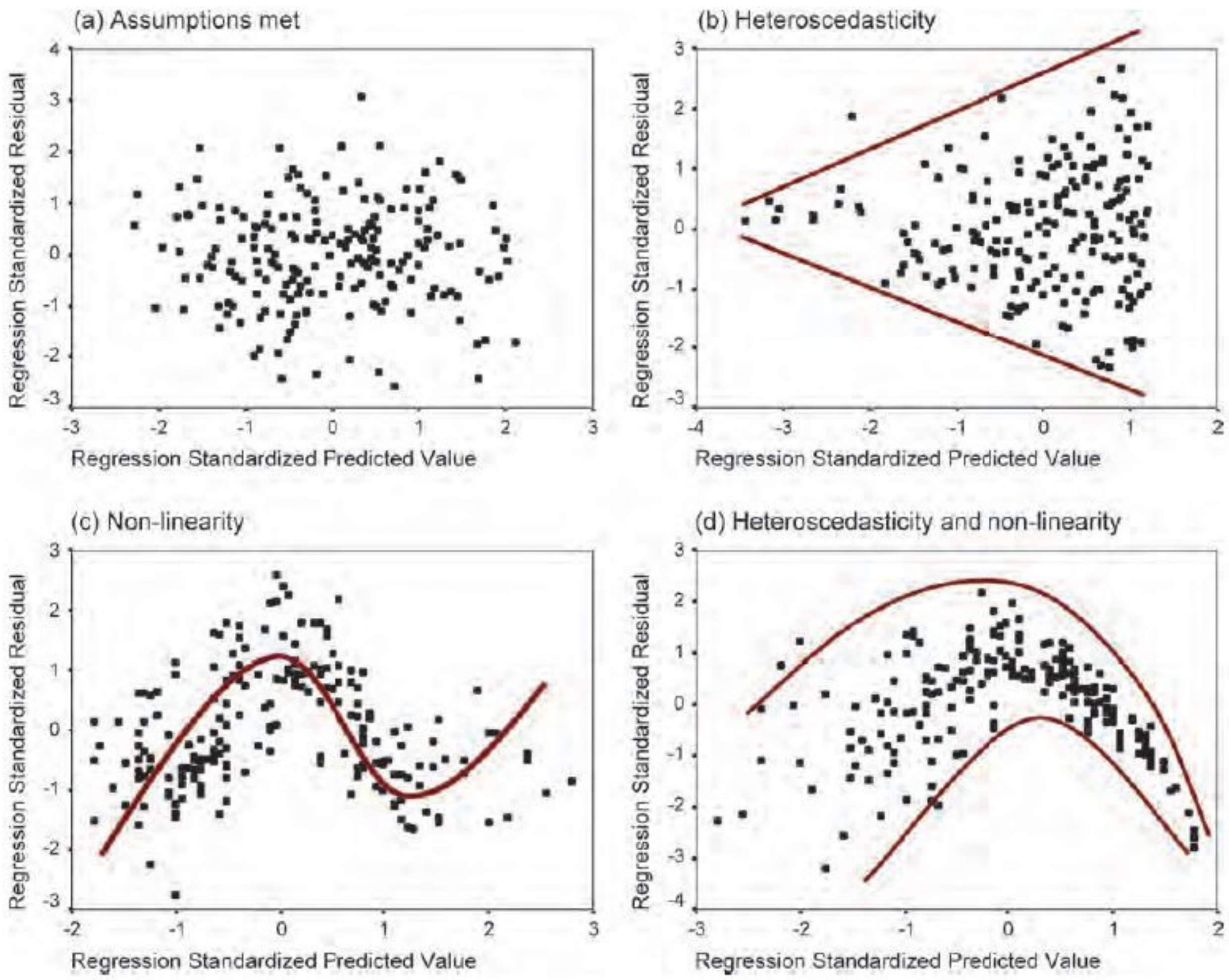
- Project A
  - Did everyone turn in their project?
  - Any concern or questions?
- Project B released today
  - Linear Regression
  - KNN Classification

Question:

Last week we talked about regression. What is supervised learning? What is regression?

Conditions for Linear Regression

- Data should be numerical and linear
- Residuals from the model should be random
    - Heteroscedasticity
- Check for outliers



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Review: Least Squares Error

We define our error as follows:

theoretical

$$\sum_{i=0}^{n}(y_i - (B_0 + B_1 x_1 + \ldots + B_p x_p))^2$$

observed

We call this **Least Squares Error**. Sum of squared *vertical* distance between observed and theoretical values.

Model "Goodness of Fit"

Common metric is called **R^2**.

- We compare our model to a **benchmark model**
  - Predict the mean y value, no matter what the x_i's are
- SST = least-squares error for benchmark
- SSE = least-squares error for our model
- $R^2 = 1 - SSE/SST$

