Week 3

Concepts in Machine Learning

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Fred Hutchinson Cancer Research Center

Week 3 Learning Objectives

- Quick CRISP-DM Review
- Supervised Learning vs Unsupervised Learning
  - Regression vs. Classification
    - Binary vs. Multiclass Classification
- Hard vs. Soft Classification
- Evaluating Classification Models
  - Soft vs Hard
- Hard Classification Metrics for Soft Classification Models
  - Confusion Matrix
  - ROC and AUC
- Discussion: Do You Really Need Hard Classification?

Definitions

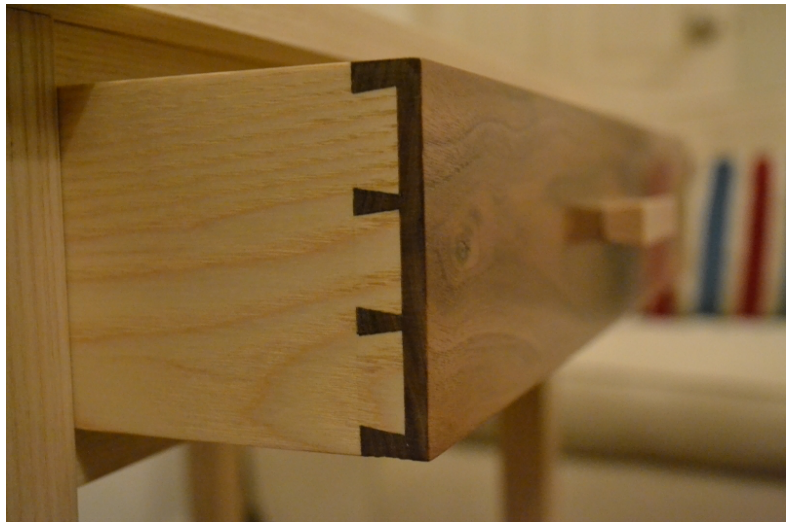
- Machine learning is an application of artificial intelligence (AI) that provides systems the ability to automatically learn and improve from experience without being explicitly programmed. (https://expertsystem.com/machine-learning-definition/)
- Machine learning (ML) is the scientific study of algorithms and statistical models that computer systems use to perform a specific task without using explicit instructions, relying on patterns and inference instead. (https://en.wikipedia.org/wiki/Machine_learning)
- Problem + Data + Algorithm(self-adjusting) + Compute ==> Insight

Experimental Design

- Difficult to master or even do well
- Close interplay between
  - Goals
  - Methods
  - Data
  - Execution
- Requires thoughtful approach and broad understanding

Capable Cabinet Maker

- Inspects and understands raw materials
- Uses the tools thoughtfully to shape and join materials
- Chooses approach and tools based on materials and goals
- Thoughtfulness born of experience



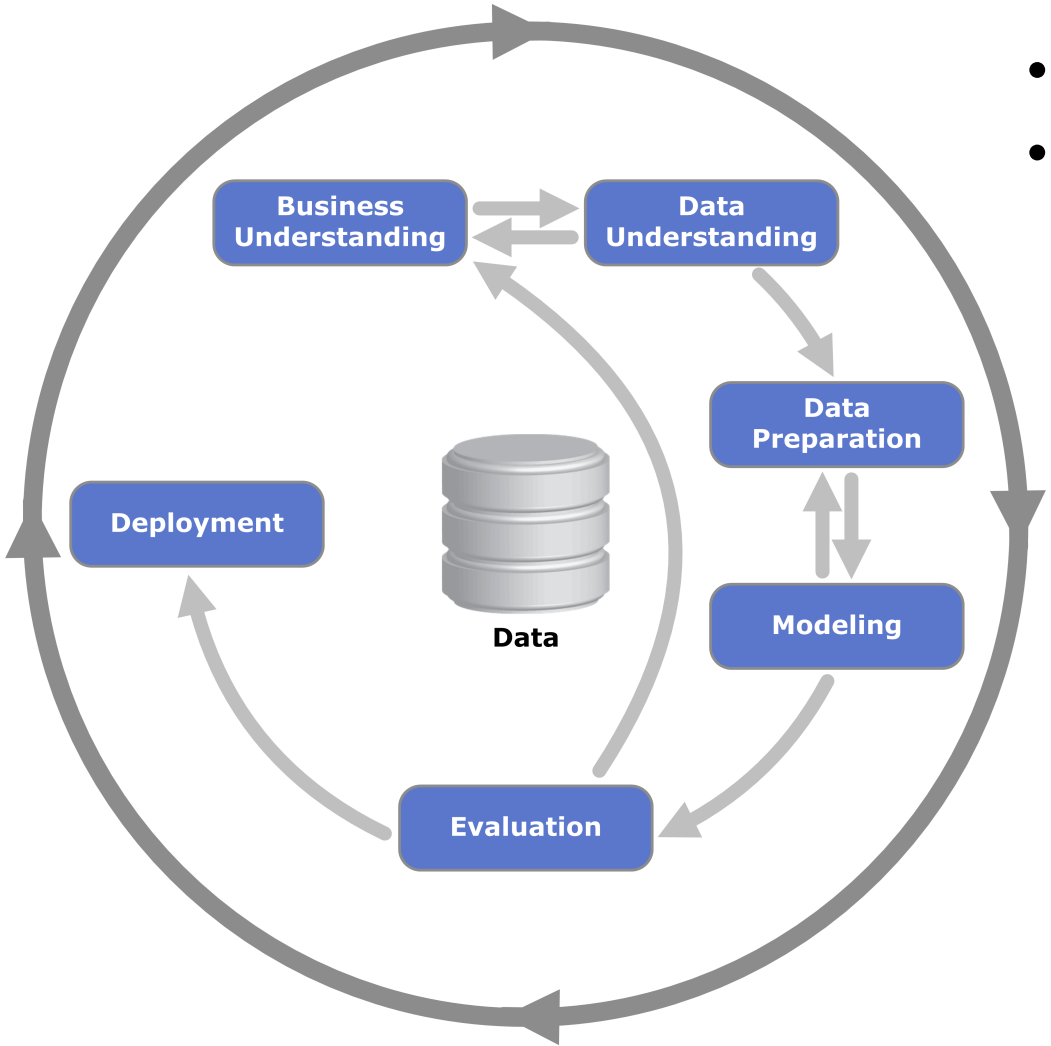
Cabinet Making?

