STAT 215A Fall 2019
Week 12

Tiffany Tang

11/15/19

Announcements

- Lab 4 Clarifications:
  - Everyone in the group submits the **same** lab4 report/files, but each person needs to push the files to their individual private repos
- Plan for the rest of the semester
  - Next week:
    - Introduce final project and discuss expectations for report
    - Additional topics?
  - December 6: Rebecca Barter guest lecture; research talk

Review: Classification methods thus far

	Logistic	Naïve Bayes	LDA	QDA
Pros	• Can do inference (with all the caveats)	• Can choose any likelihood model	• Convenient visualizations • Linearly separable	• Quadratic decision boundaries
Cons	• Problems when p>n (a solution: regularized logistic regression) • Model misspecification?	• Assumes that features are independent (a very strong assumption) • Model misspecification?	• Problems when p>n (a solution: RDA) • Model misspecification? Non-normal or non-linear decision boundaries?	• Problems when p>n (a solution: RDA) • Requires larger n to estimate more parameters adequately (compared to LDA) • Model misspecification? Non-normal or non-linear decision boundaries?

- **What about more flexible, non-parametric methods?**

Additional tools for your tool belt

- A step towards more flexible classification: k nearest neighbors
- Plan for today:
  - SVMs + Kernel Trick
  - Trees and Random Forests
- Evaluation?

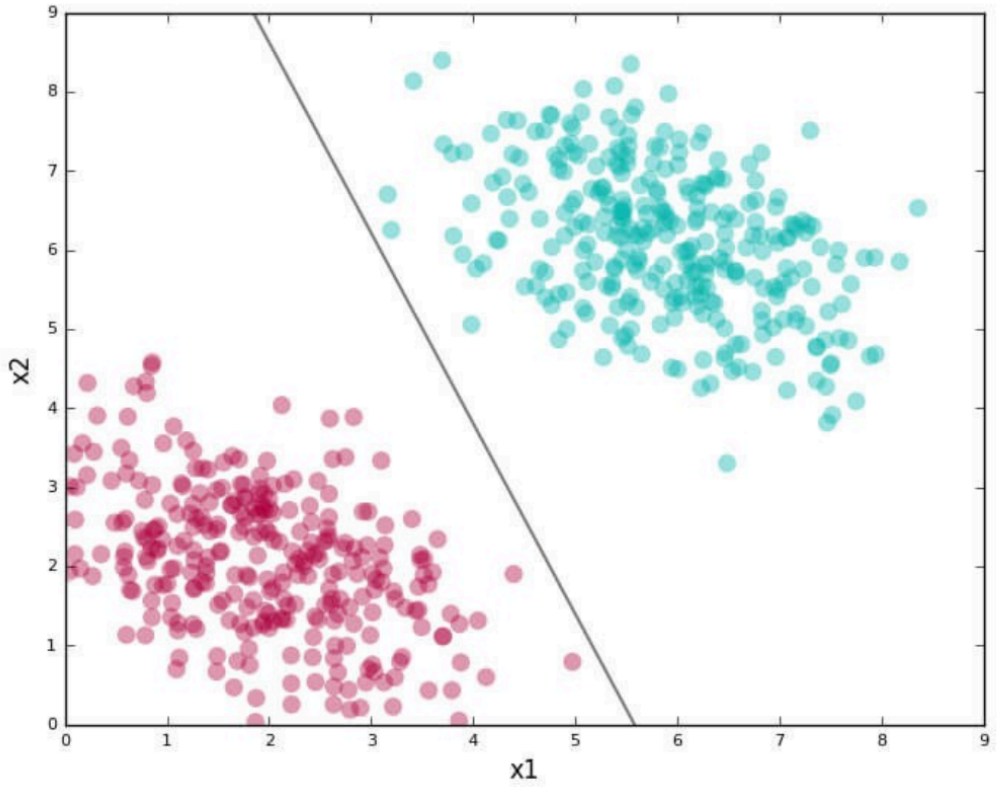
Part I: Support Vector Machines

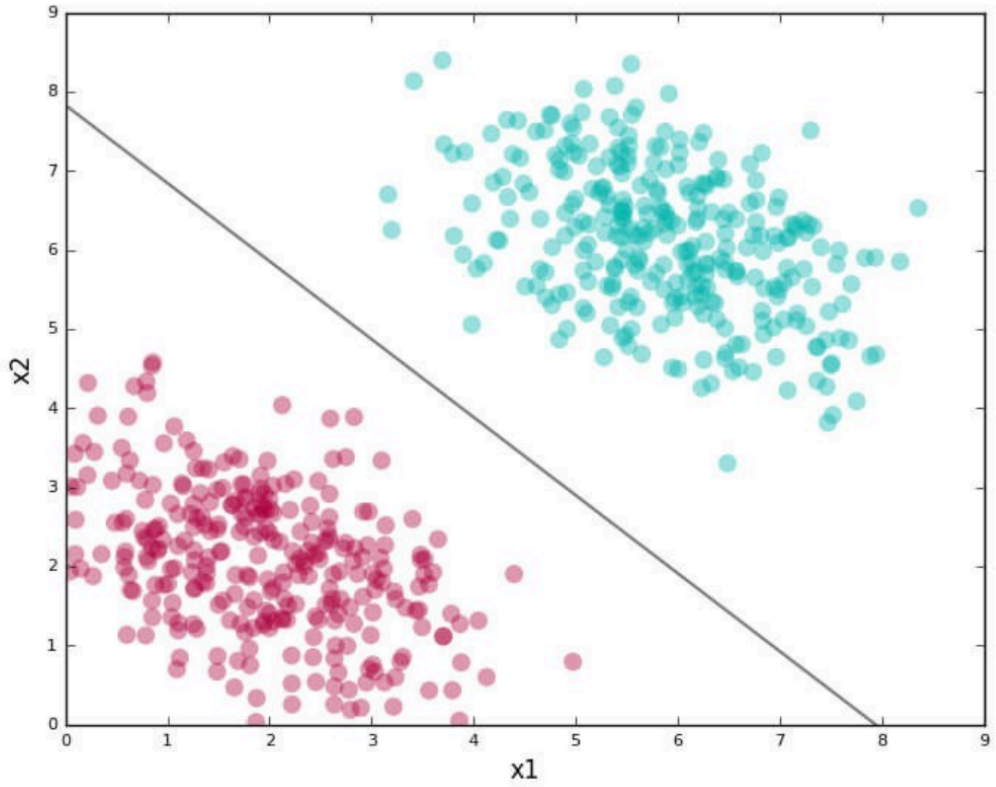
Support Vector Machines (SVM)

- One can do a lot of math here…
- Some resources
  - Gives great intuition: https://blog.statsbot.co/support-vector-machines-tutorial-c1618e635e93
  - Some discussion of the math behind SVMs:
    - https://towardsdatascience.com/understanding-support-vector-machine-part-1-lagrange-multipliers-5c24a52ffc5e
    - https://towardsdatascience.com/understanding-support-vector-machine-part-2-kernel-trick-mercers-theorem-e1e6848c6c4d
- In Elements of Statistical Learning, see p. 132 (section 4.5.2) and p. 419 (ch 12.2)
- We will focus on the intuition

Support Vector Machines (SVM)

