BIOST 546: Machine Learning for Biomedical Big Data

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Lecture 5: Classification for Biomedical Big Data - Part II
Spring 2017

Recap

- Classification using linear regression
- Fundamentals of classification, Bayes classifier and Bayes error rate
- Logistic regression, and regularization
- Batch effects and pitfalls of classification

Today's Class

- LDA & QDA
- SVM
- KNN

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Here
  - $\pi_h = P(Y = h)$ is the prior probability
  - $f_h(x) = P(X = x \mid Y = h)$ is the density function of X for an observation coming from class h
  - $p_h(x)$ is the posterior density of y given the data x

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- π_h is often easy to estimate: if we have a random sample, $\hat{\pi}_h = 1/n \sum_i I(Y_i = h)$
- However, estimating f_h can be very challenging, especially in high dimensions
- One solution is to assume a parametric form for f_h

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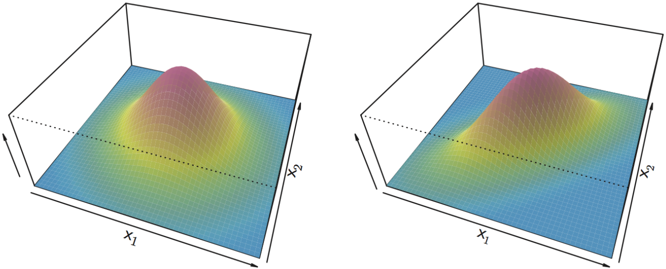

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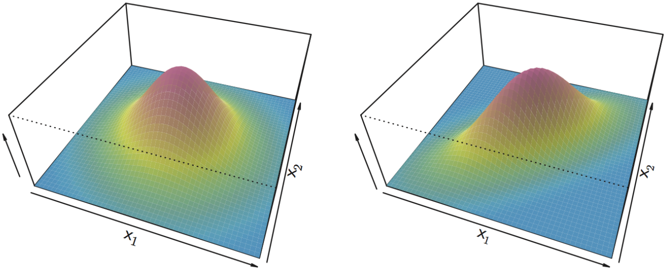

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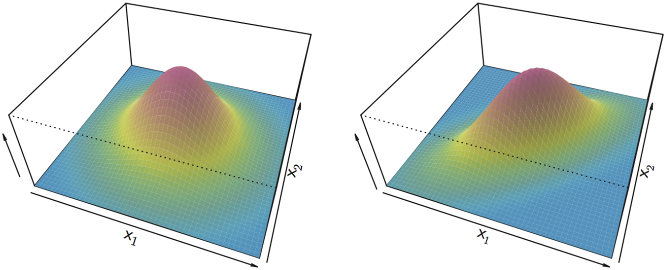

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$$X \sim \sum_{h=1}^{H} \pi_h \phi(\mu_h, \Sigma_h)$$

- LDA was developed by R. A. Fisher, and has some interesting connections to analysis of variance

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- In most cases, it is also assumed that Σ is diagonal: i.e. no correlation among covariates!!
- This latter assumption can be relaxed. However, in high dimensional settings, estimation of Σ is difficult ($\binom{p}{2}$ parameters to estimate!), and there is often not much improvements from this in HD.

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- If we further assume that $H = 2$ and $\pi_1 = \pi_2 = 0.5$, then the Bayes decision boundary is

$$\frac{\mu_1 + \mu_2}{2}$$

which is clearly linear!

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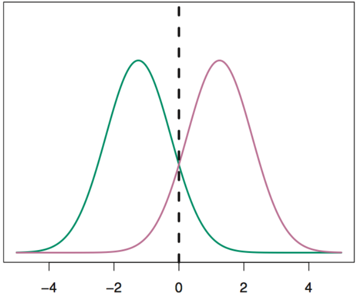