- Storage Need + Raw Materials + Tools + Work ==> Cabinet

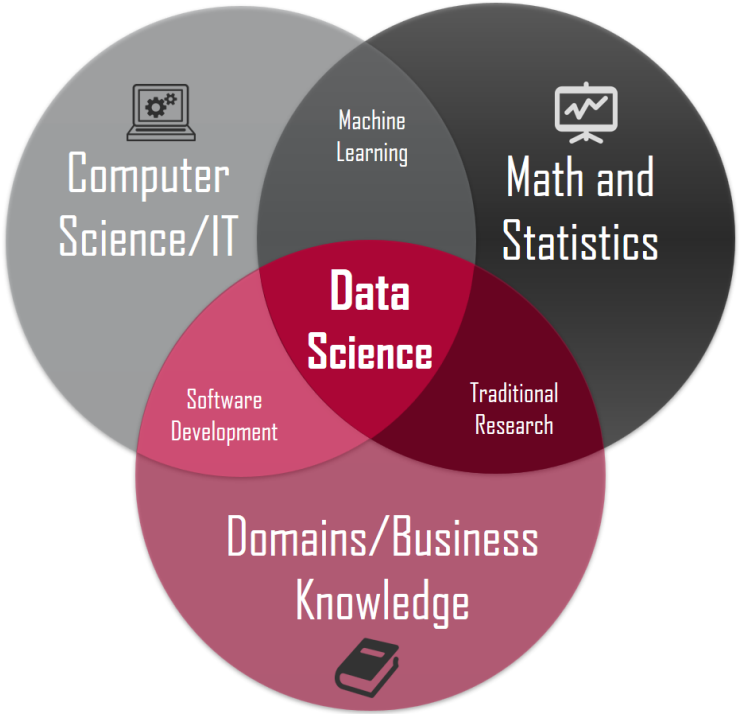
- SAT analogy format

  Tools : Cabinet Making as Algorithms : Machine Learning

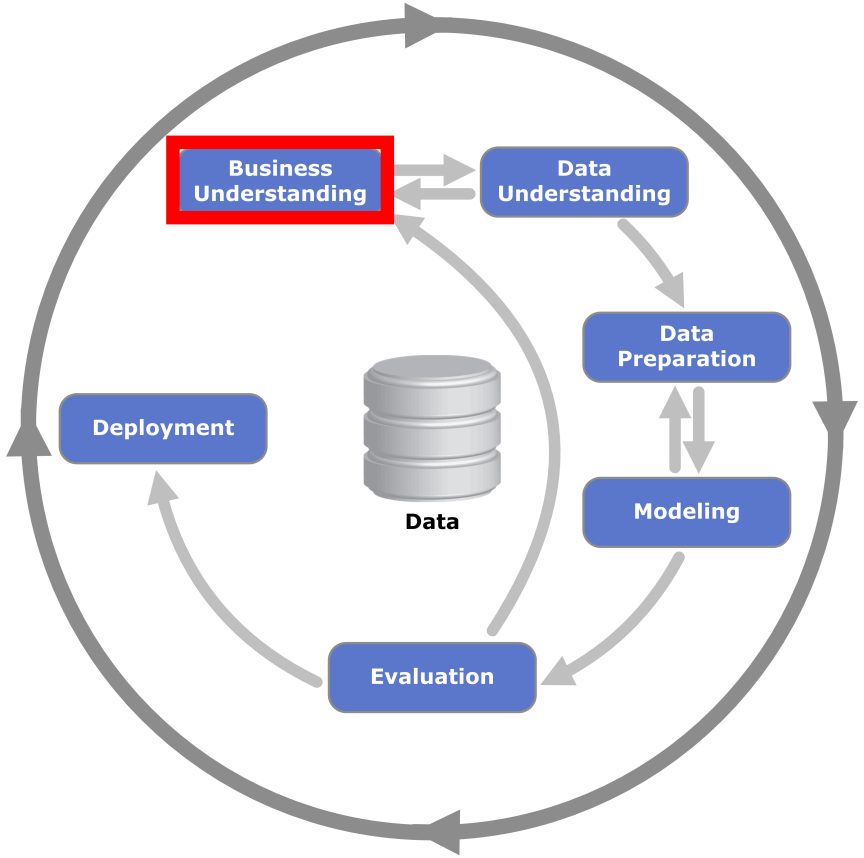
CRISP-DM
Cross-industry standard process for data mining



- Cyclical
- Iterative
- Connecting all 3 areas of the classic notion of “data science”

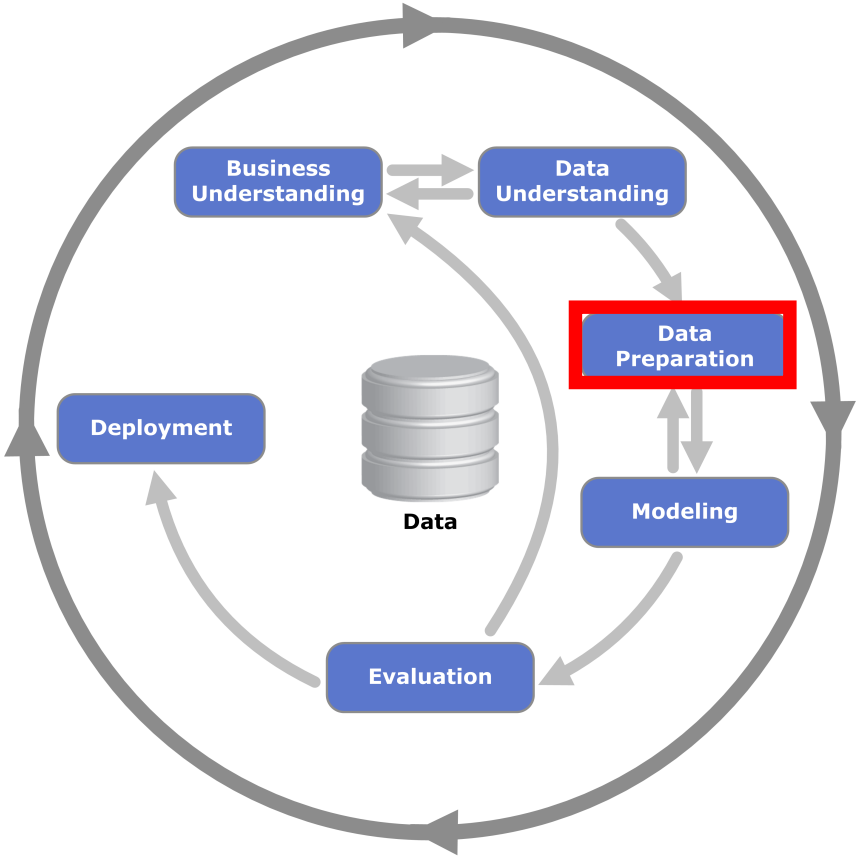


Business/Scientific Understanding



Data Understanding

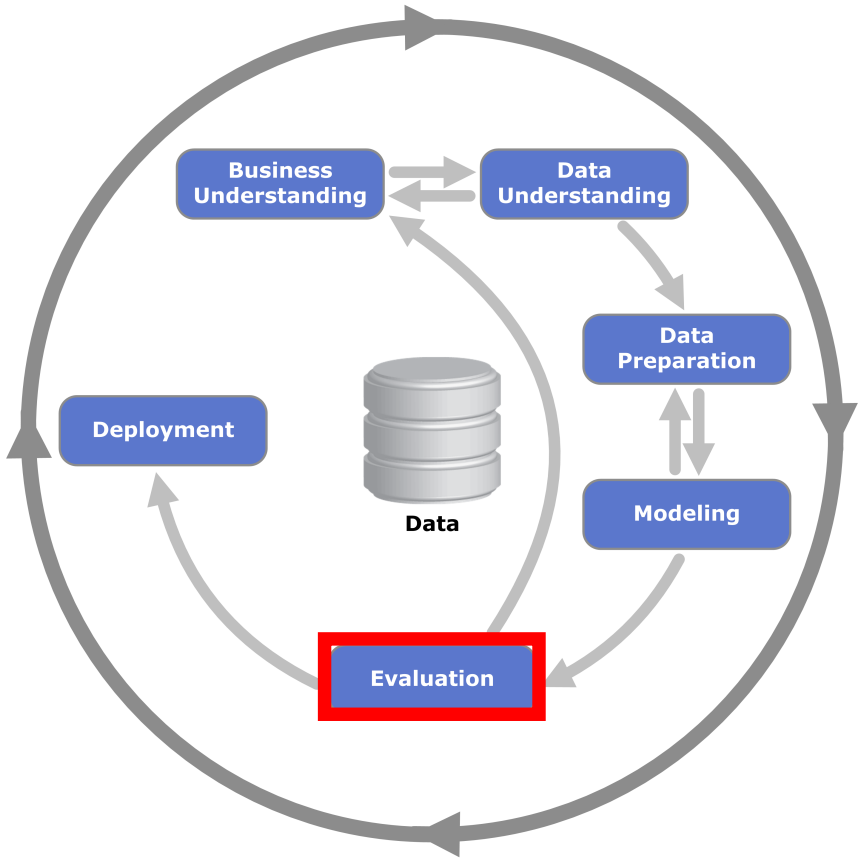
Data Preparation



Modeling


Business Understanding
Data Understanding
Data Preparation
Modeling
Evaluation
Deployment
Data

Evaluation


Business Understanding
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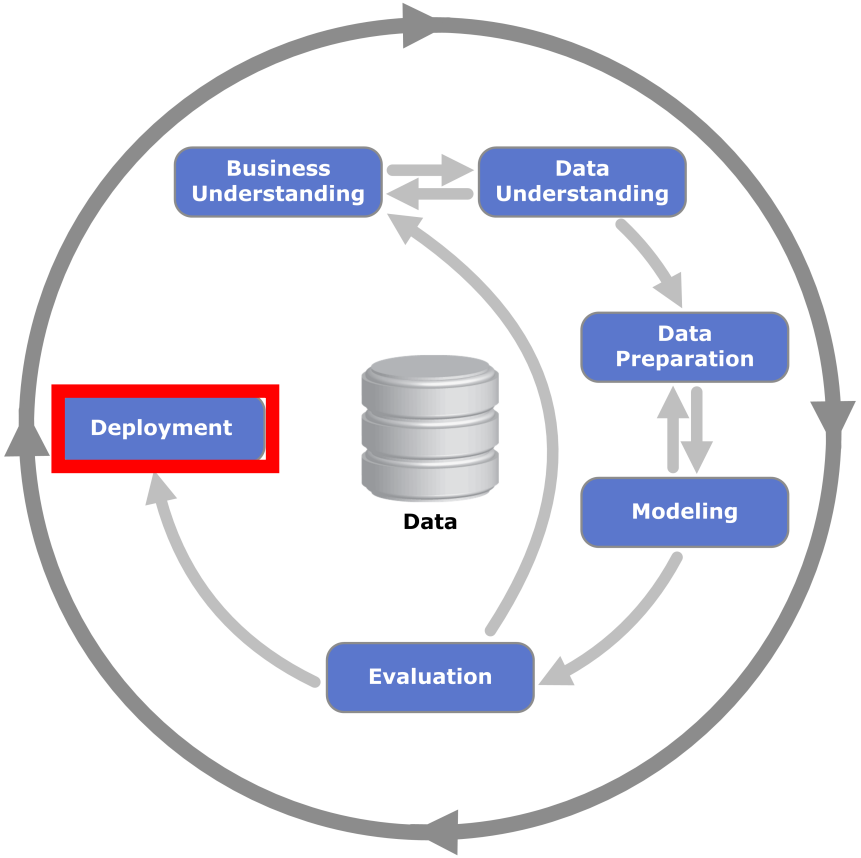
Deployment