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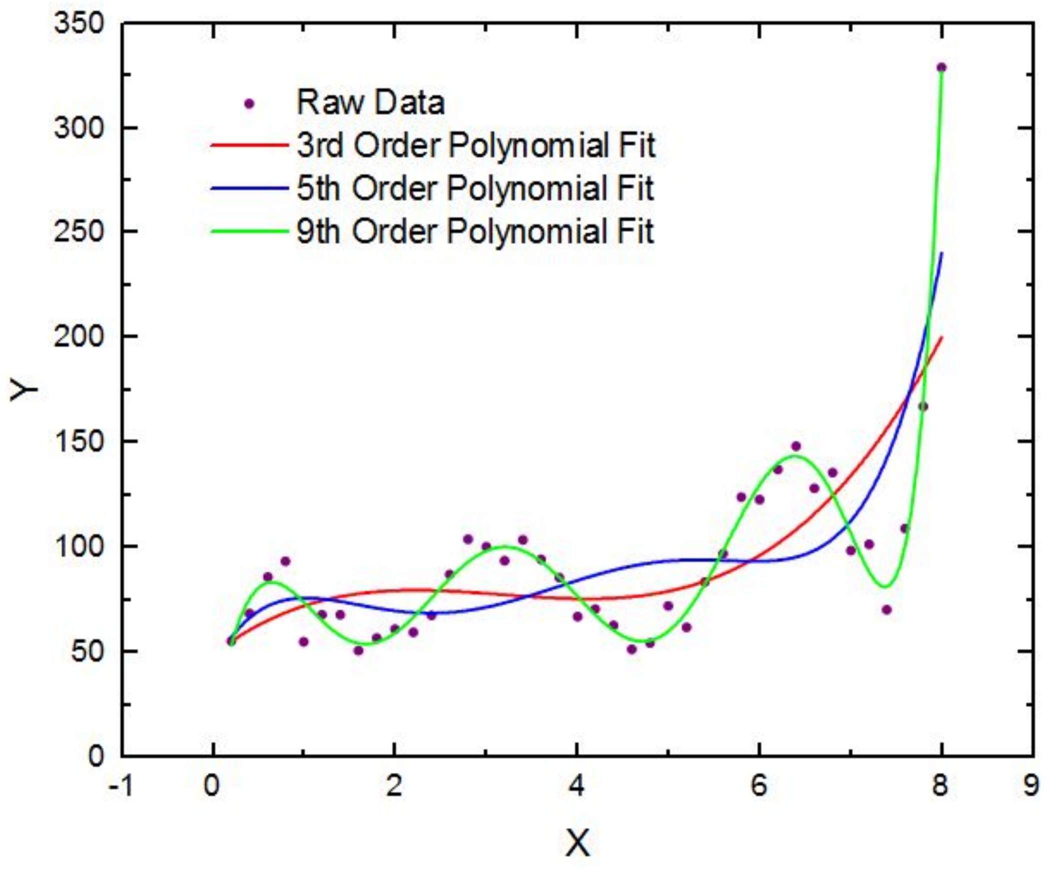
Non-Linear Regression



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- PolynomialFeatures function generates different polynomial degrees (x^2, x^3, ...)
- Curve_fit function can match your function to the model

Intro to Classification

- “What species is this?”
- “How would consumers rate this restaurant?”
- “Which Hogwarts House do I belong to?”
- “Am I going to pass this class?”

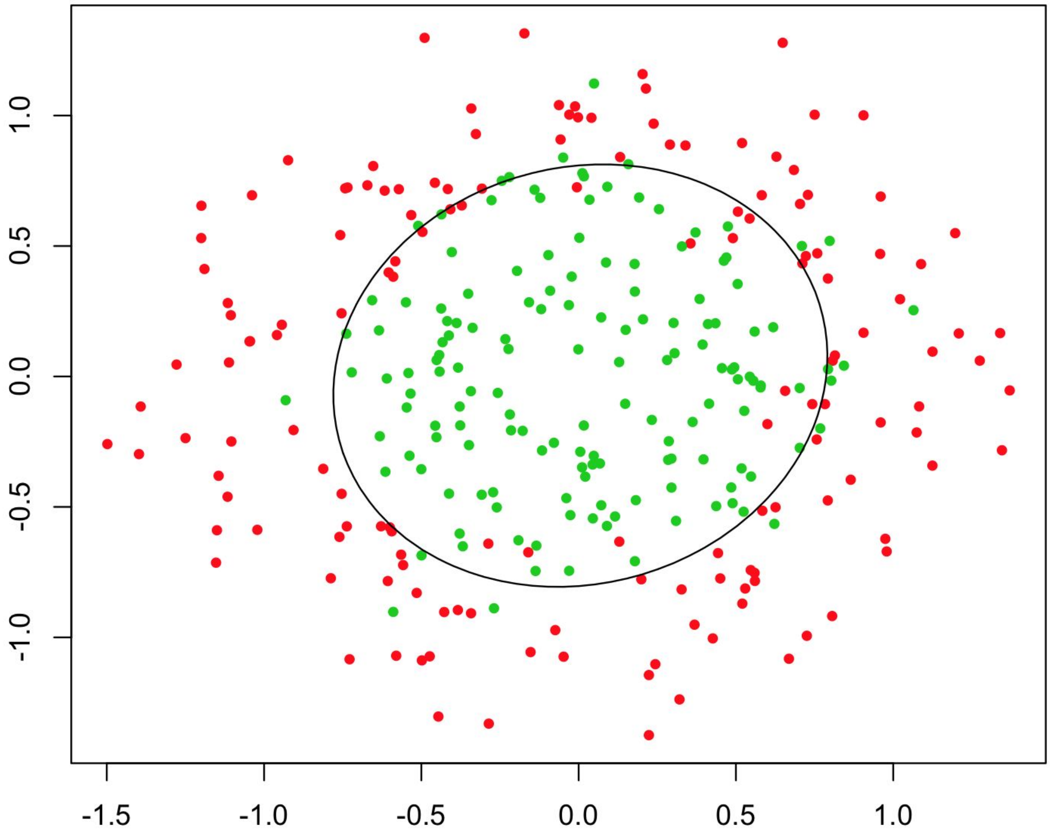
Source

The Bayesian Classifier

- The ideal classifier: a theoretical classifier with the highest accuracy
- Picks the class with the highest conditional probability for each point
- Assumes conditional distribution is known
- Exists only in theory!
    - A conceptual **Golden Standard**

Decision Boundary

- The **decision boundary** partitions the outcome space
- Classification algorithm you should use differs depending on whether the data is or is not linearly separable