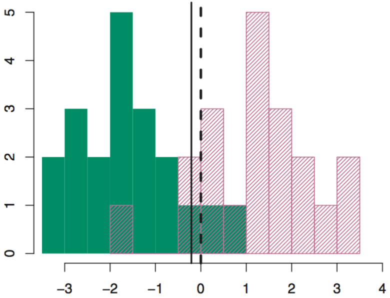

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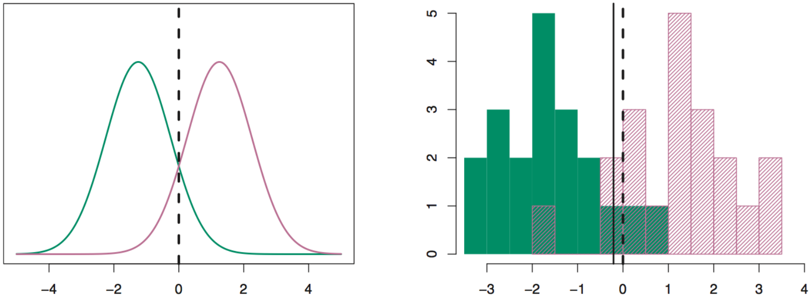

- To make this work, we need to estimate the parameters. The ML estimates are given by $\hat{\pi}_h = n_h/n$ and

$$\hat{\mu}_h = \frac{1}{n_h} \sum_{i:y_i=h} x_i \qquad \hat{\sigma}^2{}_h = \frac{1}{n-H} \sum_{h=1}^{H} \sum_{i:y_i=h} (x_i - \hat{\mu}_h)^2$$

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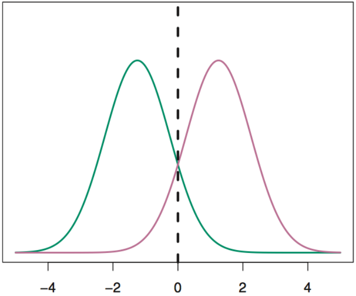

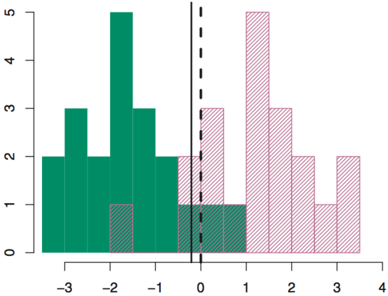

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- The picture is very similar if $H > 2$...or if $p > 1$

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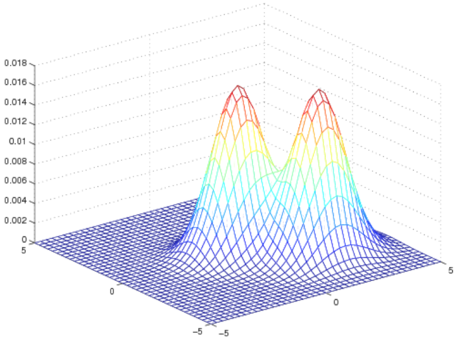

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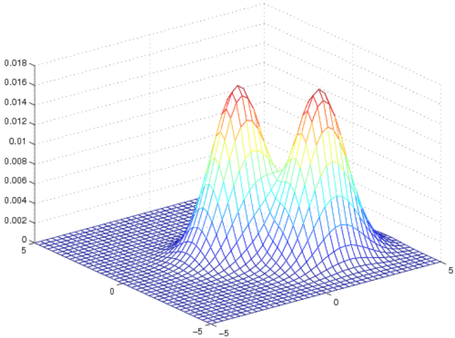

0.018
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5
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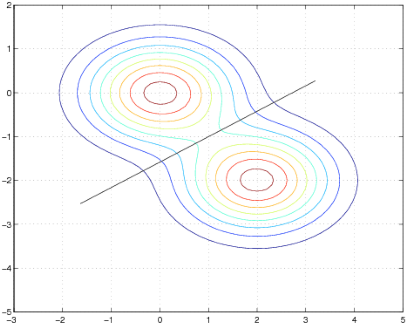
5