Business Understanding
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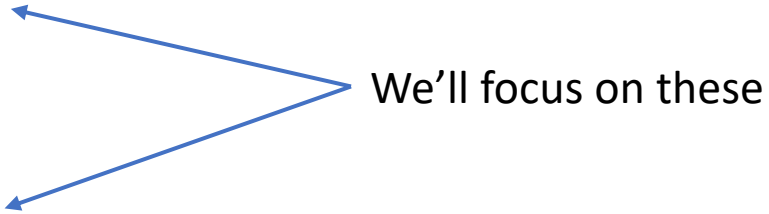
3 or 4 Machine Learning Paradigms

- Supervised Learning
- Unsupervised Learning



- Reinforcement Learning
- Semi-Supervised Learning

3 or 4 Machine Learning Paradigms

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3 or 4 Machine Learning Paradigms

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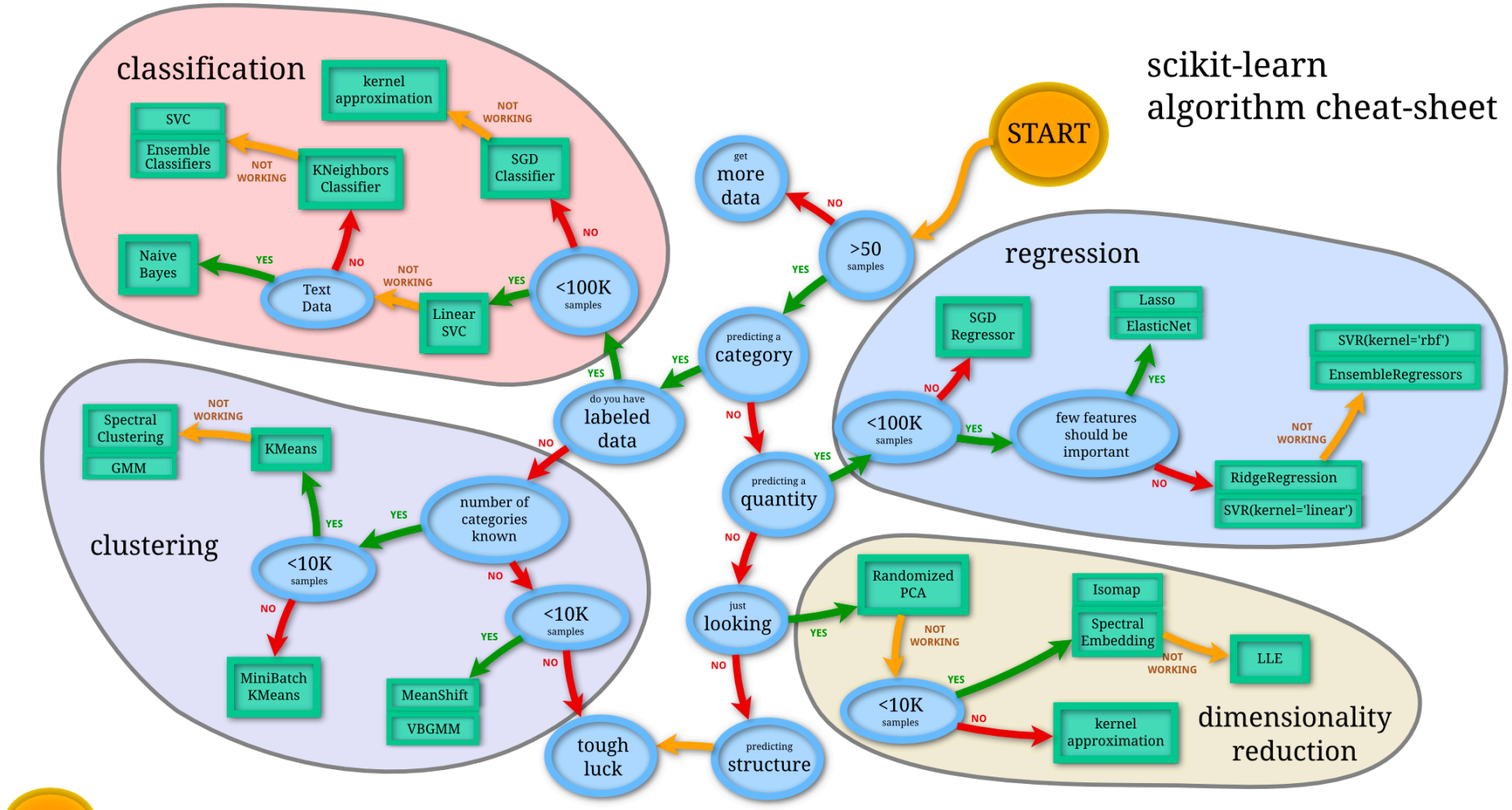
Supervised Problems: Categorical Problems

- Can we state our outcome as a choice between of A **vs.** B? (could be any number of categories)

Supervised Problems: Categorical Problems

- Can we state our outcome as a choice between of A **vs.** B? (could be any number of categories)
  - Yes, today we're interested in categories

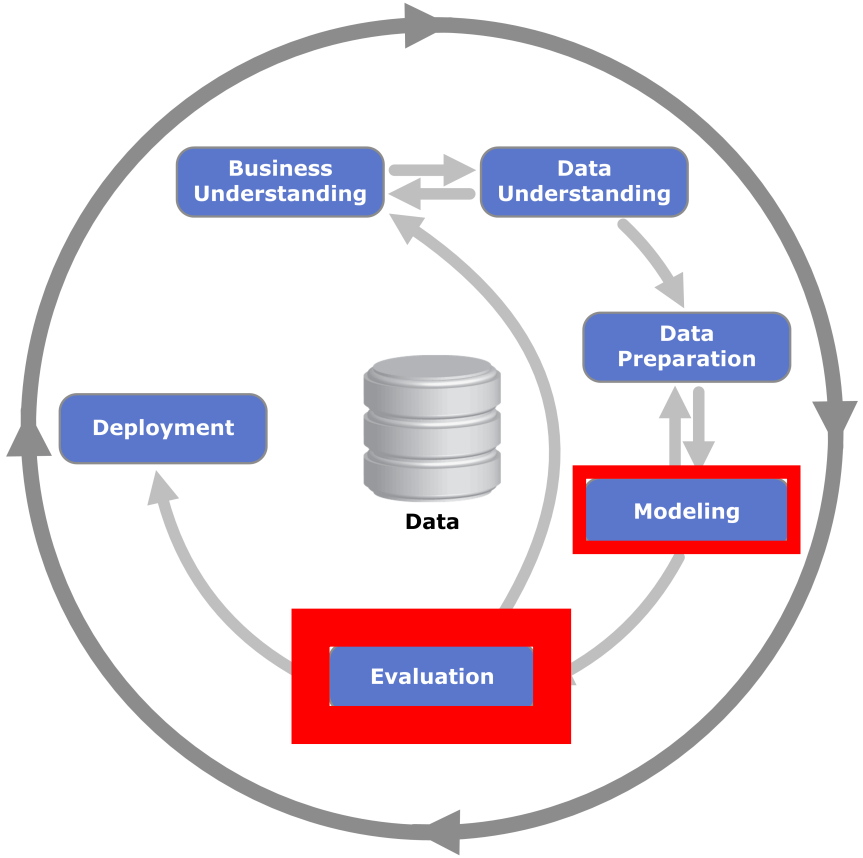
A Nifty Chart



A Nifty Chart

https://scikit-learn.org/stable/tutorial/machine_learning_map/

Modeling & Evaluation



Classification - Binary vs Multiclass

- Classification → Categorical Response
  - red, yellow, or green →Multiclass (class A or B or C or…)
  - dead or alive →Binary (A or B, A or –A)
  - HIV- or HIV+ →Binary (- or +, 0 or 1)

- Binary response → Only two values: 0 or 1
  - Most common case
  - Response 0 → negative class
  - Response 1 → positive class

Classification - Hard vs Soft

- Soft Classification:

  → Attempt to estimate probabilistic information

- Hard Classification:

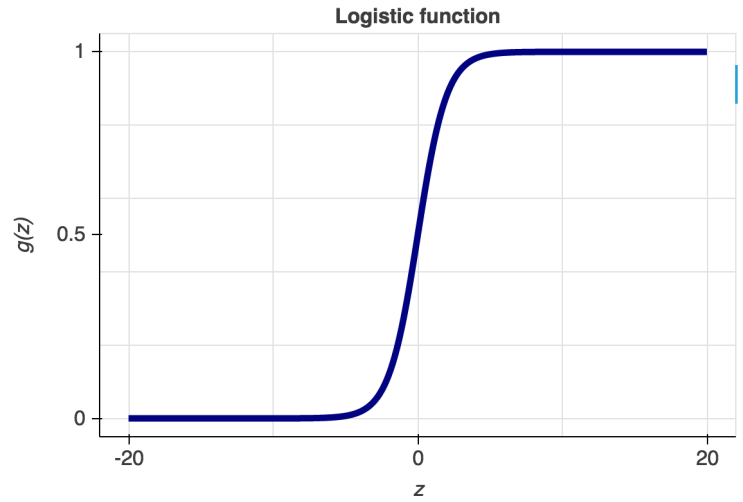
  → Only attempt to estimate class membership