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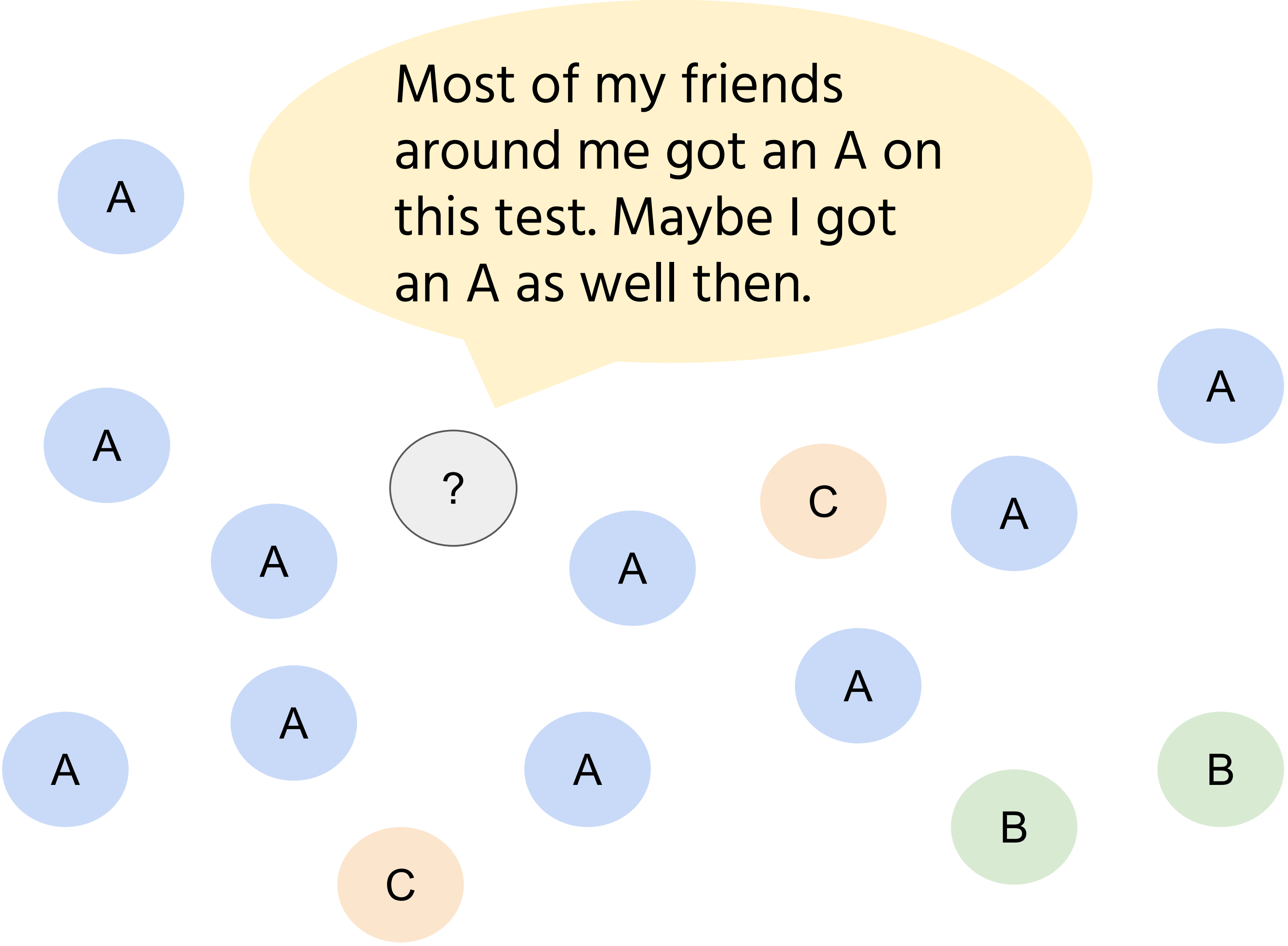
k-Nearest Neighbors (KNN)