2
1
0
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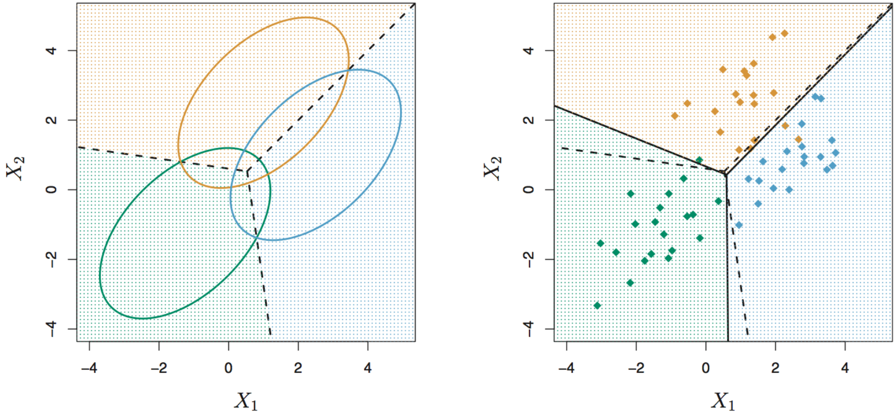

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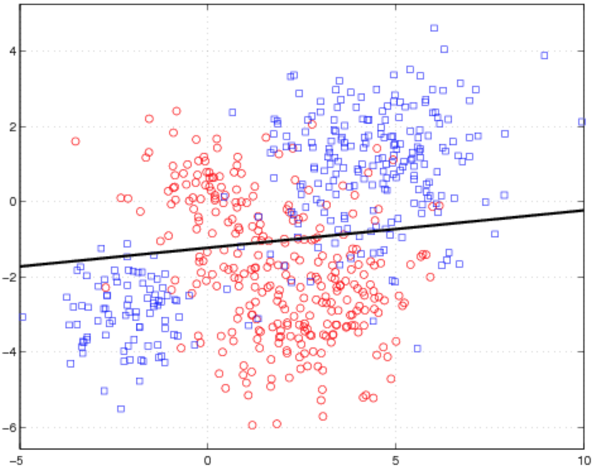

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- Note that we are still assuming that observations are from a mixture of Gaussian distributions
- QDA is much more flexible than LDA, but we need to estimate $Hp(p+1)$ parameters, which is a lot in high dimensions
- To make this a bit simpler, again we often assume that Σ_h is diagonal

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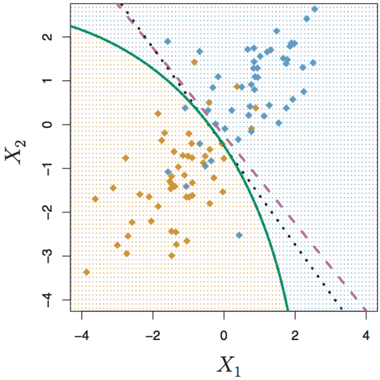

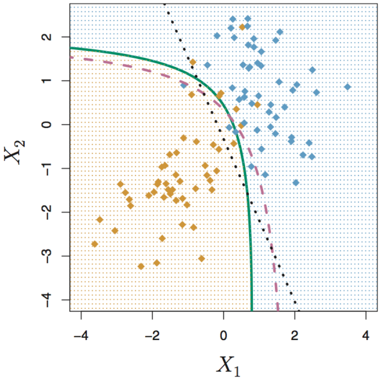

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- The alternative is to avoid making parametric assumptions; and use nonparametric models
- The simplest nonparametric approach for classification (also works for regression) is the K nearest neighbor classification method (KNN)

KNN Basics

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- As the name suggests, the simple idea behind KNN is to use the K nearest neighbor of each observation, based on the values of x, to predict its y value

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- We then apply the Bayes rule to classify x_0 to the class with largest probability

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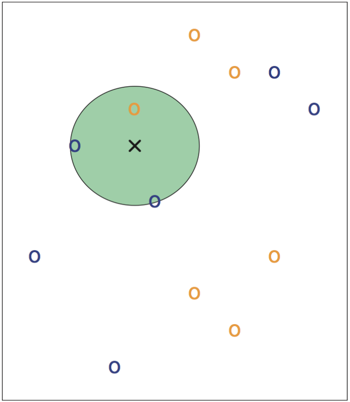