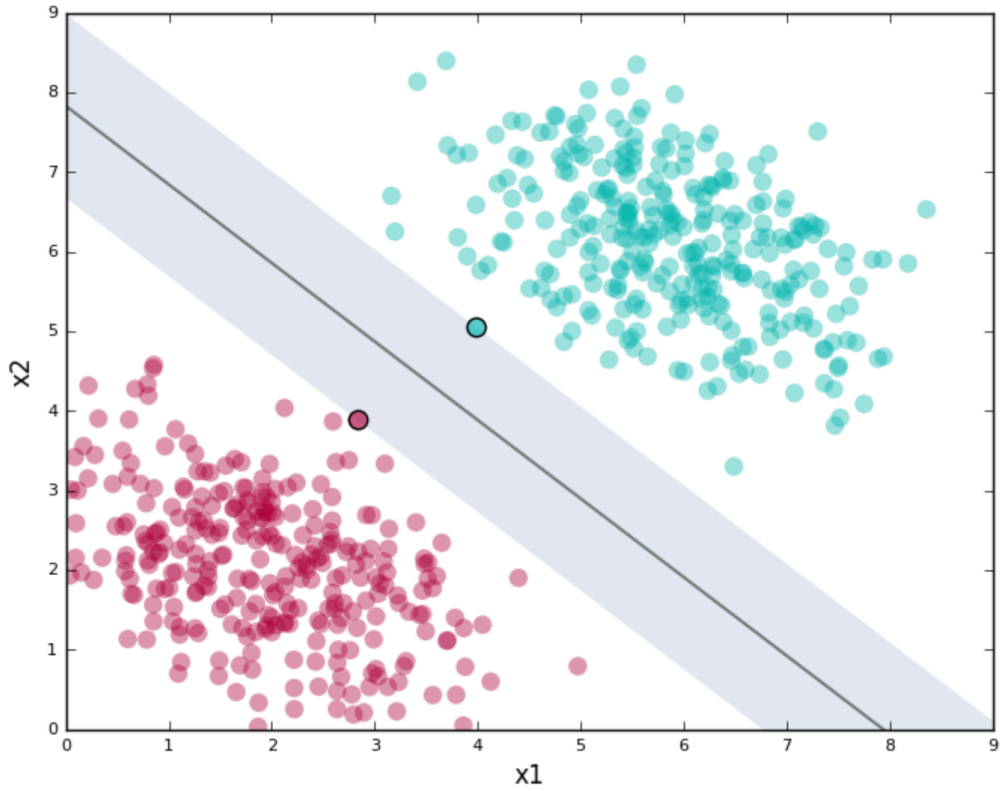
- Which classifier is better?





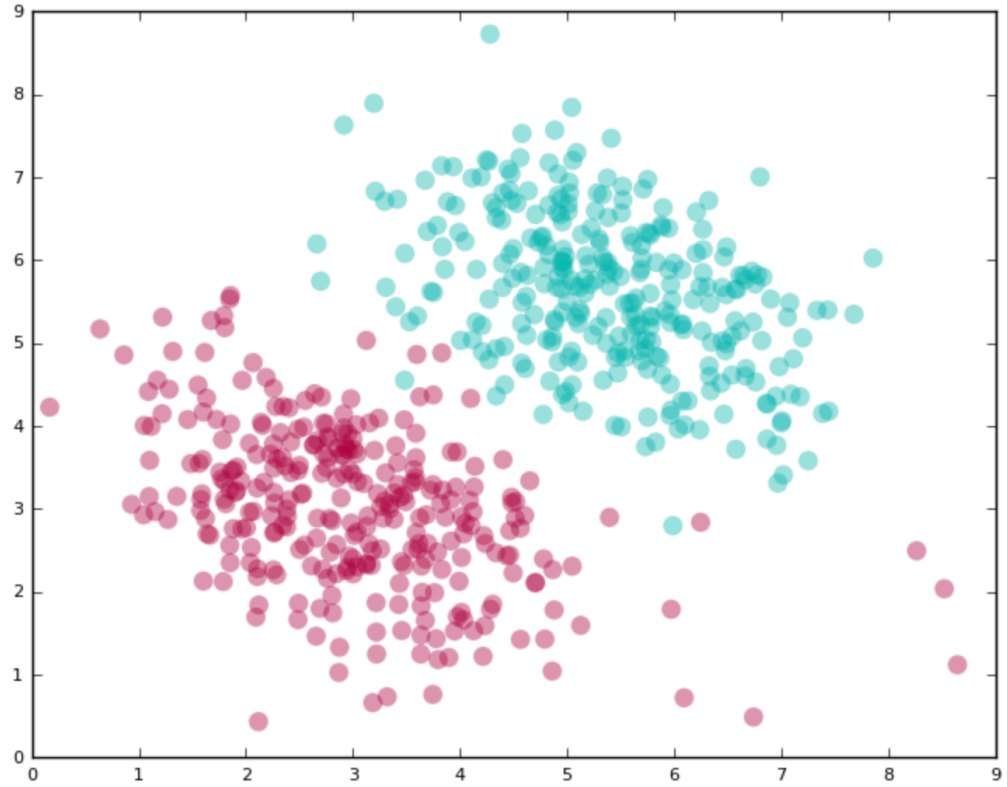
Support Vector Machines (SVM)

- **Basic Idea:**
  - Maximize the space between two hyperplanes that separate the classes
    - Called a maximum margin classifier



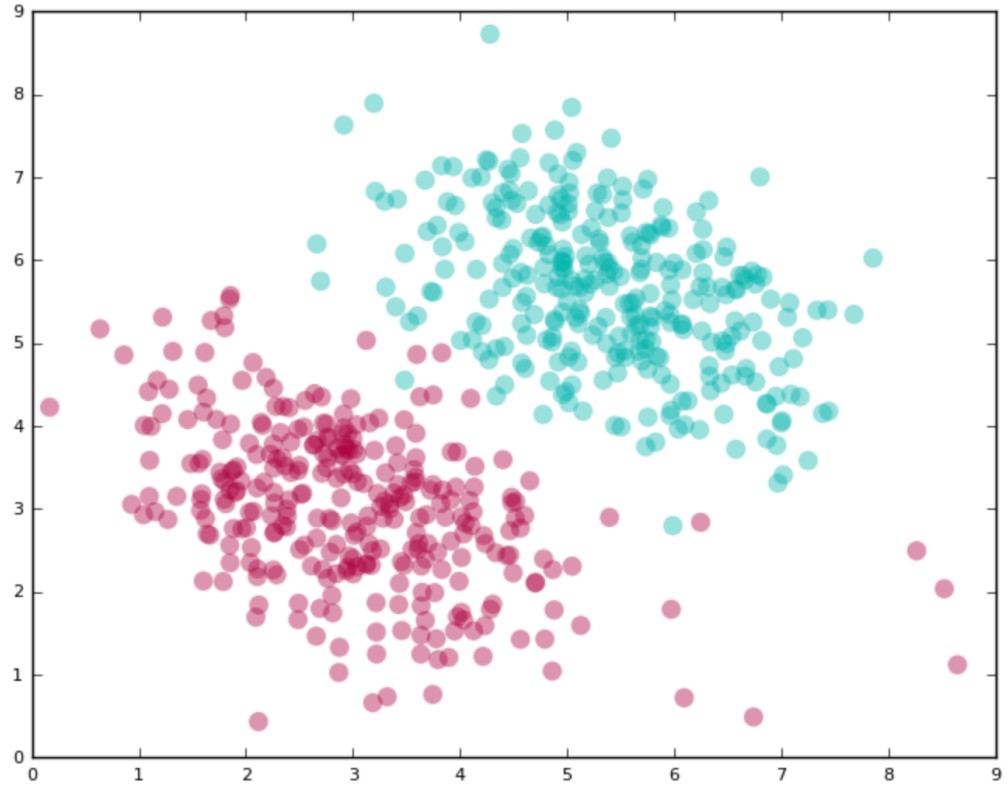
Support Vector Machines (SVM)

- What about the case where things aren't perfectly separable?



Support Vector Machines (SVM)

- **Basic Idea:**
  - Maximize the space between two hyperplanes that separate the classes while allowing for some “slack”