Soft Classification

- Model attempts to estimate the probability that an observation belongs to a class.
  - For binary: $P(y = 1 \mid X)$
  - Conditional probability
    - If we change data X, then estimate of probability changes

- Basic example is Logistic Regression

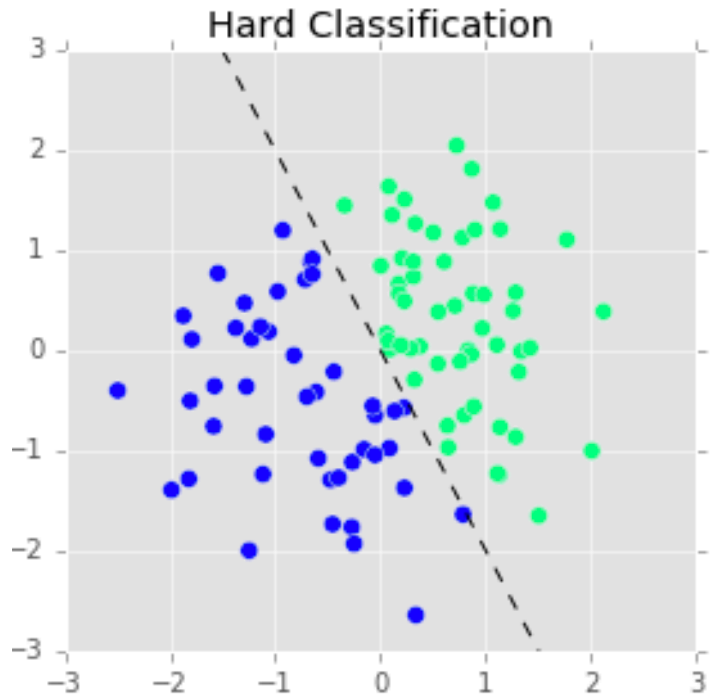
$$P(y = 1 \mid X) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k)}}$$

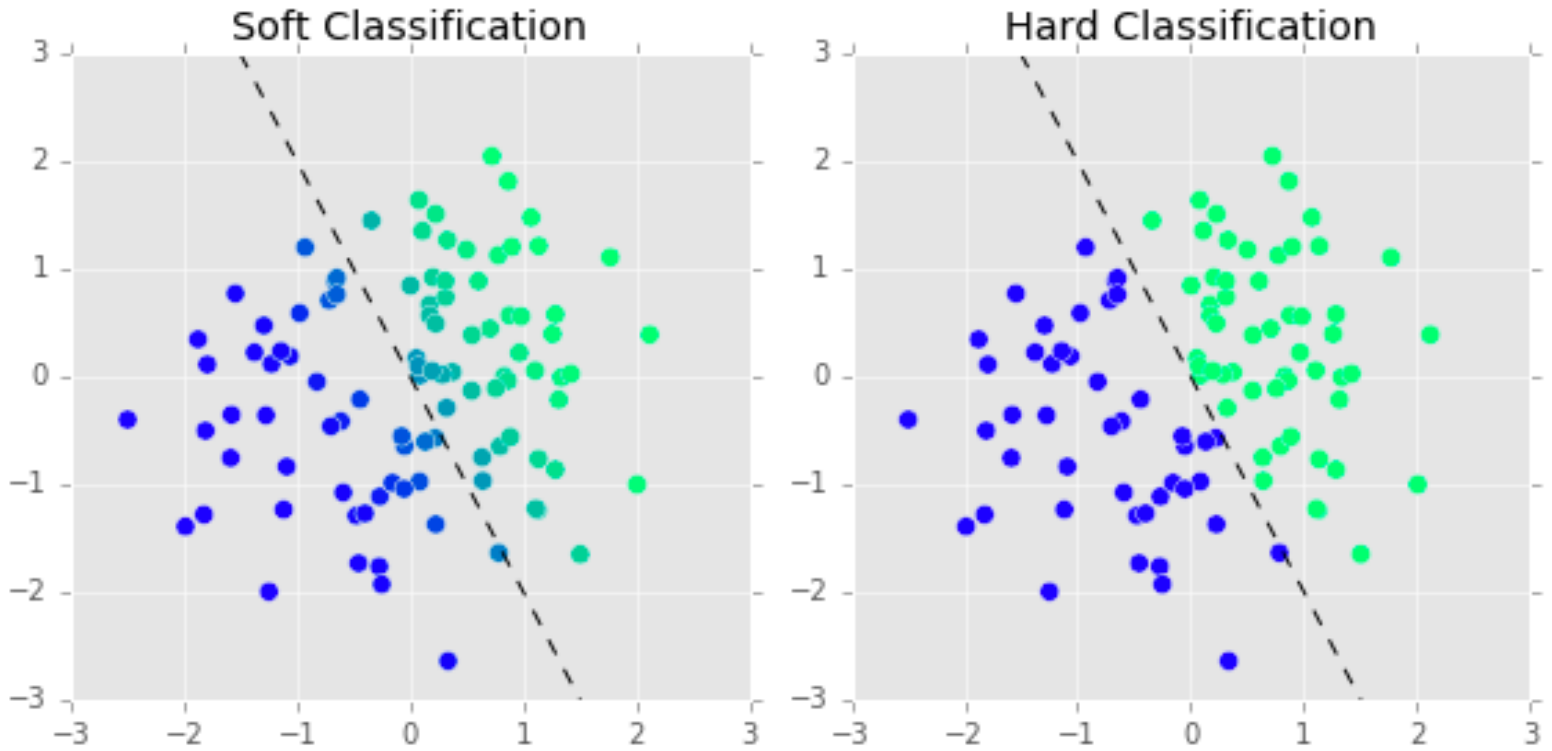


Note:
0 < y < 1

Hard Classification

- Model only attempts to estimate class membership
- Predictions are **not** probabilities
- Predictions are either zeros or ones





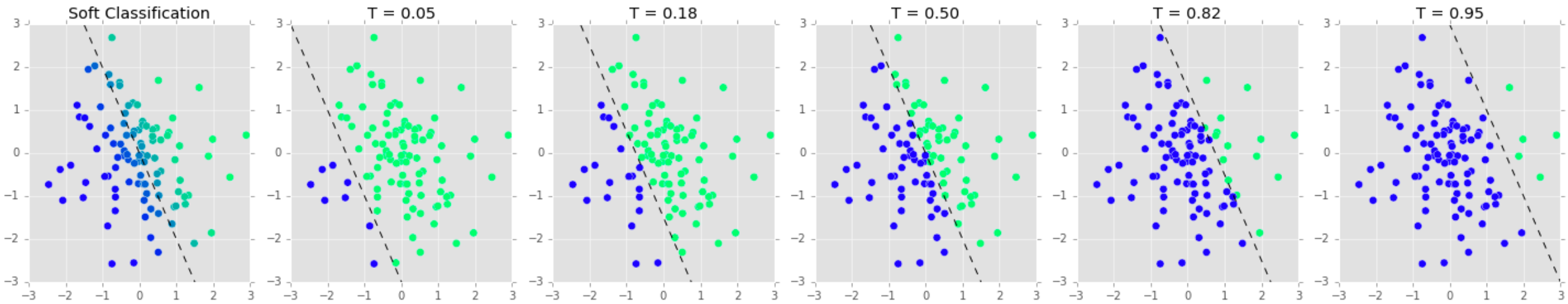
- Common misconception: **All** classification models are hard classifiers
  - **Not true!**
- There **are** some models strictly designed to be hard classifiers
  - For instance SVMs (Support Vector Machines)
- Often, soft classification is a better strategy!