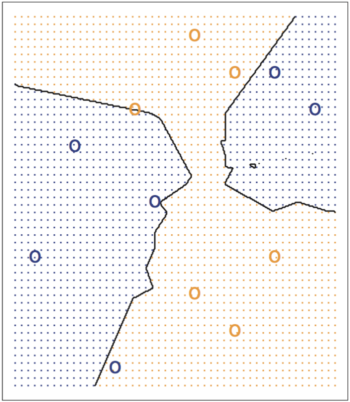

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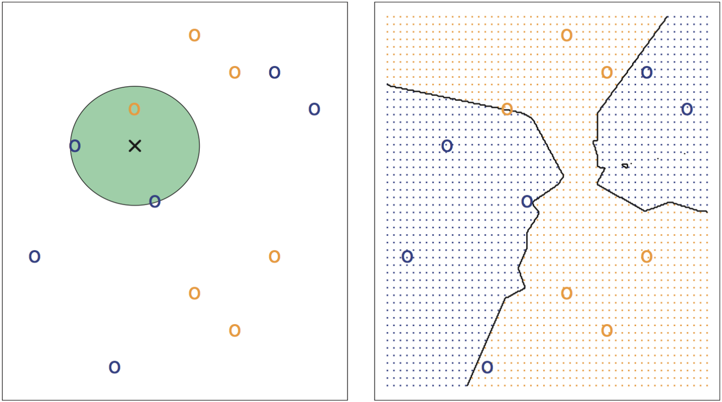

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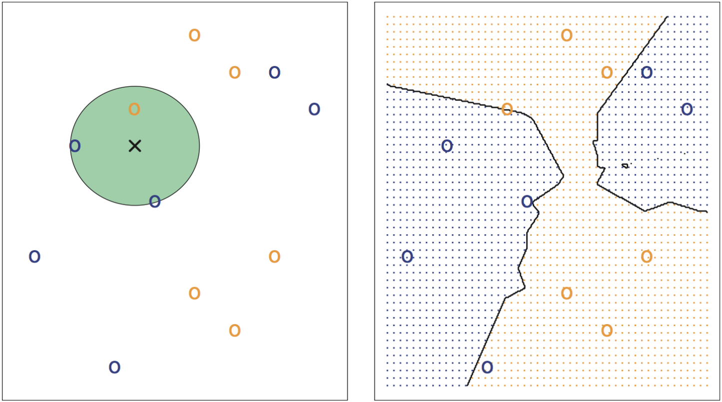

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- Large K: less flexible classifier, and a smoother decision boundary $\Rightarrow$ high bias and low variance

Bias-Variance Tradeoff for KNN

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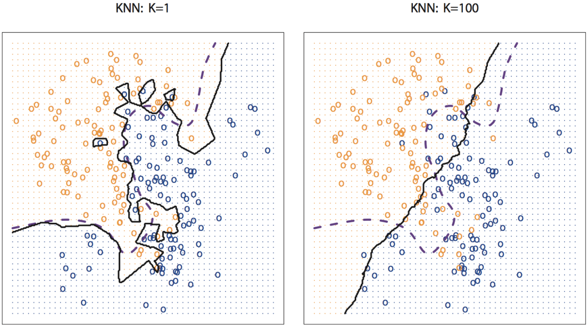

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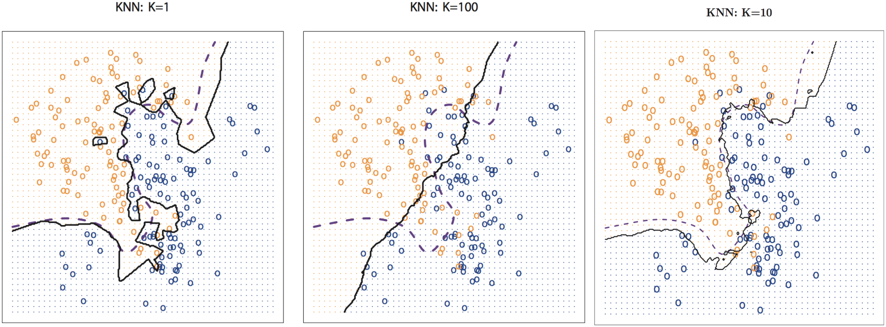