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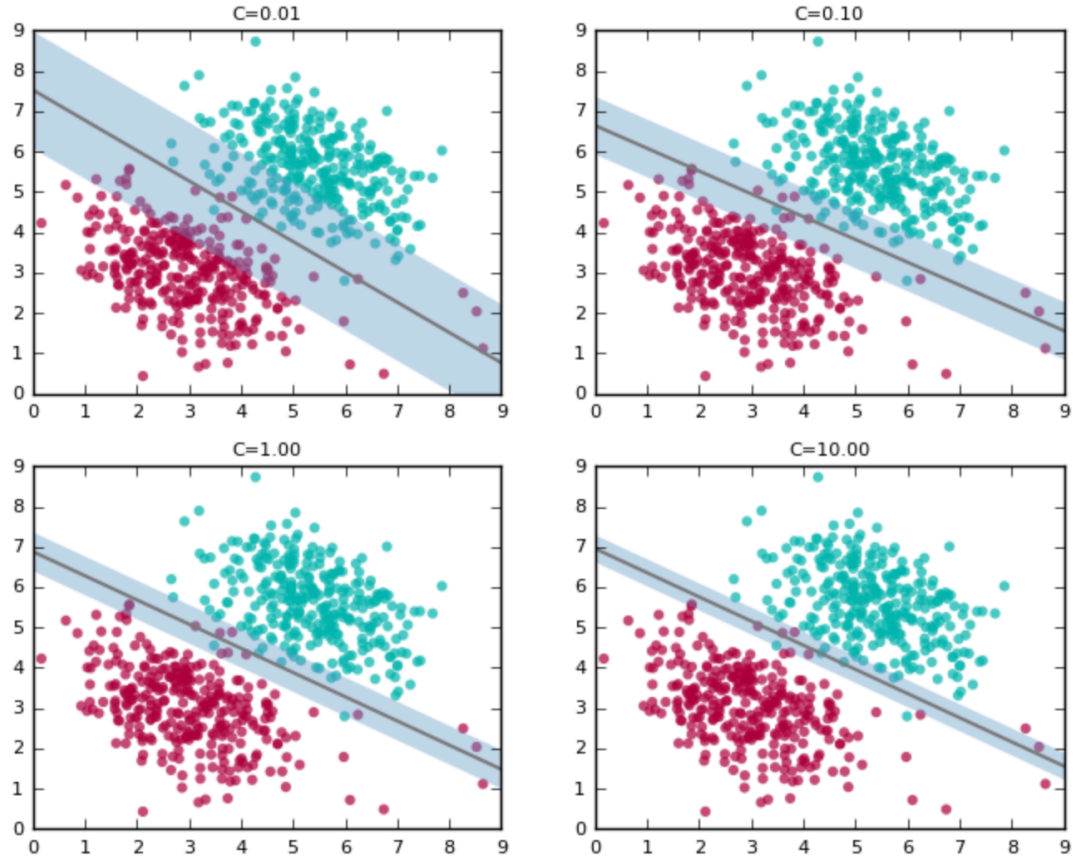
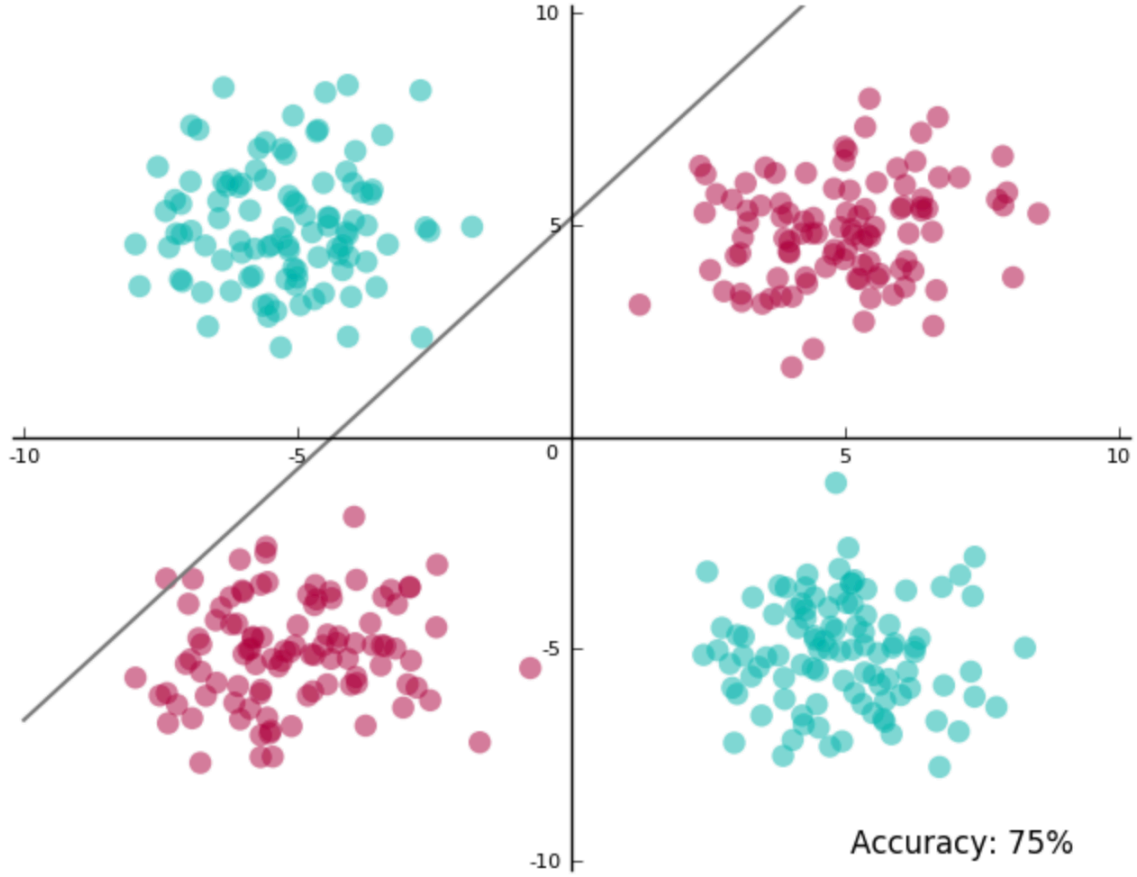


Support Vector Machines (SVM)

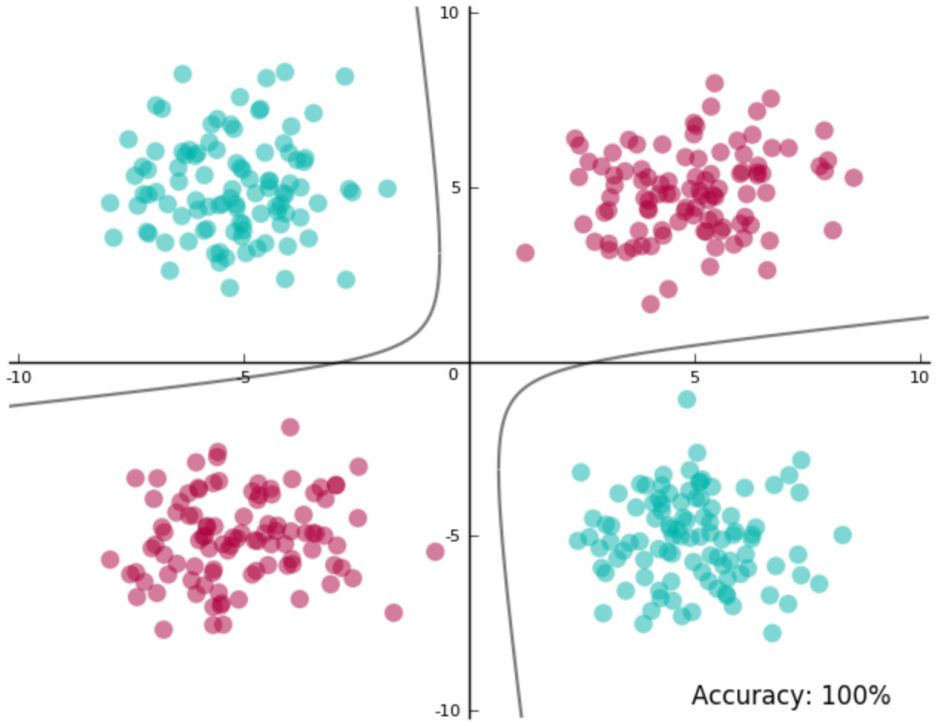
- So far so good with the linearly separable case, but what about non-linearly separable data

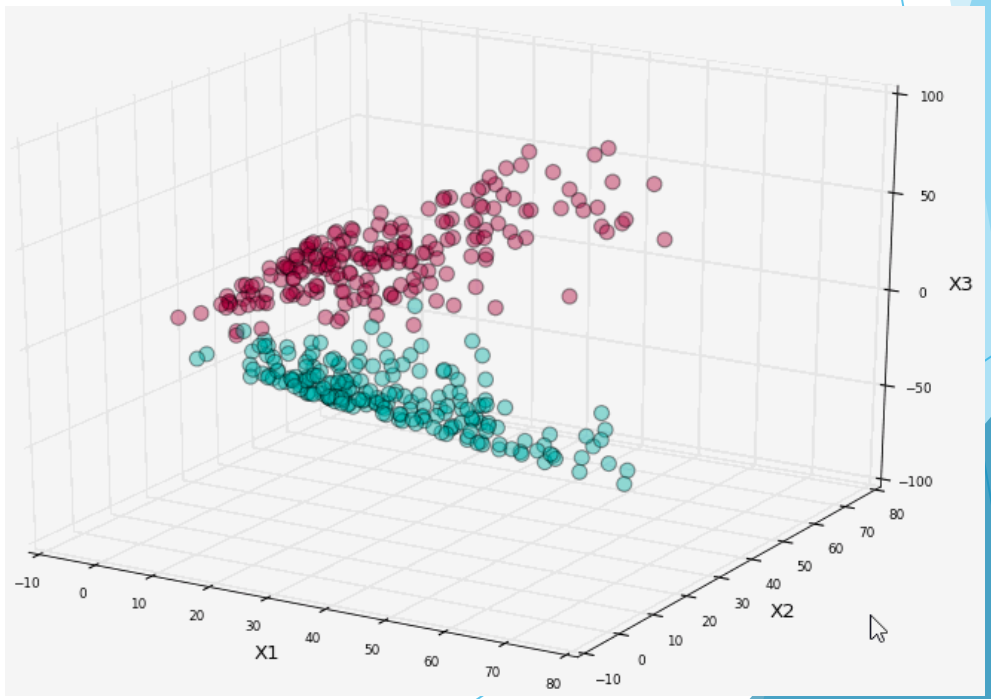


Support Vector Machines (SVM)