Easy to interpret

Fast calculation

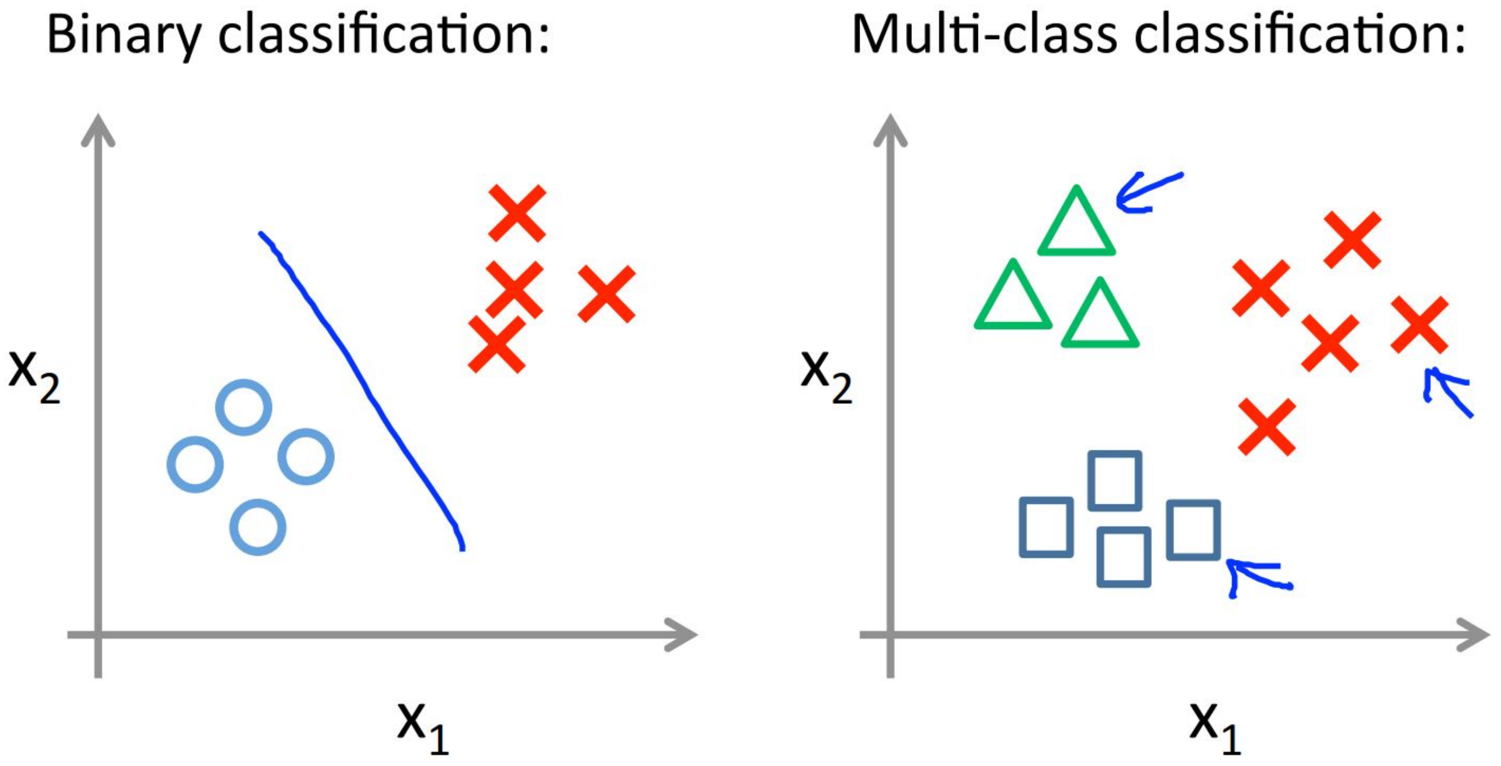
No prior assumptions

Good for coarse analysis



Multi-Class Classification

Classifying instances into three classes or more



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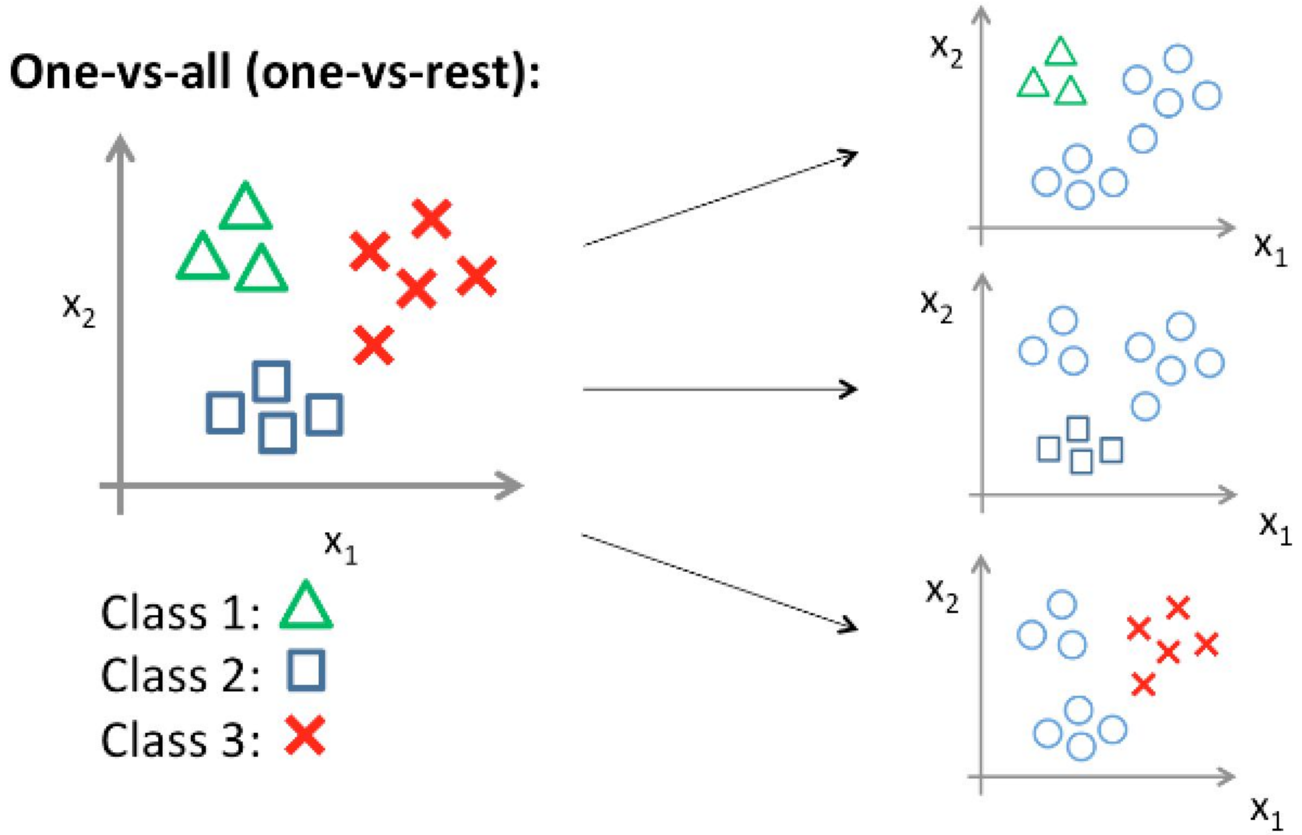
One-vs-All

- Train a single classifier per class
- All samples of that class classified as positive, all other samples as negative



KNN

How does it work?

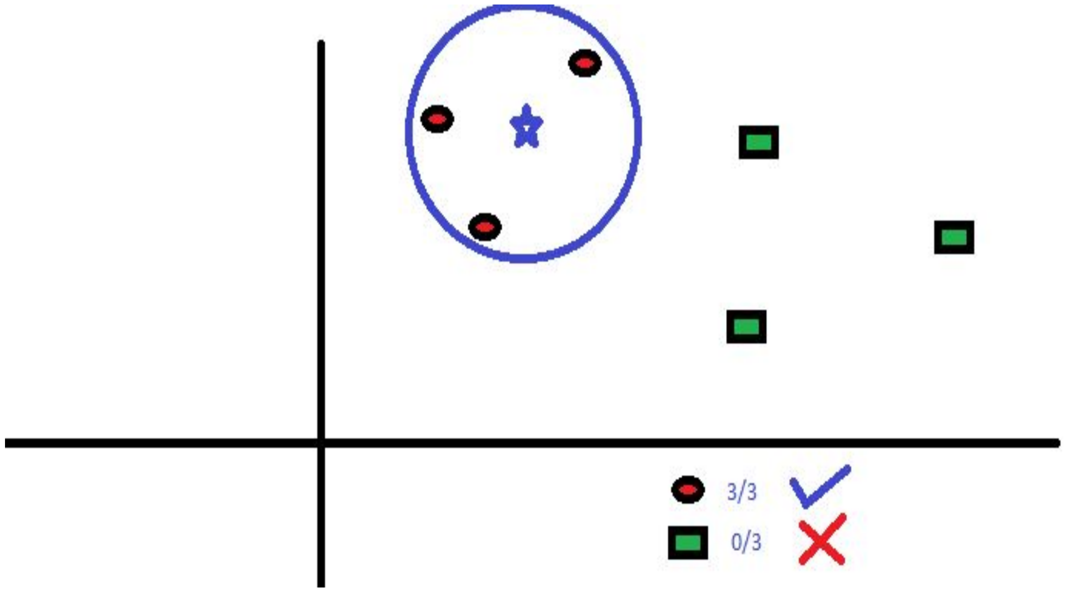
Define a *k* value (in this case k = 3)

Pick a point to predict (blue star)

Count the number of closest points

Increase the radius until the number of points within the radius adds up to 3

Predict the blue star to be a red circle!