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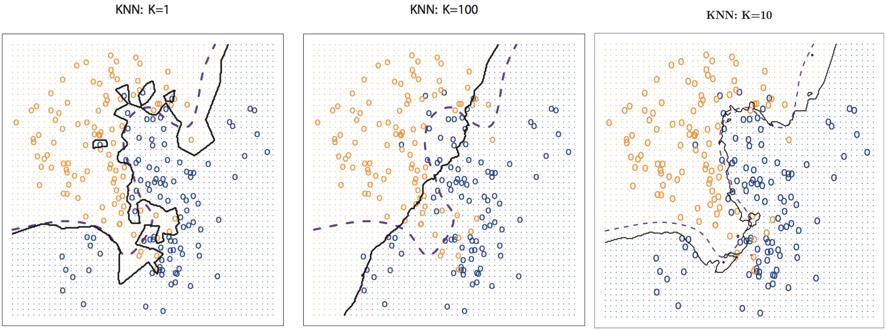

- We again have to face our beloved bias-variance tradeoff, and need to choose K that gives good test error

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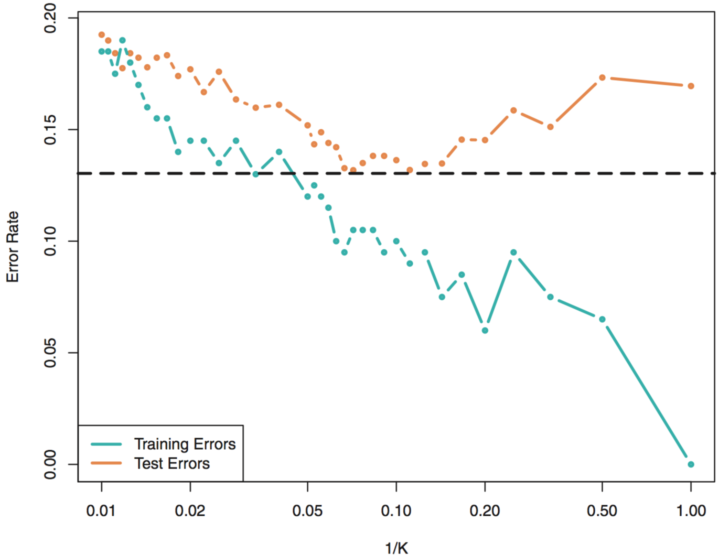

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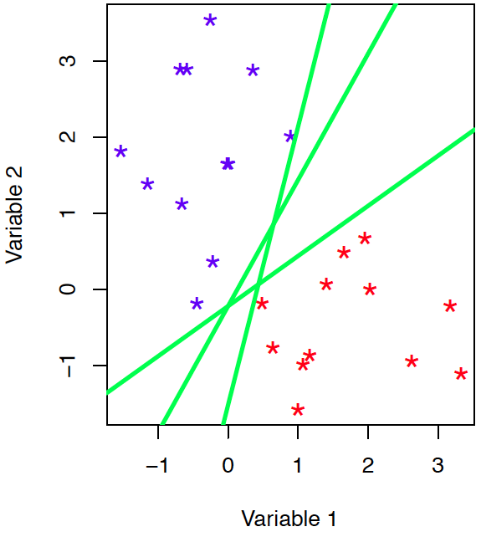
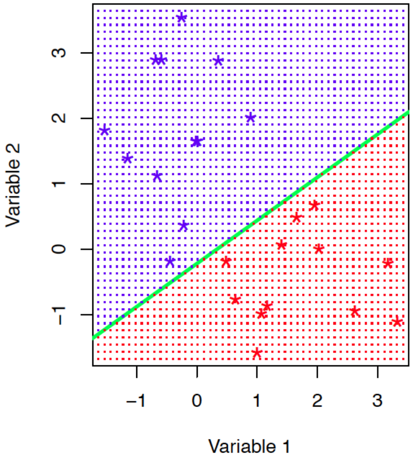
- Fundamentally and numerically very similar to logistic regression (more later).
- However, has a very different motivation and is a very nice idea.