- **Idea:** find a higher-dimensional projection such that in that higher-dimensional space, the data becomes linearly separable

$$X_1 = x_1^2$$
$$X_2 = x_2^2$$
$$X_3 = \sqrt{2}x_1x_2$$





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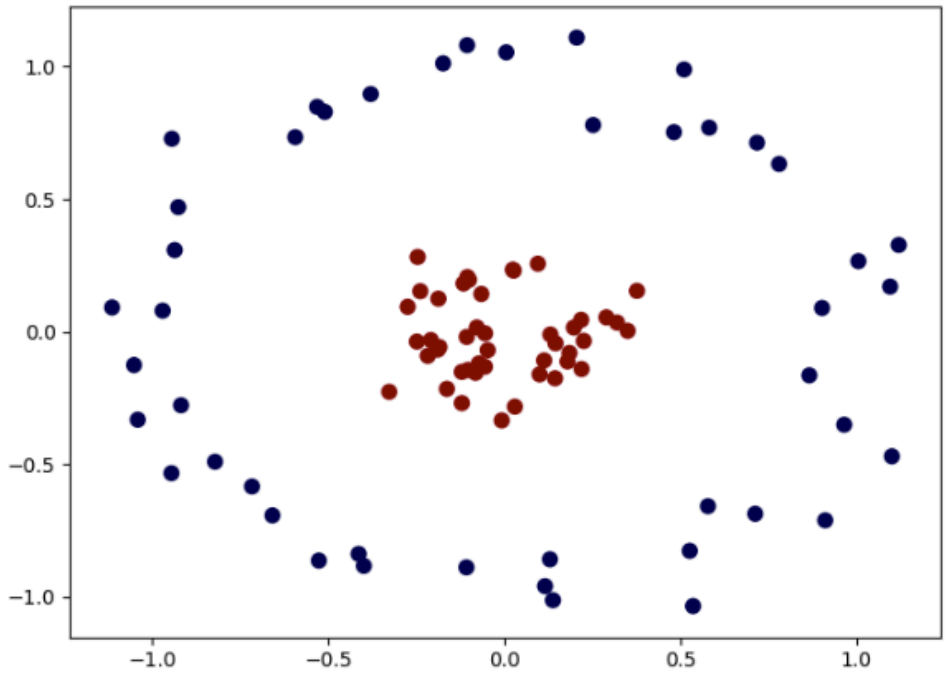

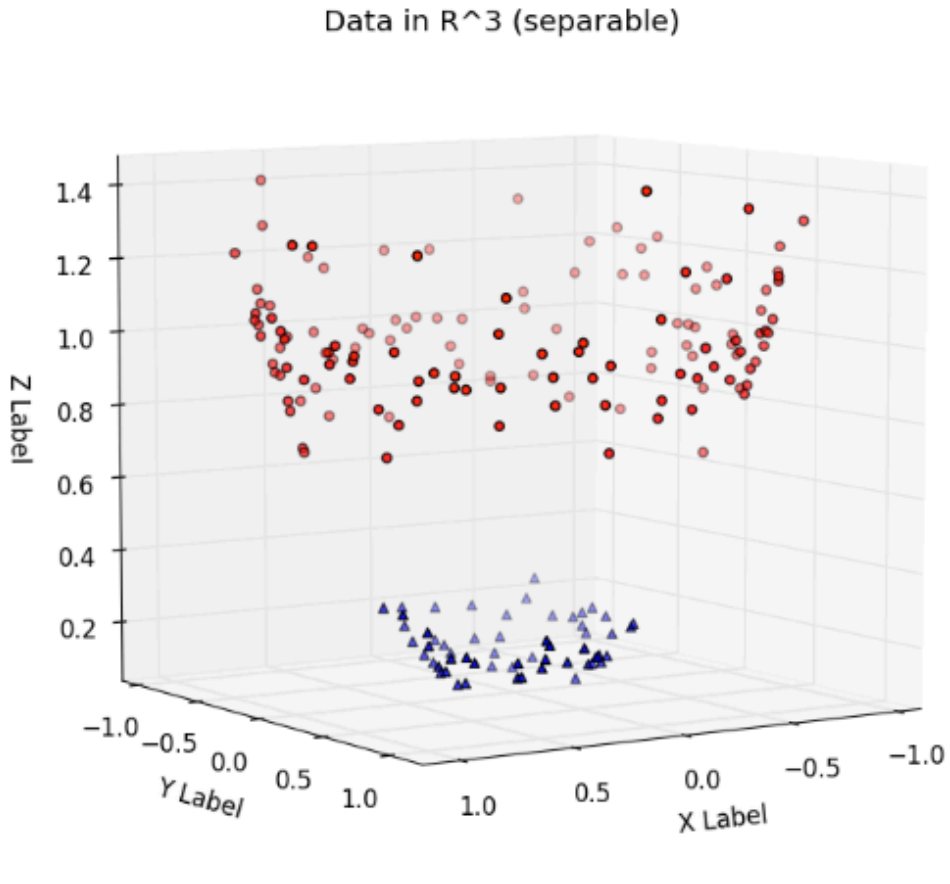

Support Vector Machines (SVM)

- How to perform this “lifting” trick in a computationally feasible way? SVMs take advantage of the **kernel trick**

- Can show that by maximizing the margins while allowing for slack, SVM solves the following optimization problem:

$$\text{maximize} \quad \mathcal{L}_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to} \quad \sum_i \alpha_i y_i = 0$$

$$\alpha_i \geq 0 \ \ \forall i$$

- Main point: this is a function of the inner product between data points

Kernel Trick

- SVM simply needs the inner product between data points: $x_i^T x_j$
- Leveraging the idea of projecting onto a higher dimensional space, we can replace the usual inner product $x_i^T x_j$ with

$$\varphi(x_i)^T \varphi(x_j)$$

where φ is some map from R^p to a higher-dimensional space (possibly even infinite dimensional)

- What is the trick? No need to even figure out what φ is
  - This is great news for us! Imagine trying to compute an infinite dimensional function…
- Instead of explicitly computing φ, just need kernel function:

$$K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$$

Kernel Trick

Some common kernel functions: $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$

- Linear kernel: $K(x, z) = x^T z$
- Naïve polynomial kernel: $K(x, z) = (x^T z)^d$
- Polynomial kernel: $K(x, z) = (1 + x^T z)^d$
- Gaussian kernel: $K(x, z) = e^{-\frac{1}{2\sigma^2}||x - z||_2^2}$
- Radial basis kernel: $K(x, z) = e^{-\gamma||x - z||_2^2}$
- Sigmoid kernel: $K(x, z) = \tanh(\eta \cdot x^T z + \nu)$

Kernel Trick

- Let's show that we can write the Gaussian kernel as

$$K(x,z) = e^{-\frac{1}{2\sigma^2}(x-z)^2} = \varphi(x)^T\varphi(z)$$

$$\begin{aligned}
K(x,z) = e^{-\frac{1}{2\sigma^2}(x-z)^2} &= e^{-\frac{x^2+z^2}{2\sigma^2}} e^{\frac{xz}{\sigma^2}} \\
&= e^{-\frac{x^2+z^2}{2\sigma^2}} \left(\sum_{n=0}^{\infty} \frac{(xz)^n}{\sigma^{2n} n!} \right) \\
&= e^{-\frac{x^2+z^2}{2\sigma^2}} \left(\sum_{n=0}^{\infty} \sqrt{\frac{1}{\sigma^{2n} n!}} x^n \cdot \sqrt{\frac{1}{\sigma^{2n} n!}} z^n \right) \\
&= e^{-\frac{x^2}{2\sigma^2}} e^{-\frac{z^2}{2\sigma^2}} \left[1 \cdot 1 + \sqrt{\frac{1}{\sigma^2 1!}} x \cdot \sqrt{\frac{1}{\sigma^2 1!}} z + \sqrt{\frac{1}{\sigma^4 2!}} x^2 \cdot \sqrt{\frac{1}{\sigma^4 2!}} z^2 + \dots \right] \\
&= \phi(x)^\top \phi(z)
\end{aligned}$$

where $\phi(x) := e^{-\frac{x^2}{2\sigma^2}} \left(1, \sqrt{\frac{1}{\sigma^2 1!}} x, \sqrt{\frac{1}{\sigma^4 2!}} x^2, \dots \right) = e^{-\frac{x^2}{2\sigma^2}} \left(\sqrt{\frac{1}{\sigma^{2n} n!}} x^n \right)_{n=0}^{\infty}$

Kernel Trick

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&= \phi(x)^\top \phi(z)
\end{aligned}$$

- **Takeaway:** by replacing the usual inner product $x_i^T x_j$ with the Gaussian kernel, it's as if we were projecting the data into an infinite dimensional space and finding a separating hyperplane in that infinite dimensional space!