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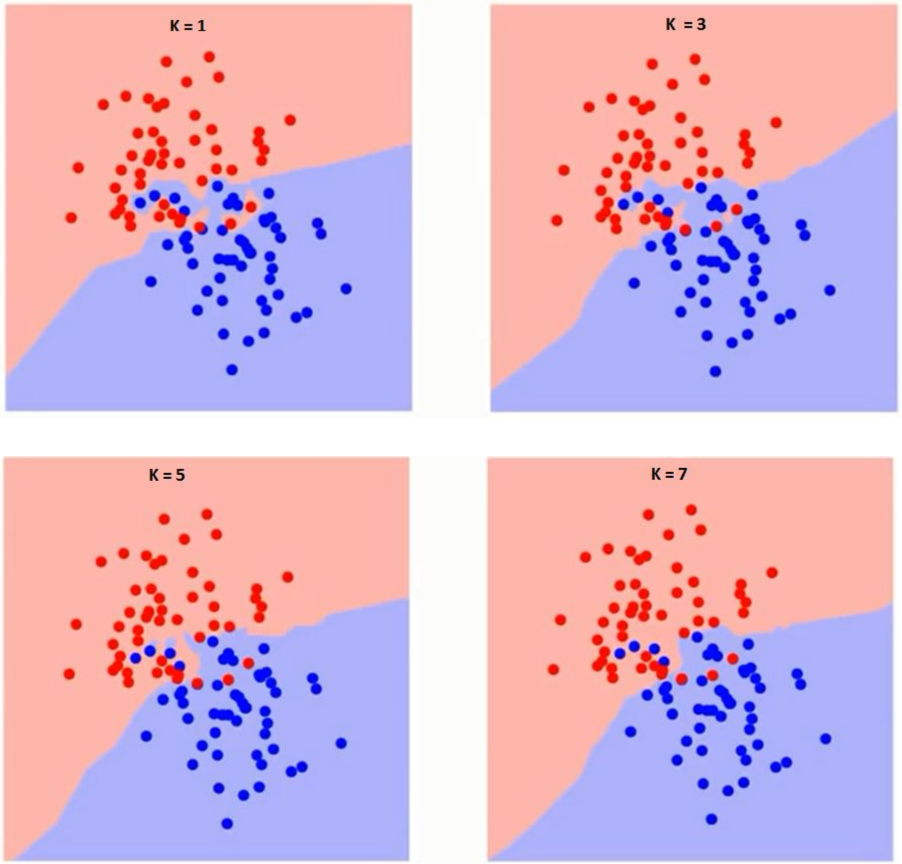
Demo

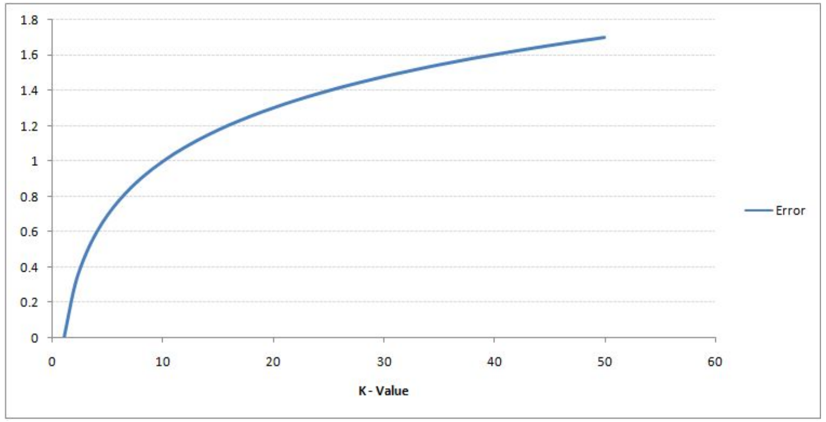
Question:

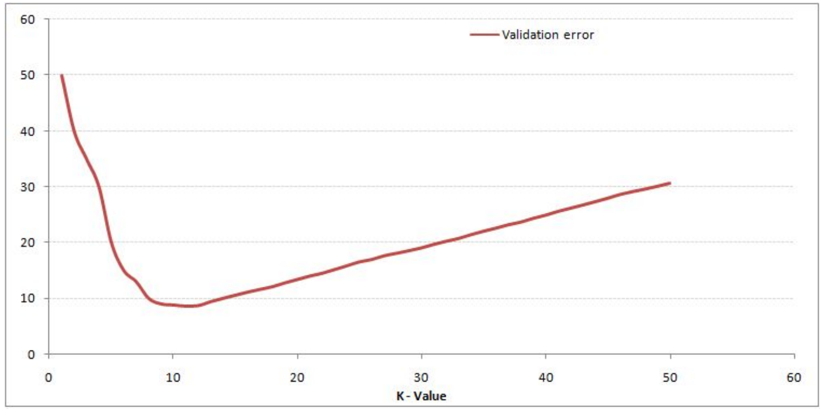
What defines a good *k* value?

KNN

The *k* value you use has a relationship to the fit of the model.