Relationship: Soft and Hard Classifiers

- You can always turn a soft classifier into a hard classifier!
- For binary soft classifiers, this is called **Thresholding**
- Pick a **cutoff** or **threshold T**

$$\text{If } P(y = 1 \mid X) < T \text{ then classify } \hat{y} = 0$$

$$\text{If } P(y = 1 \mid X) \geq T \text{ then classify } \hat{y} = 1$$



Evaluating Classification Models: Two Basic Approaches

- Evaluate probabilities directly

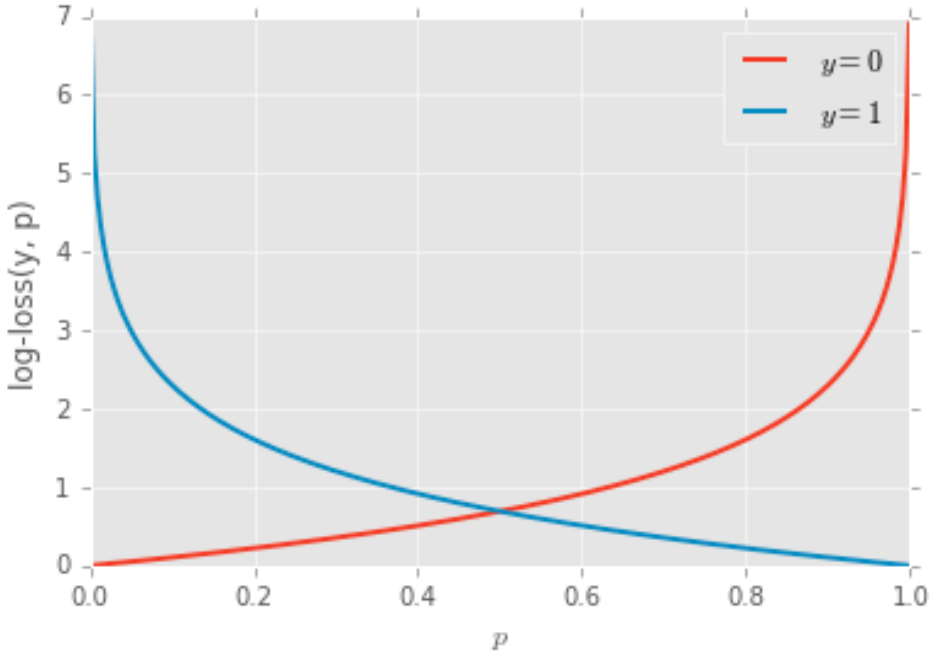
or

- Evaluate ordering of probabilities
  - i.e. something predicted as more probable than something else actually **is** more probable

Evaluating Classification Models: Soft

- Soft classification models are best evaluated and compared on the basis of their predicted probabilities (*not* by converting them to hard classifiers and evaluating the result)
- The gold standard metric for evaluating soft classification models is the log-loss

$$\text{log-loss}(y, p) = -\sum_i y_i \log(p_i) + (1 - y_i) \log(1 - p_i)$$



Evaluating Classification Models: Hard

- When evaluating hard classifications, there are only four possibilities for each data point:
  - **True Negative**: Actual 0, Predicted 0.
  - **False Positive**: Actual 0, Predicted 1.
  - **False Negative**: Actual 1, Predicted 0.
  - **True Positive**: Actual 1, Predicted 1.
- Arranged in a grid → Confusion Matrix
  - Many hard classification evaluation metrics can be derived from this table

	Predicted 1	**Predicted 0**
Actual 1	True Positive	False Negative
Actual 0	False Positive	True Negative

Accuracy

- The simplest and most natural thing to do is compute the proportion of predictions that we got correct
- Lots of problems here

$$\text{Accuracy} = \frac{\#\text{ True Positives} + \#\text{ True Negatives}}{\text{Total \# of Data Points}}$$

or

$$\text{Accuracy} = 1 - \frac{\#\text{ False Positives} + \#\text{ False Negatives}}{\text{Total \# of Data Points}}$$

False Positive and True Positive Rate

- While the accuracy measures how our predictions perform across all of our dataset, the **false positive rate** and **false negative rate** focus on the positive and negative classes individually.

$$\text{FP Rate} = \frac{\#\text{ False Positives}}{\#\text{ False Positives} + \#\text{ True Negatives}}$$

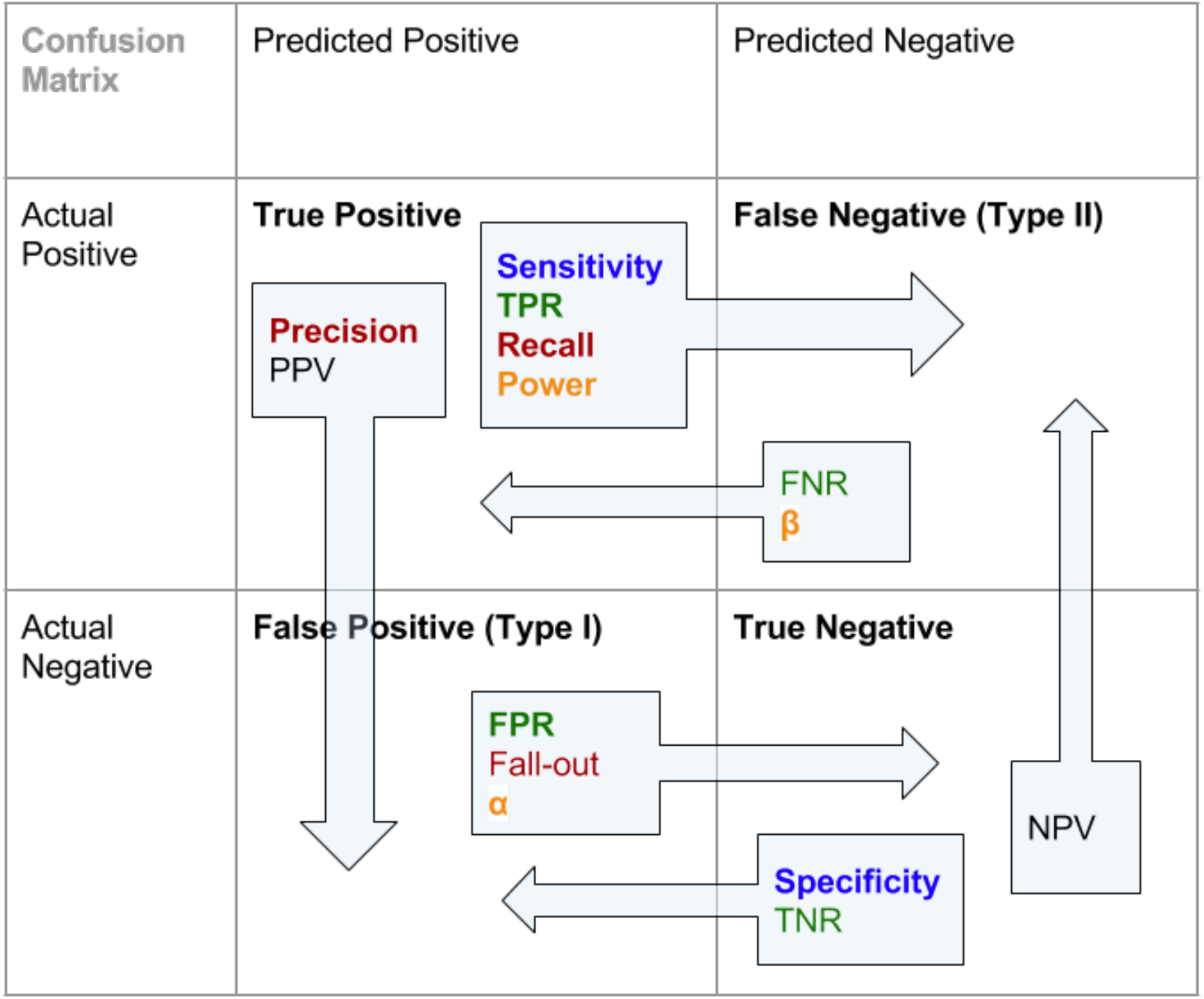
$$\text{TN Rate} = 1 - \frac{\#\text{ False Positives}}{\#\text{ False Positives} + \#\text{ True Negatives}} = \frac{\#\text{ True Negatives}}{\#\text{ False Positives} + \#\text{ True Negatives}}$$

$$\text{TP Rate} = \frac{\#\text{ True Positives}}{\#\text{ False Negatives} + \#\text{ True Positives}}$$

Grand Confusion Matrix

- Each is a ratio
- (TP, TN, FP, FN) /

  sum of 2 others
- Numerator given by label location
- Denominator given by locations spanned by arrow