Kernel Trick

- Can do something similar with other kernels: e.g., polynomial kernels for 2-dimensional data

$$k(\mathbf{x}, \mathbf{y}) = (1 + \mathbf{x}^T \mathbf{y})^2 = (1 + x_1\, y_1 + x_2\, y_2)^2 =$$
$$= 1 + x_1^2 y_1^2 + x_2^2 y_2^2 + 2x_1 y_1 + 2x_2 y_2 + 2x_1 x_2 y_1 y_2$$

- This is an inner product between two 6-dimensional vectors:

$$\varphi(x) = \varphi(x_1, x_2) = \left(1, x_1^2, x_2^2, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1 x_2\right)$$
$$\varphi(y) = \varphi(y_1, y_2) = (1, y_1^2, y_2^2, \sqrt{2}y_1, \sqrt{2}y_2, \sqrt{2}y_1 y_2)$$
$$\Longrightarrow \quad K(x, y) = \varphi(x)^T \varphi(y)$$

- What happens if we use the kernel $K(x, y) = (x^T y)^2$

Recap of SVMs + Kernel Trick

- **Basic idea:** find separating hyperplane that maximizes margins (with some slack) between classes

- Turns out the optimization problem corresponding to this idea is:

$$\text{maximize} \quad \mathcal{L}_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{ij} \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$

$$\text{subject to} \quad \sum_i \alpha_i y_i = 0$$

$$\alpha_i \geq 0 \ \forall i$$

- Because the optimization problem depends only on the inner product $x_i^T x_j$, can use the kernel trick to "lift" the data into a higher-dimensional space to hopefully find an optimal separating hyperplane

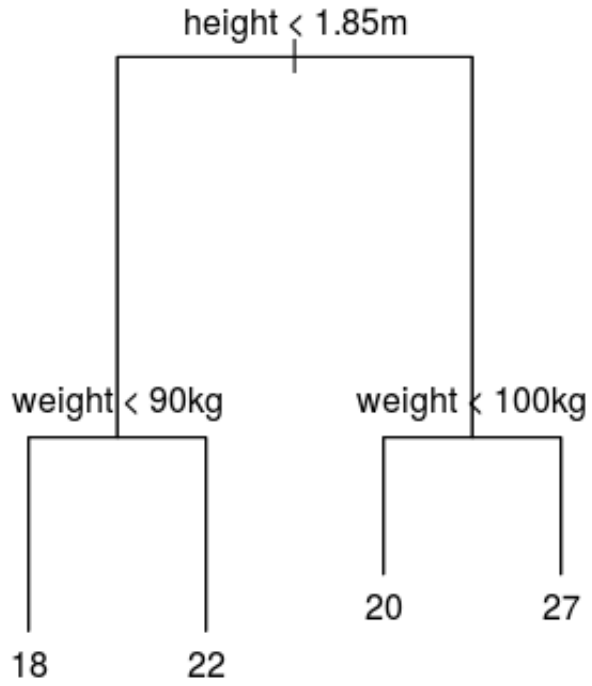
Practical Notes on SVM

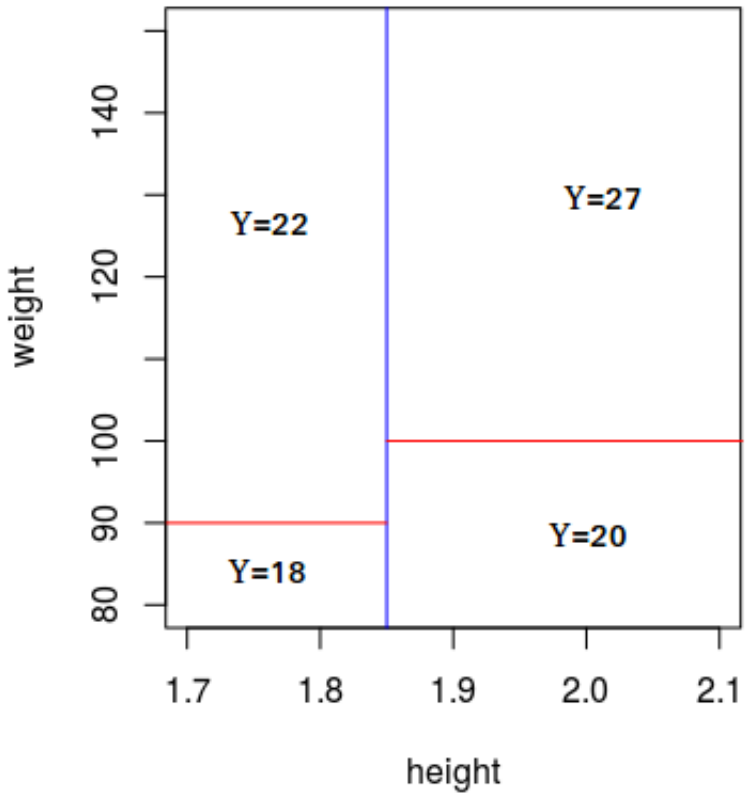
- Kernel trick allows for extreme flexibility
- But with flexibility, there is a greater danger of overfitting, especially if p is large
- Lots of other methods based upon this kernel trick: kernel PCA, kernel ridge regression, etc.

Trees and Random Forests

CART (Classification and Regression Trees)

- **Idea:** recursively partition the data space via binary splits and fit a simple model for each result region





CART (Classification and Regression Trees)

- At each split in the tree, how to choose what **variable** (j) to split on and what **threshold** (t)?
- For now, assume we have a regression problem: at each split, we want to optimize L_2 loss

$$\min_{j,t} \left\{ \min_{\mu_L} \sum_{i:x_{ij} \leq t} (y_i - \mu_L)^2 + \min_{\mu_R} \sum_{i:x_{ij} > t} (y_i - \mu_R)^2 \right\}$$

- Can find global minimum for each split via a brute force search
  - Note: we cannot necessarily find the global minimum for the entire tree

CART (Classification and Regression Trees)

- Brute force search algorithm:
  - For each feature j:
    - Sort X: $x_{(1)j} \leq \cdots \leq x_{(n)j}$ → O(nlogn)
    - Scan from left to right and threshold t_j that minimizes L_2 loss → O(n)
  - Out of the p possible splits, take the best t_j
- Total complexity: O(pnlogn + pnK) where K = number of splits → Not too bad!
- For classification, can replace L_2 loss with classification error, Gini index, etc.