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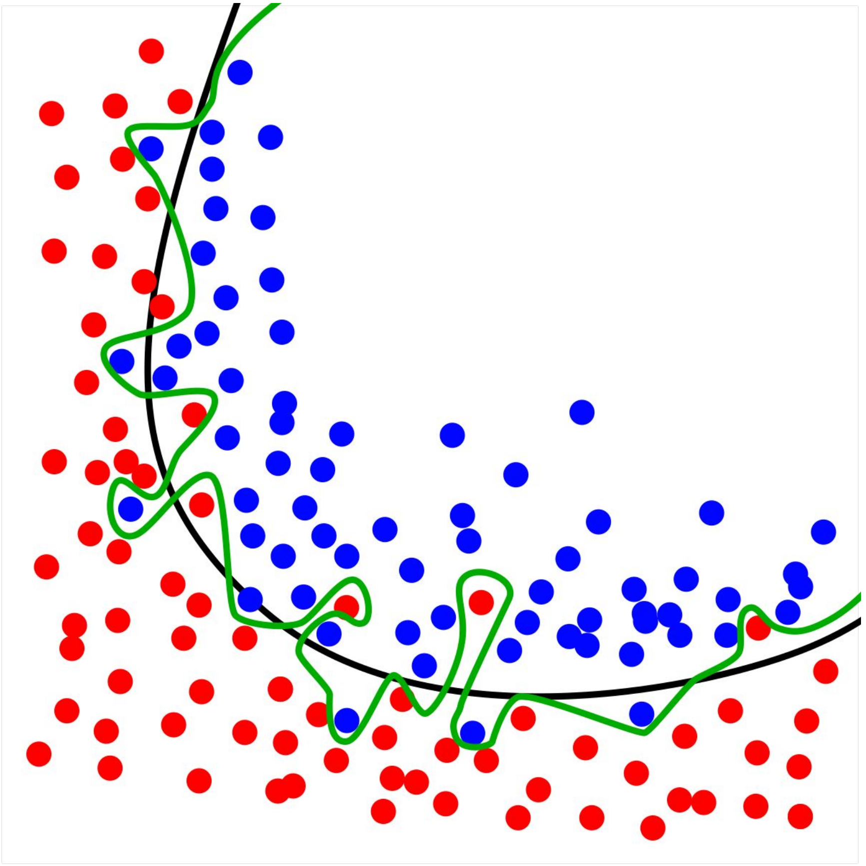
Overfitting

When the model corresponds too closely to training data and then isn't transferable to other data.

Can fix by:

- Splitting data into training and validation sets
- Decreasing model complexity



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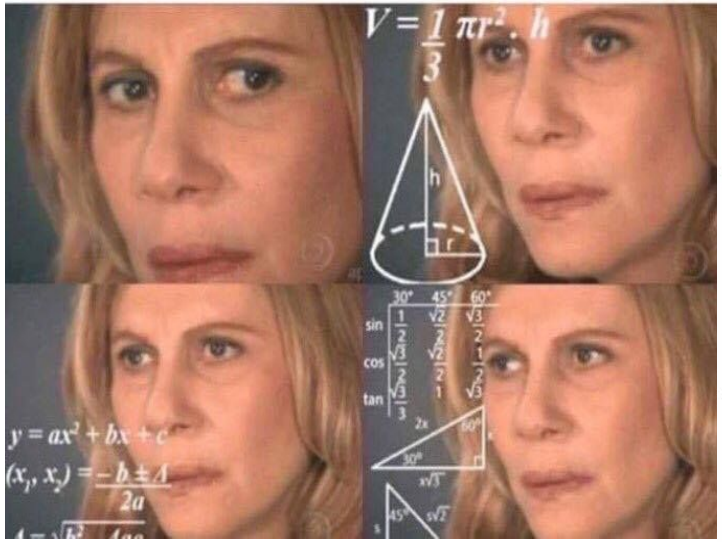
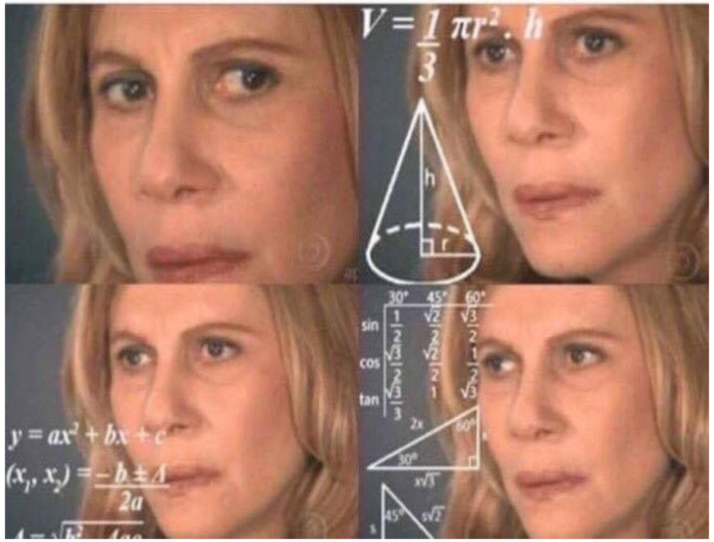
Confusion Matrix



	p' (Predicted)	n' (Predicted)
p (Actual)	True Positive	False Negative
n (Actual)	False Positive	True Negative



Sensitivity

Sensitivity = True Positive / (True Positive + False Negative)

Also called **True Positive Rate**.

How many positives are correctly identified as positives?

Optimize for:

- Airport security
- Initial diagnosis of fatal disease

Source

Specificity

Specificity = True Negative / (True Negative + False Positive)

Also called **True Negative Rate**.

How many negatives are correctly identified as negative?

Question:

Name some examples of situations where you'd want to have a high specificity.

Specificity

Specificity = True Negative / (True Negative + False Positive)

Also called **True Negative Rate**.

How many negatives are correctly identified as negative?