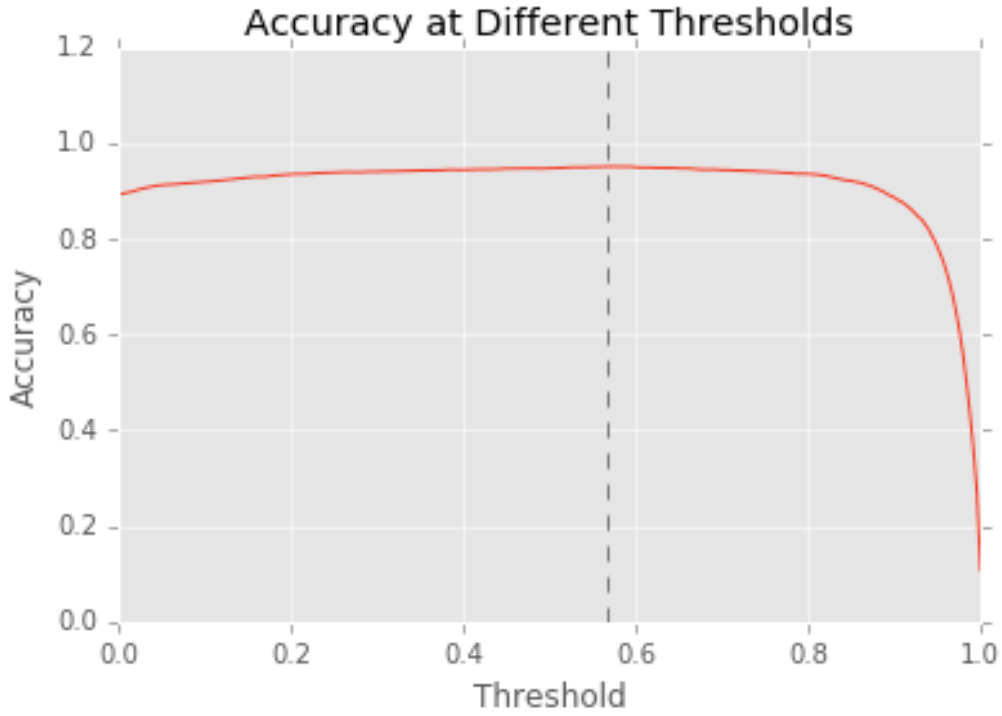


Hard Classification Metrics for Soft Classification Models

- Some metrics that can be used to evaluate both hard and soft classifiers.
  - Since a soft classifier can be made into a hard classifier by thresholding the predicted probabilities at a fixed level…
  - …any metric designed for hard classification models can, after thresholding, be applied to a soft classification model.
- Interesting to see how each of these metrics behaves as we vary the threshold.
- The following slides have plots of some of these measures for a logistic regression on a testing data set.

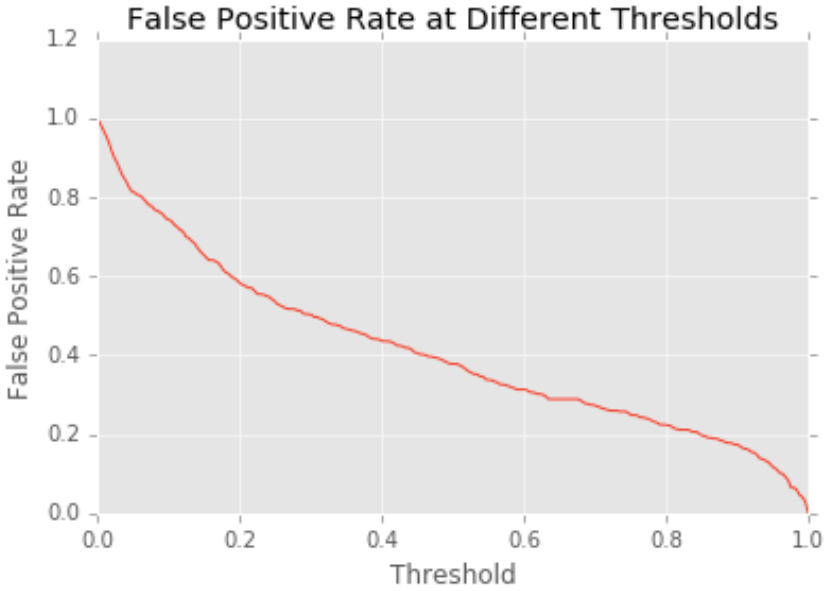
Thresholds - Accuracy

- Tons of things to talk about here, but the main takeaway is that accuracy is rarely a good metric to evaluate hard classifiers
- Example: HIV test with >99% accuracy?
  - Easy!
  - Classify everyone as HIV-
  - For most populations, that's >99% accurate
- Can be a decent metric in rare cases
  - Balanced dataset
  - Scaling minority class to balance data?
    - Not worth it just to use accuracy

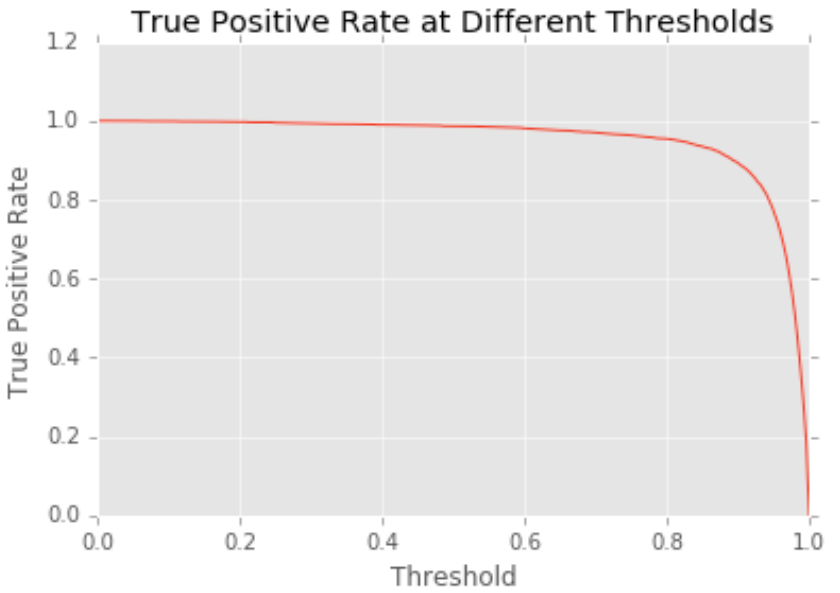


Thresholds - False Positive and True Positive Rates

- Intuitively, as threshold increases
  - FP rate decreases
- At the extremes
  - A threshold of zero classifies everything as positive, so all our negative classes are falsely classified
  - A threshold of one we classify nothing as positive, so all the negative classes are correctly classified.

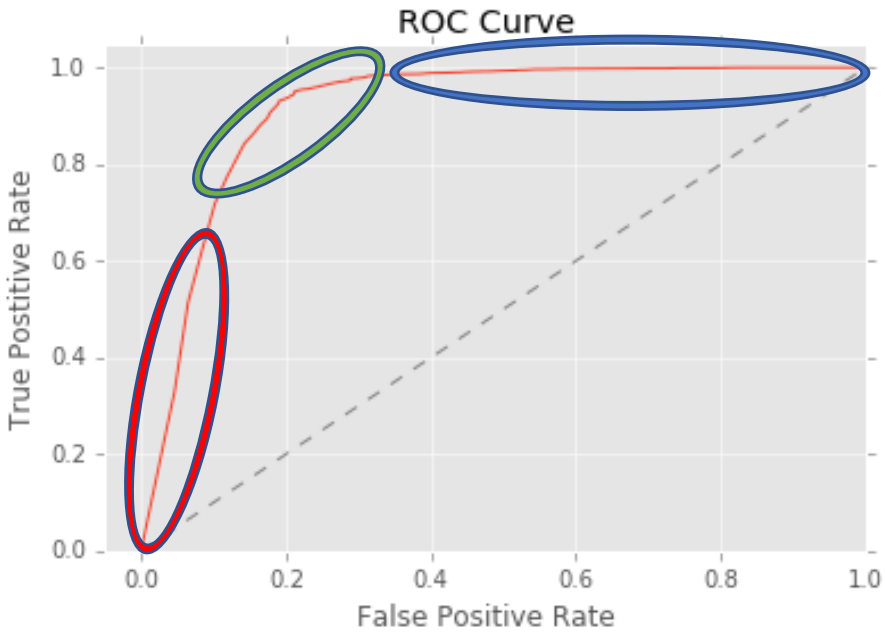


- We interpret behavior of TP rate curve similarly



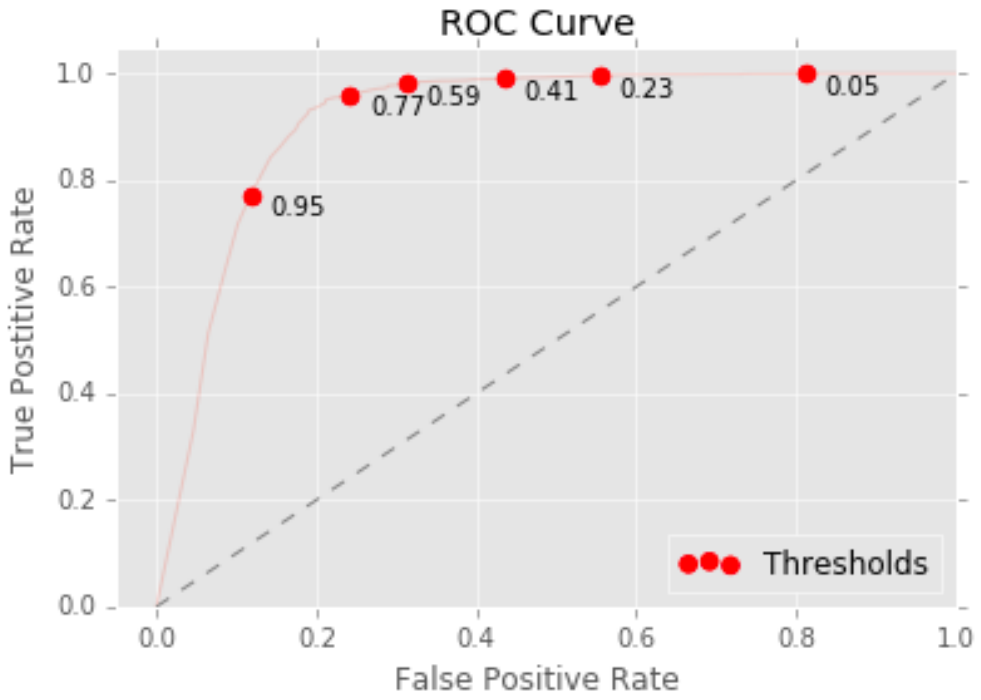
ROC Curves

- A trade-off when setting the threshold of a soft classifier if a hard classification is needed
  - If the threshold is set too low, then we will be very liberal in what observations we classify as positive, which drives up the false positive rate of the model.
  - If the threshold is set too high, then we will be very conservative in what observations we classify as positive, which will drive down the true positive rate.
  - We suspect that in the middle there is some sweet spot, where we have balanced a trade-off between the false positive and true positive rates.
- An **ROC** (receiver operating characteristic) **curve** expresses this relationship in one picture.