CART (Classification and Regression Trees)

- **Advantages:**
  - Can deal with continuous, categorical, binary, count features all at the same time
  - Doesn’t depend on scale of X!!
  - Easily interpretable, fairly flexible, and fast
- **Disadvantages:**
  - Potentially too simple
  - Not a great balance between bias-variance tradeoff
    - As depth of tree increases, massively overfit to the training data → no bias, high variance
    - If tree is too shallow, massively underfit → high bias, low variance

Random Forest

- **Idea:** try to reduce both the bias and variance using decision trees
- To reduce the bias, grow deep trees (i.e., grow trees to purity so that in each of the leaf nodes, we have 1-3 observations left)
- To reduce the variance,
  - Grow many trees (e.g., 500 trees) using bootstrap samples of the data and average over this ”forest”
  - Try to force these trees to be close to iid: at each split, select m_{try} out of p variables randomly to search and potentially split on

Random Forest Algorithm

- **Inputs:** number of trees to grow (B), number of variables to randomly select at each split (m_{try}), number of leaf/terminal nodes (M)
- For each tree b = 1, …, B:
  - Bootstrap data → X^{*b}
  - Grow decision (CART) tree T^b such that
    - At each split in the tree, randomly choose m_{try} out of p variables to try and potentially split on
    - Grow until tree has M leaf/terminal nodes
- Make prediction: $\hat{y}(x) = \frac{1}{B}\sum_{b=1}^{B} T^b(x)$

Random Forest in Practice

- Because we are bootstrapping the data before constructing each tree, we essentially have a “test set” for each tree that we can exploit
  - We call this left out data due to bootstrapping the **out-of-bag (OOB) data**, from which we can compute the OOB error
  - OOB error can be used like CV error to tune parameters like m_{try}
- Can obtain marginal feature importances from RF

Random Forest in Practice

- Advantages:
  - Doesn’t depend on scale of X
  - Great prediction for lots of problems
  - Reduces bias and variance simultaneously unlike CART
- May not be optimal with correlated features or p >> n
- No longer easily interpretable
- Two useful packages:
  - library(randomForest)
  - library(ranger)
  - ranger is much faster than randomForest

Another useful tool in practice

- Caret package
- See tutorial created by Rebecca Barter in the week12 folder

Evaluation Metrics for Classification

How to evaluate your classification methods

- Going beyond classification error…
- What if we have class imbalance?
  - Ex. sample of 100 people and only 10 have the disease → always predict healthy and get 90% classification accuracy!!

Confusion Matrix

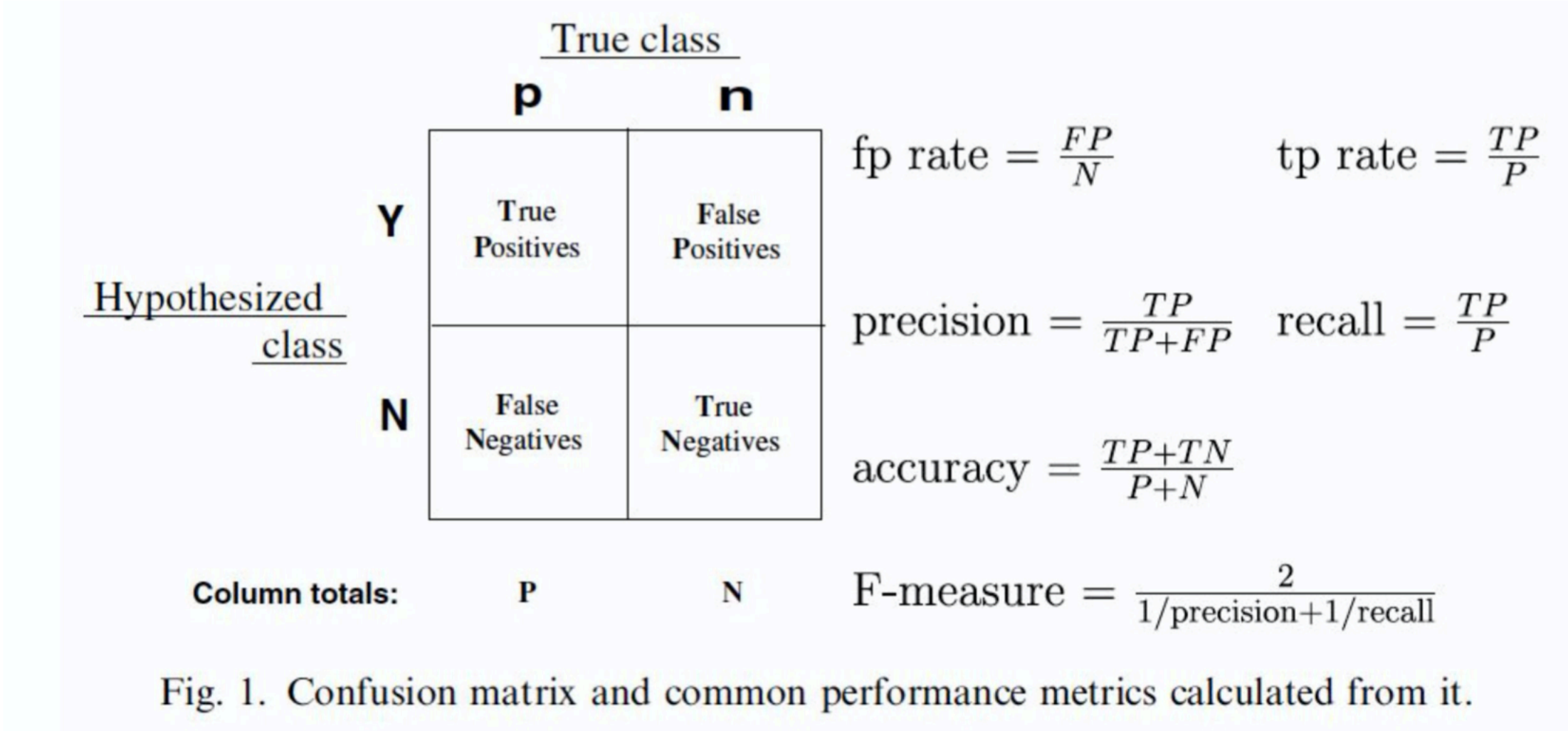
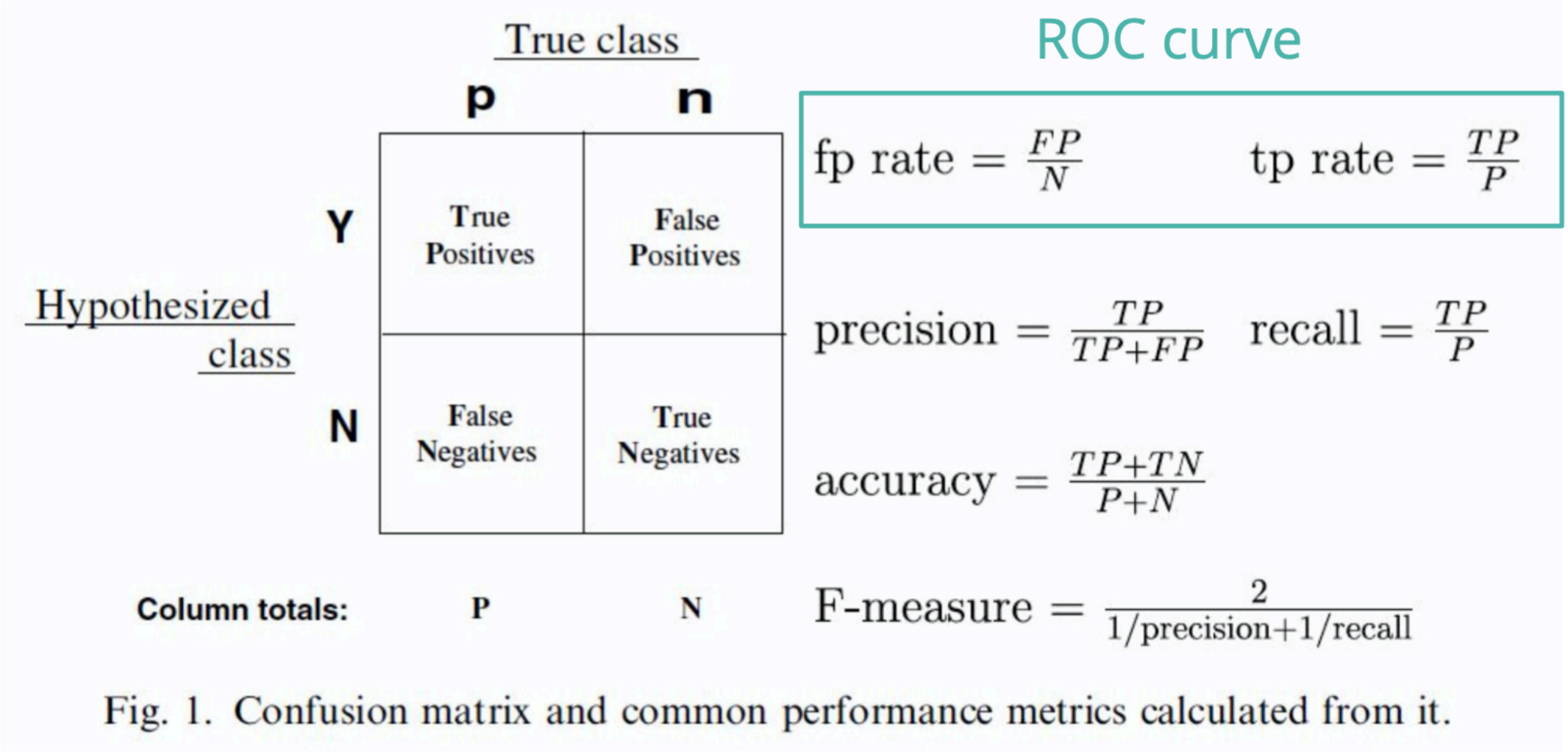


Fig. 1. Confusion matrix and common performance metrics calculated from it.