Optimize for:

- Testing for a disease that has a risky treatment
- DNA tests for a death penalty case

Source

Other Important Measures

- **Overall accuracy** - proportion of correct predictions
- **Overall error rate** - proportion of incorrect predictions
- **Precision** - proportion of correct positive predictions among all positive predictions

Accuracy =
(True Positive + True Negative)/Total
Error Rate =
(False Positive + False Negative)
/Total

Precision =
True Positive
/(True Positive + False Positive)

Example

Given this confusion matrix, what is the:

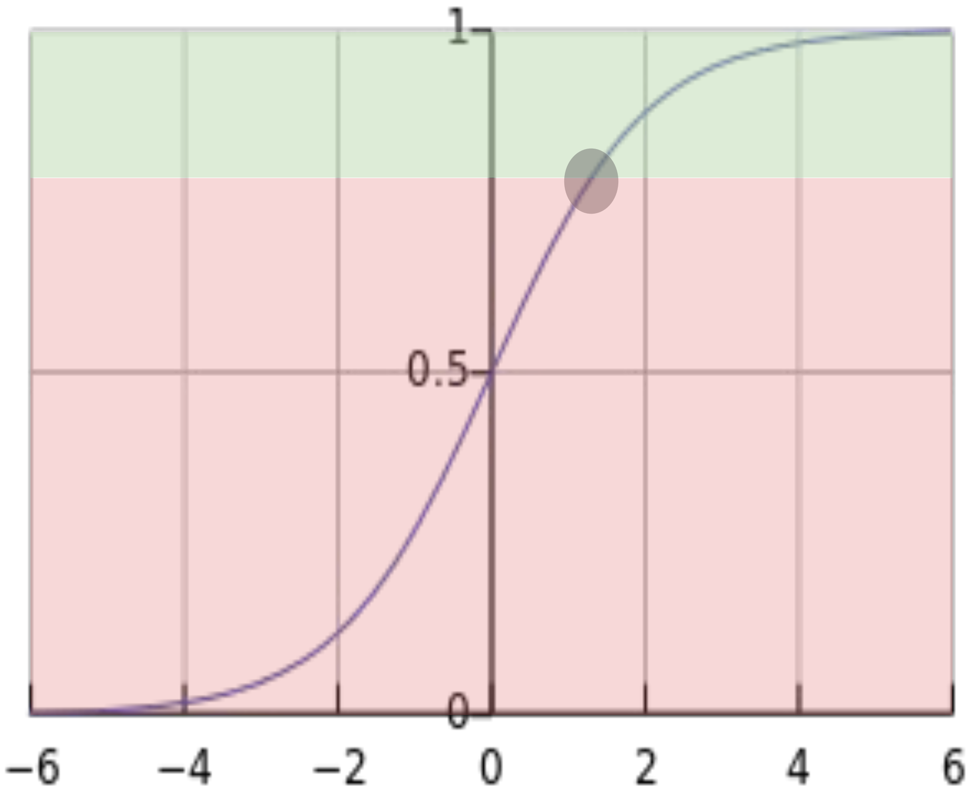
- Specificity?
- Sensitivity?
- Overall error rate?
- Overall accuracy?
- Precision?

	p' (Predicted)	n' (Predicted)
p (Actual)	146	32
n (Actual)	21	590

Threshold

Where between 0 and 1 do we draw the line?

- $P(x)$ below threshold: predict 0
- $P(x)$ above threshold: predict 1



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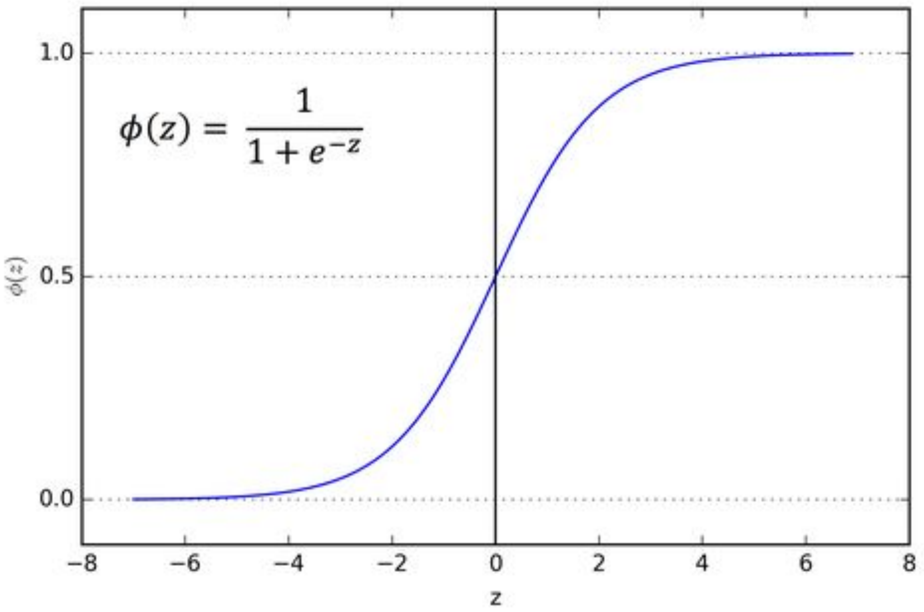
Thresholds Matter (A Lot!)

What happens to the specificity when you have a

- Low threshold?
  - Sensitivity increases, specificity decreases
- High threshold?
  - Sensitivity decreases, specificity increases