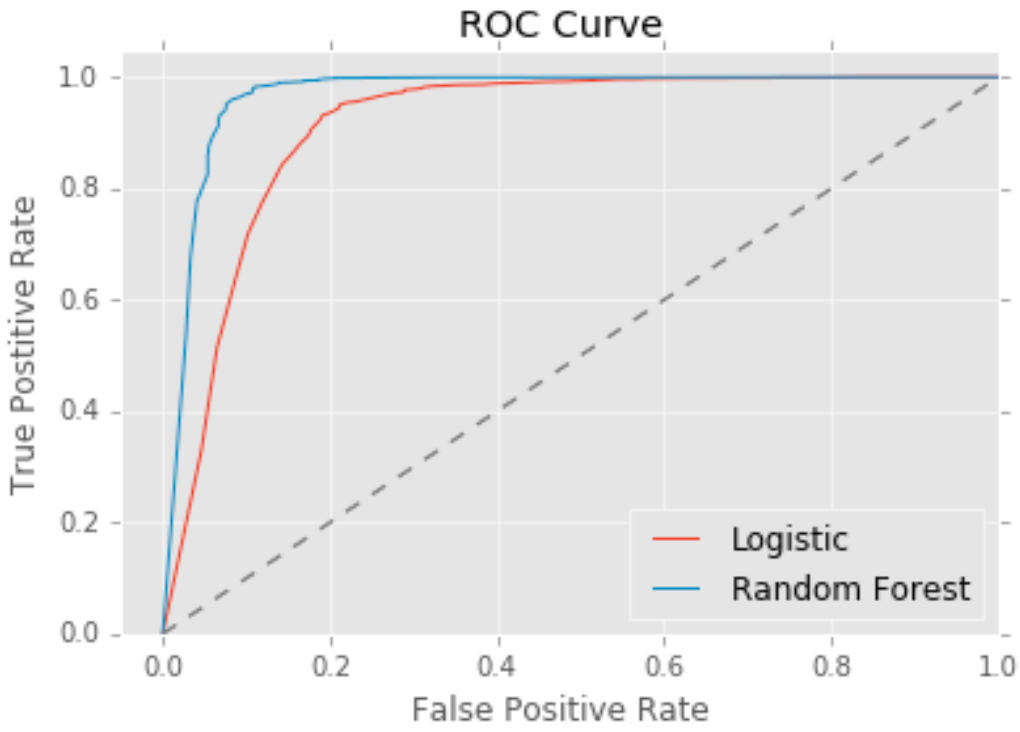
ROC Curves

- An ROC curve visualizes the trade-offs between false positives and true positives as we vary the threshold on a soft classification model.
- Each choice of the threshold results in **one** point on the ROC curve
- Dashed line between (0, 0) and (1, 1)
  - Traditional to include
  - Represents random class assignment
  - Curve above line
    - Predictive power better than random guess



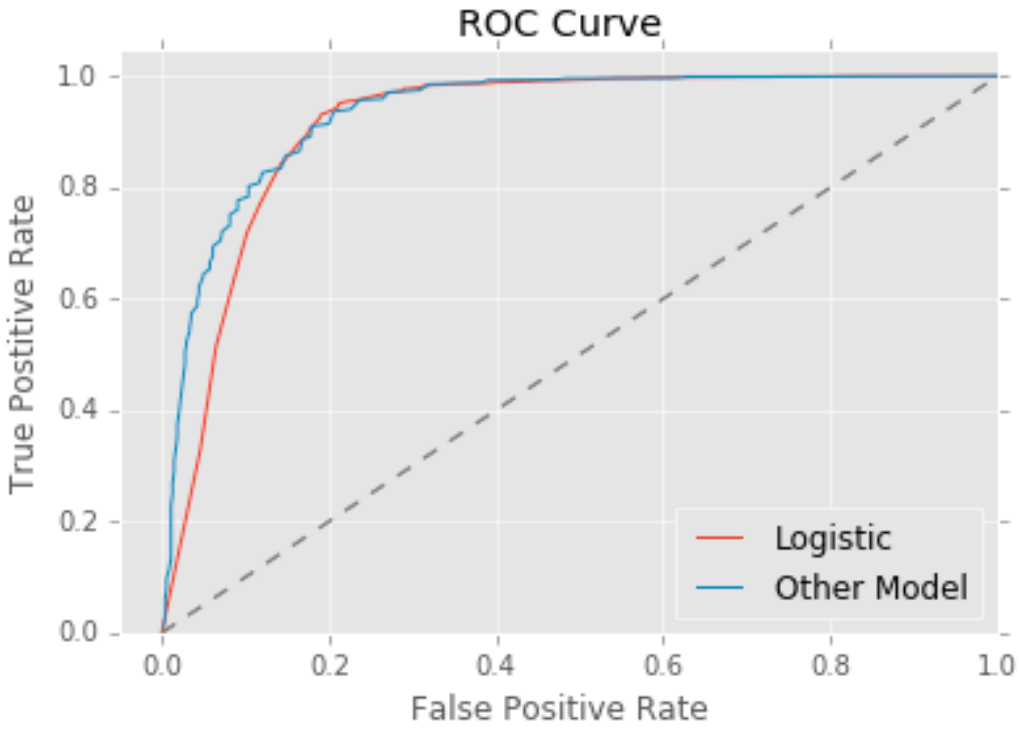
ROC Curves

- Common to inspect ROC curves of competing classifiers
  - Get a feel for how models make tradeoffs for FP and FN rates
- Here, random forest does a better job of distinguishing the positive from negative classes.



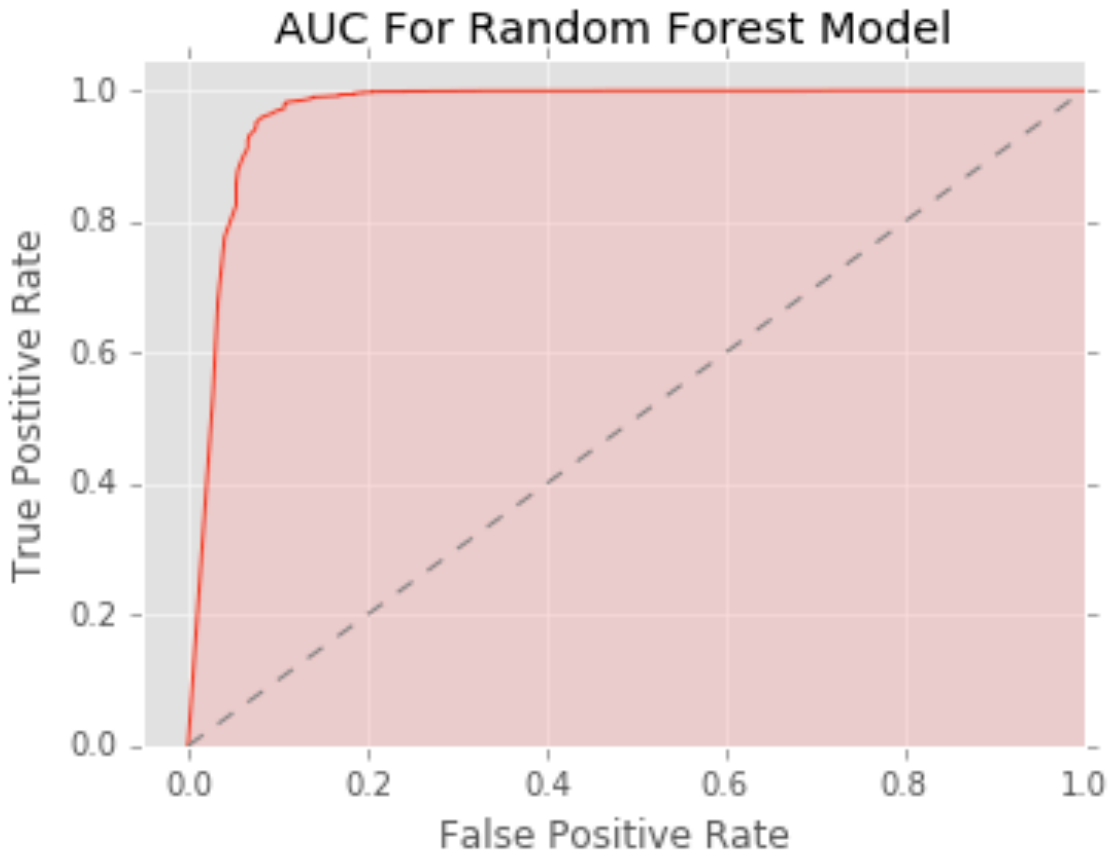
ROC Curves

- In some cases, the ROC curves for the models being compared will cross
- ROC curves give us no statistical reason to prefer one model over another
  - It depends on the costs of false positive and false negative errors in our decision problem.
  - Profit curves useful in business questions, but each problem space will need its own approach