Source: Fawcett (2005)

Confusion Matrix



Hypothesized class	True class: p	True class: n
Y	True Positives	False Positives
N	False Negatives	True Negatives
Column totals:	P	N

ROC curve

$$\text{fp rate} = \frac{FP}{N} \qquad \text{tp rate} = \frac{TP}{P}$$

$$\text{precision} = \frac{TP}{TP+FP} \qquad \text{recall} = \frac{TP}{P}$$

$$\text{accuracy} = \frac{TP+TN}{P+N}$$

$$\text{F-measure} = \frac{2}{1/\text{precision}+1/\text{recall}}$$

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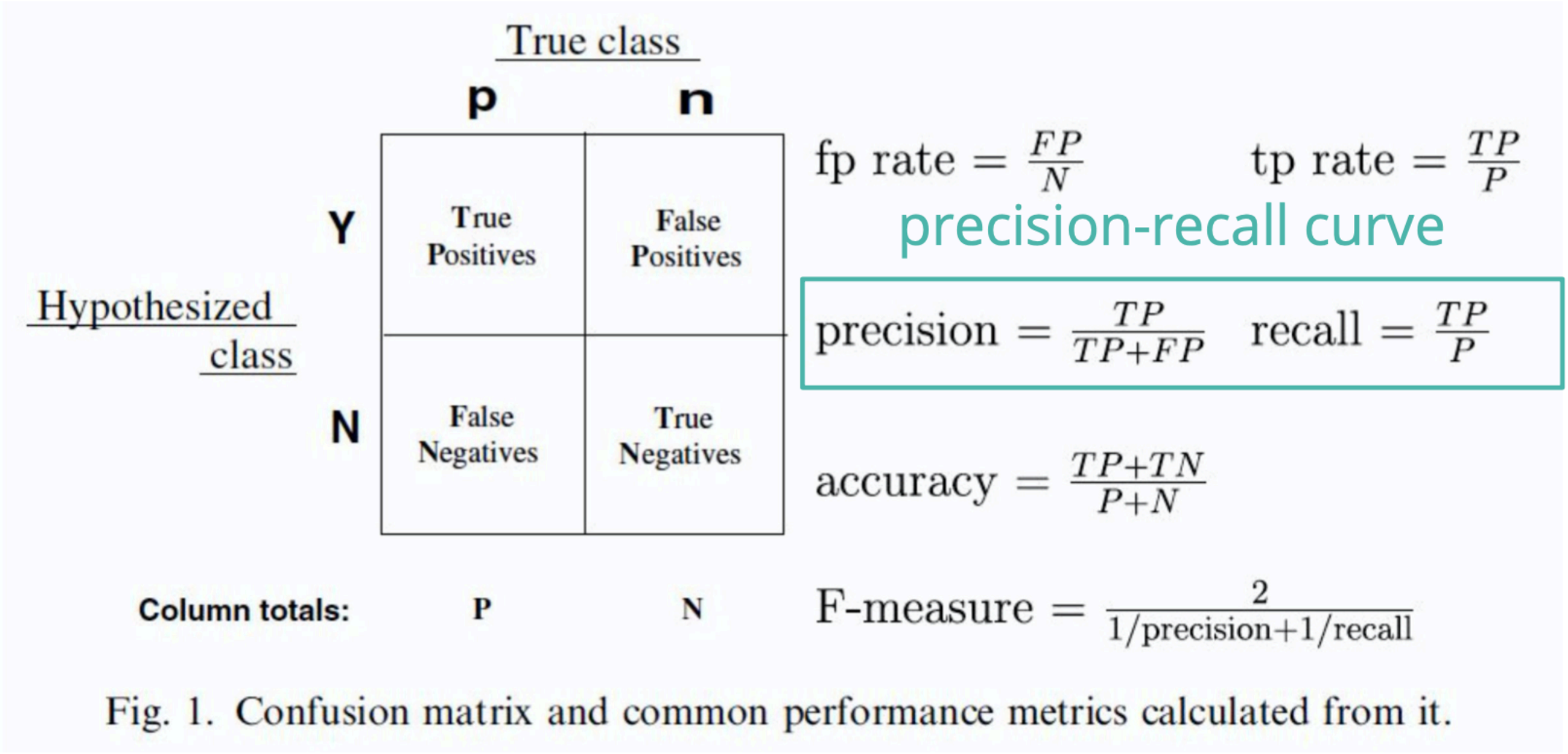

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precision-recall curve

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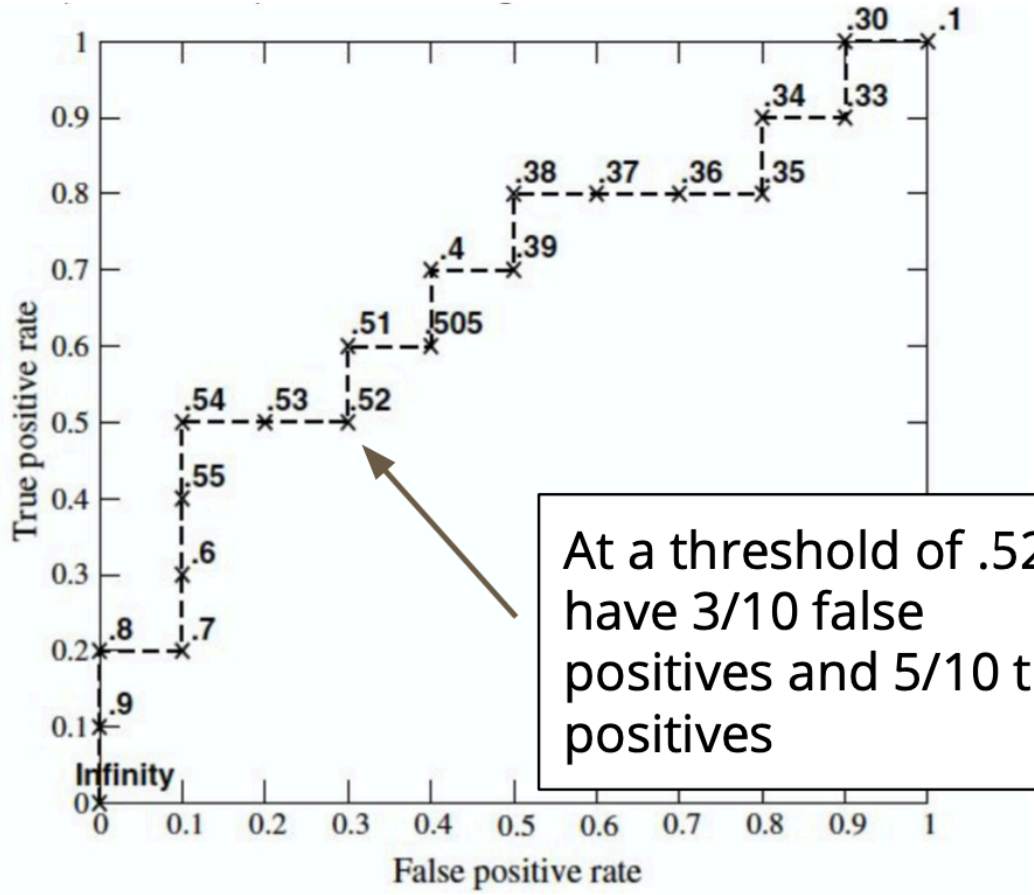
Receiver operating characteristics (ROC) curve

We can generate an ROC curve when the output of a classifier is a probability and we must choose a threshold for the final predicted class

Inst#	Class	Score	Inst#	Class	Score
1	p	.9	11	p	.4
2	p	.8	12	n	.39
3	n	.7	13	p	.38
4	p	.6	14	n	.37
5	p	.55	15	n	.36
6	p	.54	16	n	.35
7	n	.53	17	p	.34
8	n	.52	18	n	.33
9	p	.51	19	p	.30
10	n	.505	20	n	.1