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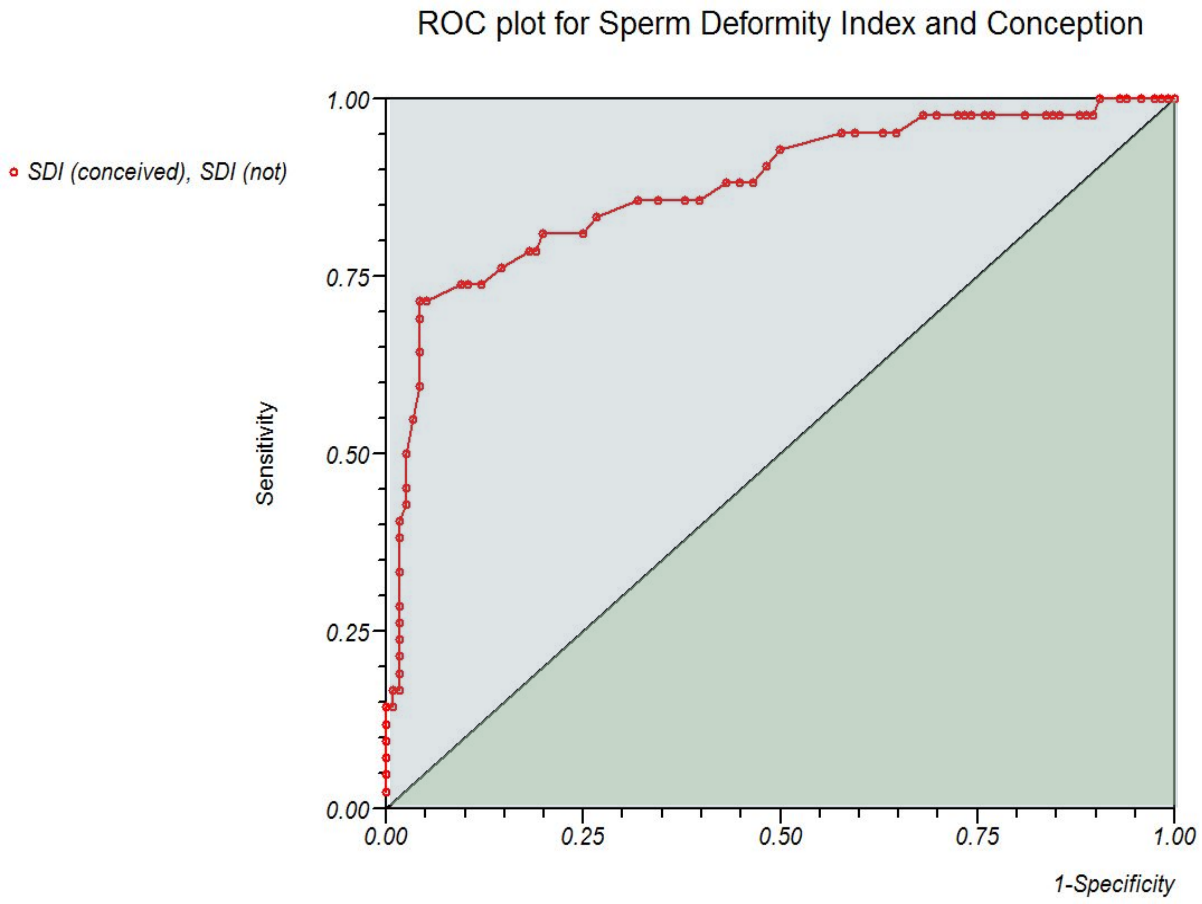
ROC Curve

Receiver **O**perating **C**haracteristic

- Visualization of trade-off
- Each point corresponds to a specific threshold value



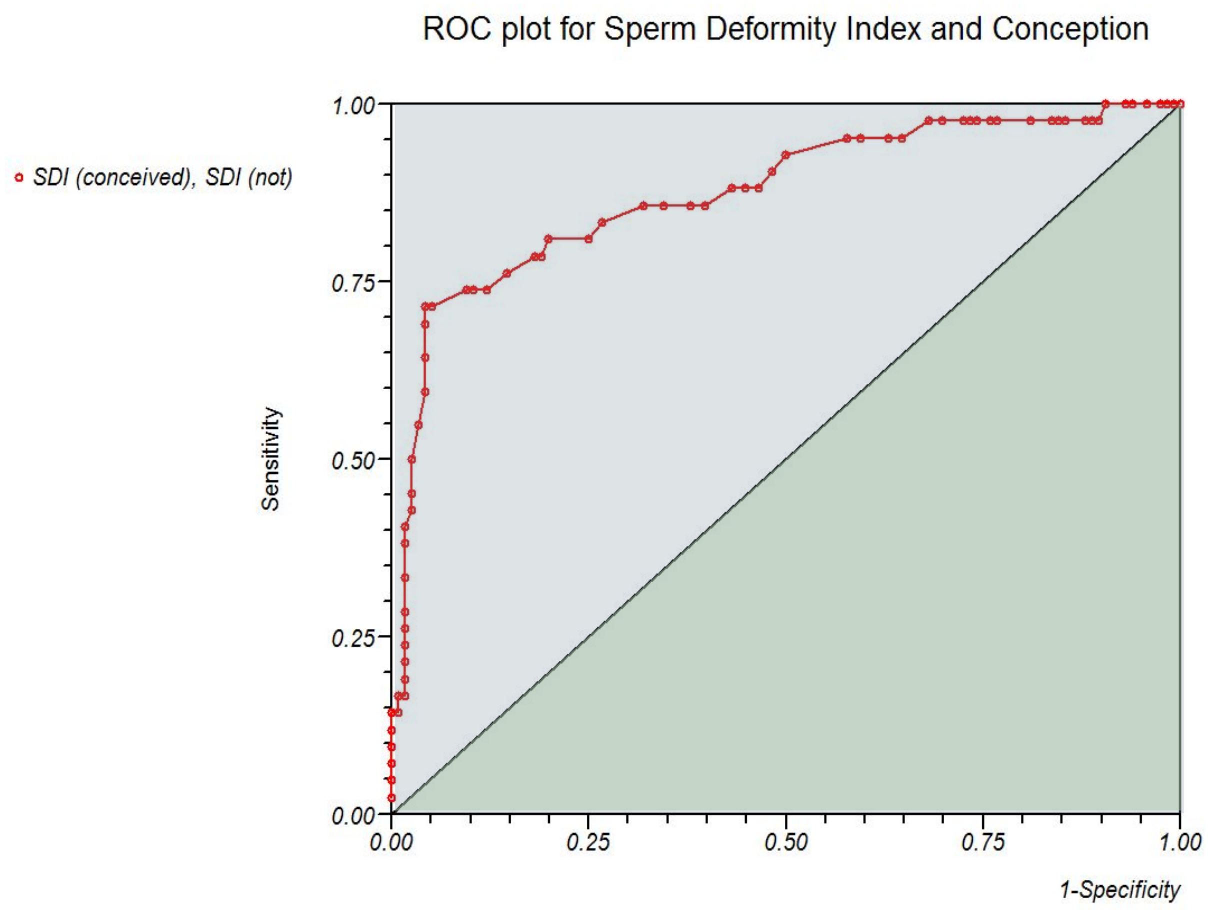
Area Under Curve

$$\text{AUC} = \int ROC\ curve$$

Always between 0.5 and 1.

Interpretation:

- 0.5: Worst possible model
- 1: Perfect model



Coming Up

Your problem set: Start working on Project Part B

Next week: More classifiers (SVM!)

See you then!