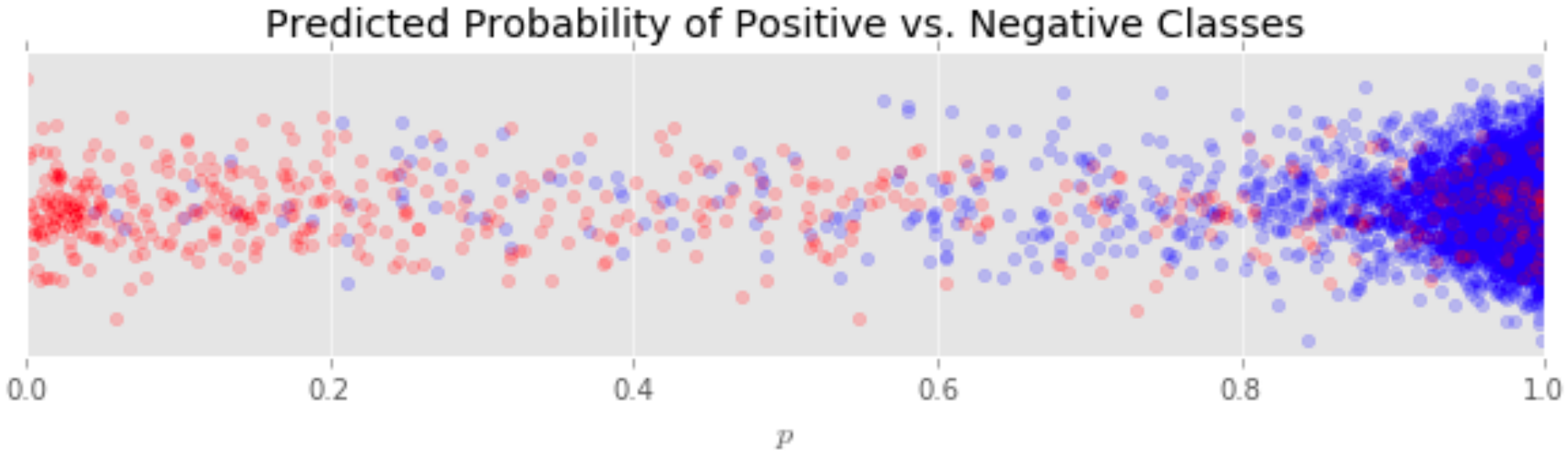
The AUC

- The **area** under the ROC curve is a numeric measure of a model's overall ability to distinguish between positive and negative classes.
- AUC is a nice measure of model fit, as it averages over **all** thresholds.



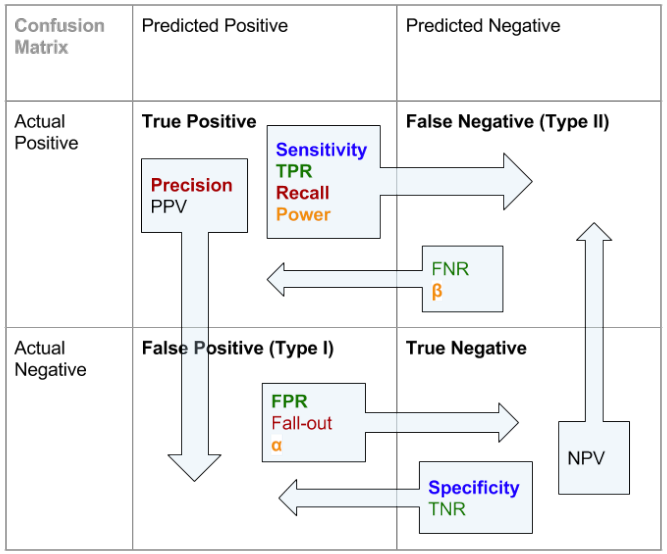
Interpretation of AUC

- The AUC has a very nice probabilistic interpretation:
  - The probability of our model predictions *ranking* a randomly chosen positive class higher than a random negative class
- The AUC statistic measures **the chance that a random pair of (red, blue) points is ranked in the correct order**

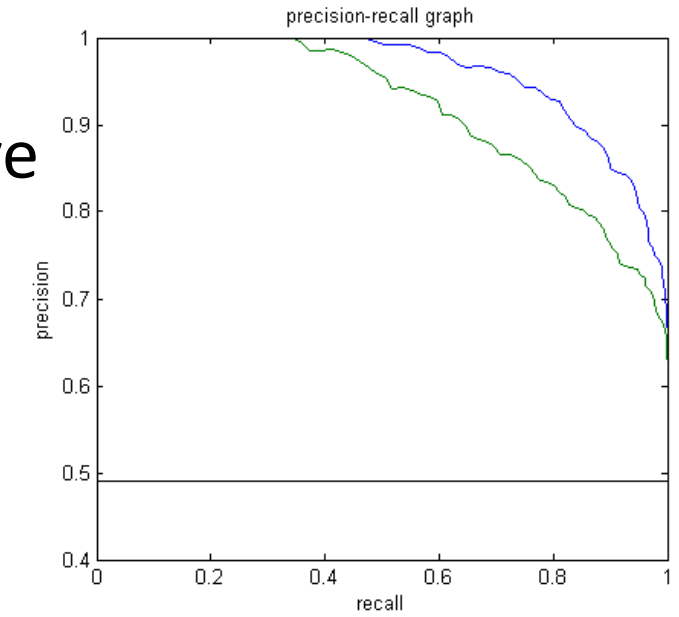


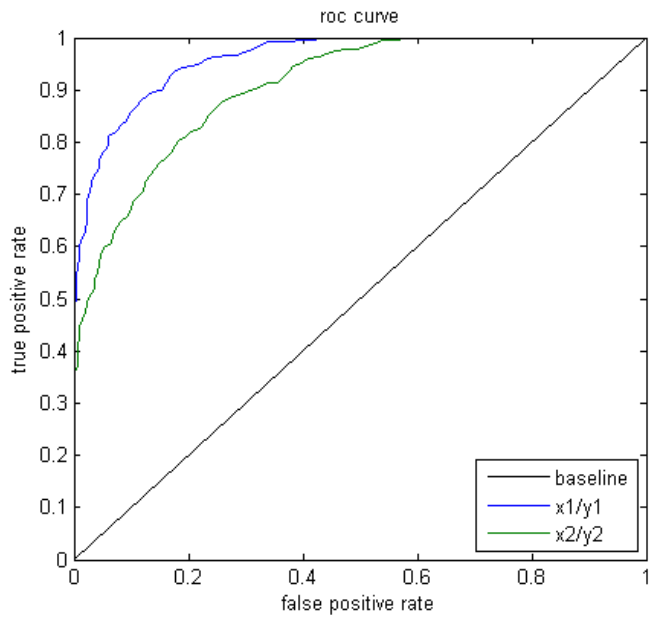
Precision-Recall Curve

- Another chart used to describe the trade-off at different thresholds
- Also parameterized by the threshold (like the ROC)
- But plots the precision (the ratio of true positives over predicted positives) against the recall (a.k.a. sensitivity a.k.a. TPR).



- Precision-recall curve
  - x is recall
  - y is precision





- ROC curve
  - x is FPR
  - y is TPR

Conclusion:
Discussion - Do You Really Need Hard Classification?

- The most persistent mistake in this area is the *overuse of hard classification models*. Let's be explicit: soft classification models are more flexible in practice, and they should generally be preferred.
- But many business or scientific problems **do** call for hard classification, especially when some decision must be made
  - e.g. we are going to do this or not, we are going to invest in this or that, etc.
- It is important to distinguish in our problem solving process between:
  - Estimating the probability of uncertain events.
  - Using those probabilities to make hard decisions or develop decision rules.
- The best general principle
  - Convert your probabilities into decisions as late into the process as possible.