Source: Fawcett (2005)

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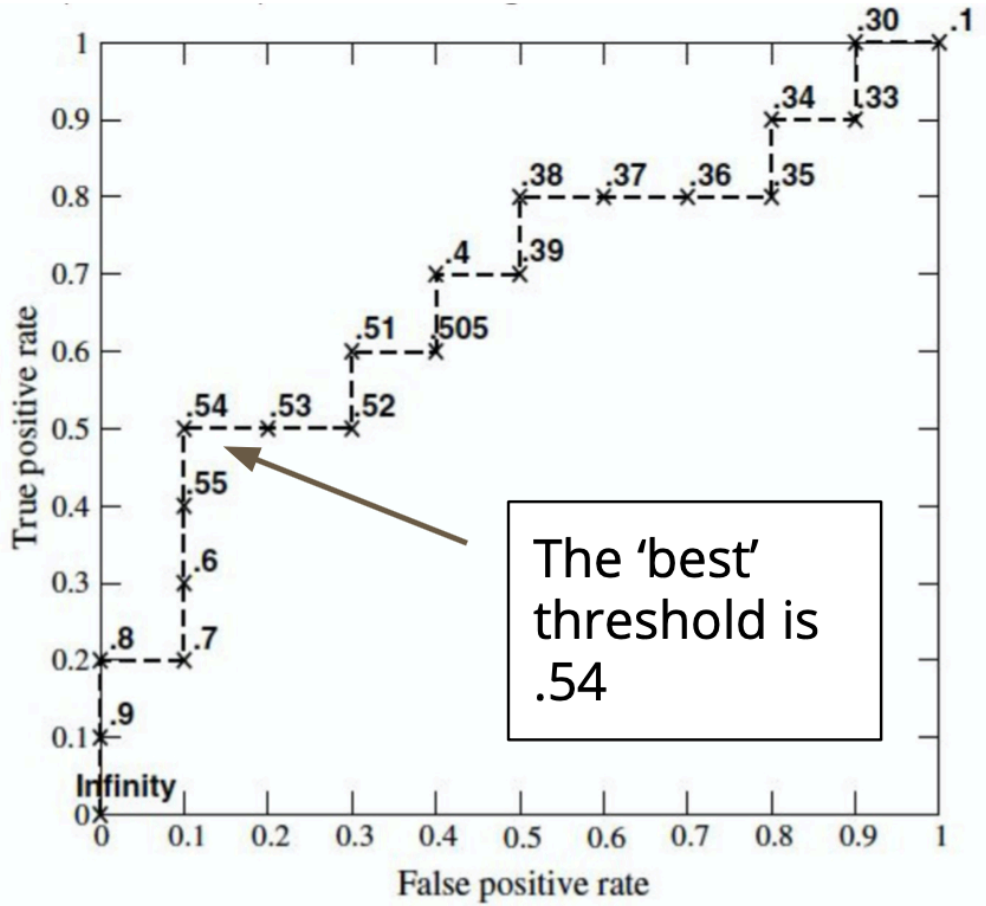
6	p	.54	16	n	.35
7	n	.53	17	p	.34
8	n	.52	18	n	.33
9	p	.51	19	p	.30
10	n	.505	20	n	.1



Source: Fawcett (2005)

Area under the curve

The area under the curve (AUC) is a method for comparing algorithms and evaluating classifiers.

The AUC has an important statistical property:

> *The AUC of a classifier is equivalent to the probability that the classifier will rank a randomly chosen positive instance higher than a randomly chosen negative instance*

Source: Fawcett (2005)

Area under the curve

Care should be taken when using ROC curves to compare classifiers

- The ROC graph is often used to select the best classifiers simply by graphing them in ROC space and seeing which one dominates.
- This is misleading: it is analogous to taking the maximum of a set of accuracy figures from a single test set.
- Without a measure of **variance** we cannot compare classifiers

It is a good idea to the average of multiple ROC curves (e.g. via cross validation)

See Fawcett (2005) for examples on how to average

Source: Fawcett (2005)

ROC vs Precision-Recall (PR) Curves

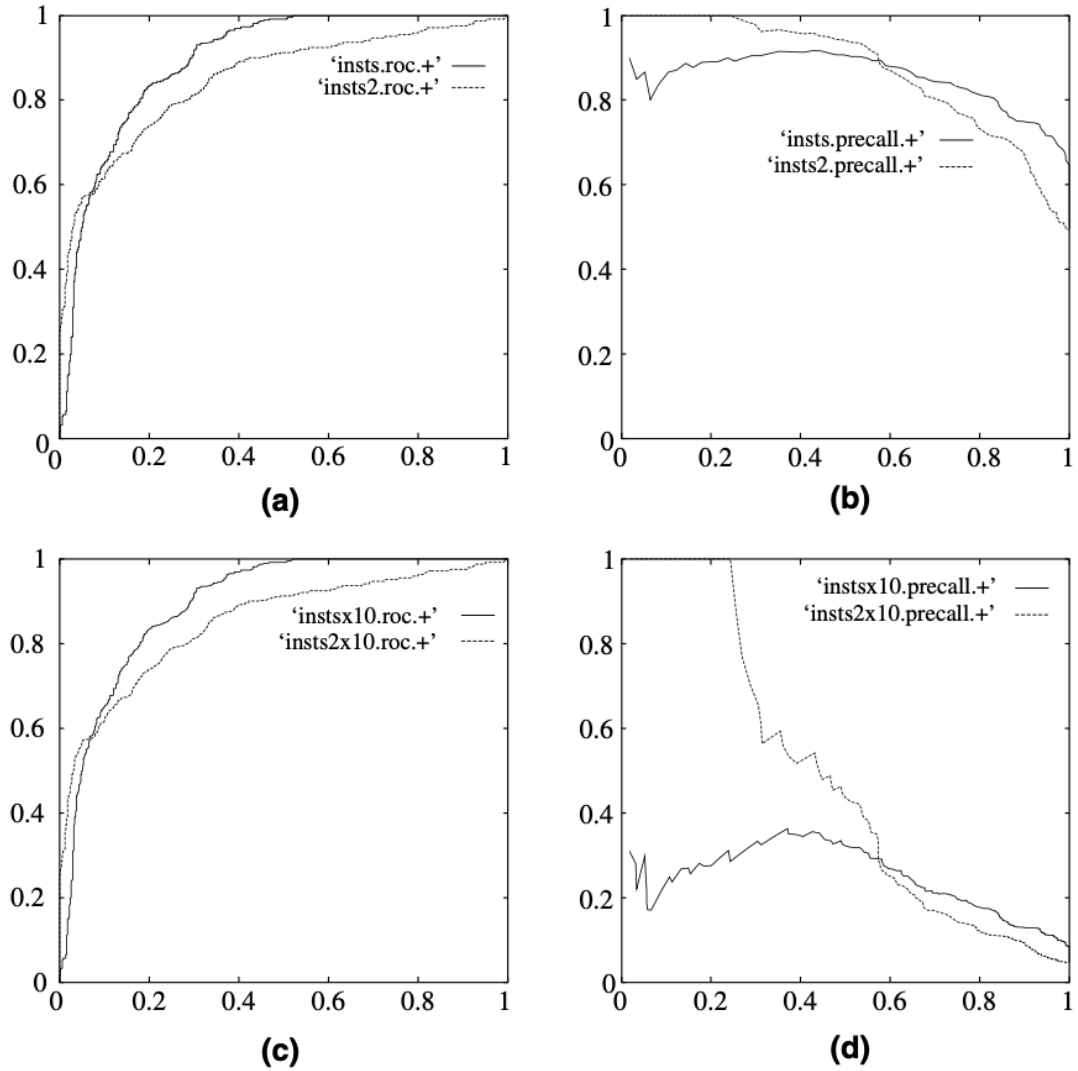


Fig. 5. ROC and precision-recall curves under class skew. (a) ROC curves, 1:1; (b) precision-recall curves, 1:1; (c) ROC curves, 1:10 and (d) precision-recall curves, 1:10.

ROC vs PR Curves

- Generally, precision-recall curves are preferred when there is class imbalance
- ROC curves tend to paint an overly optimistic view of the model on datasets with class imbalance
- PR calculations do not involve the true negatives rate and hence do not typically present such an optimistic view