Separating Hyperplane



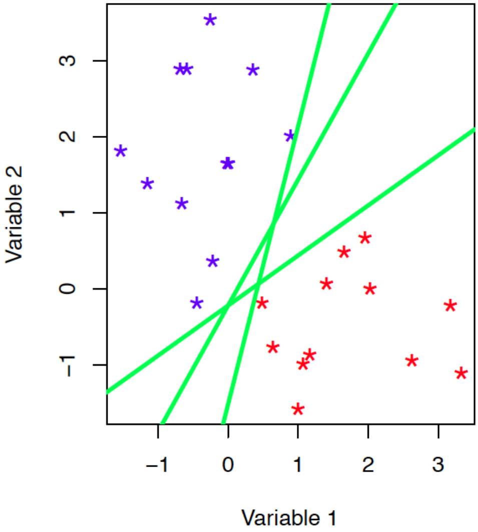
Classification via Separating Hyperplanes



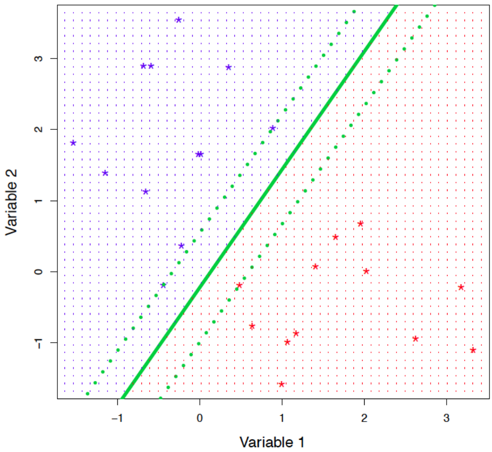
Blue class if $\beta_0 + \beta_1 X_1 + \beta_2 X_2 > c$; red class otherwise.

Which hyperplane?

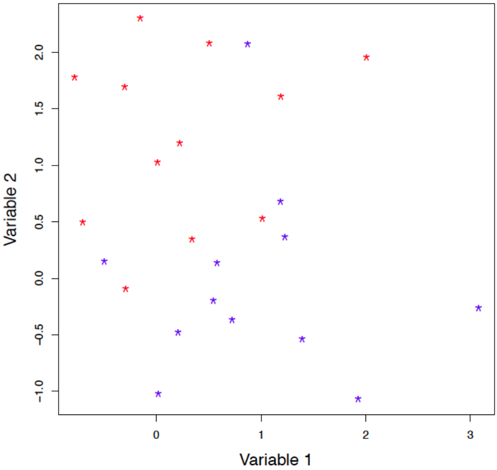
There are potentially many hyperplanes...



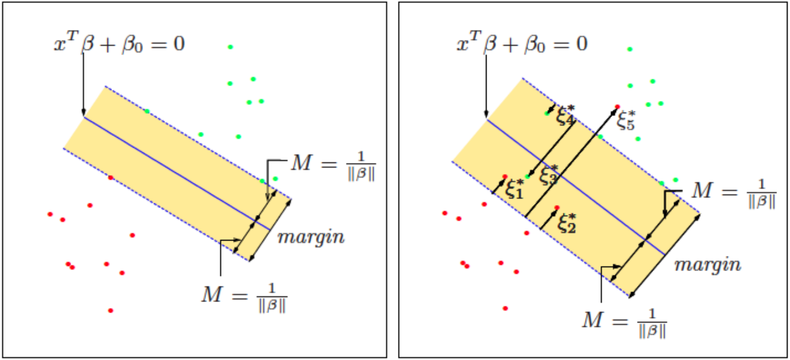
Maximally Separating Hyperplane



What if There is No Separating Hyperplane?



Support Vector Classifier: Allow for Violations



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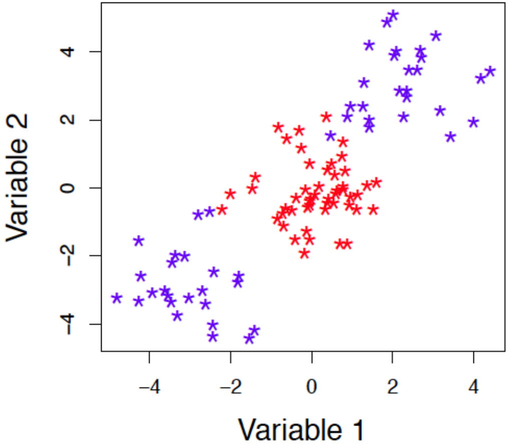
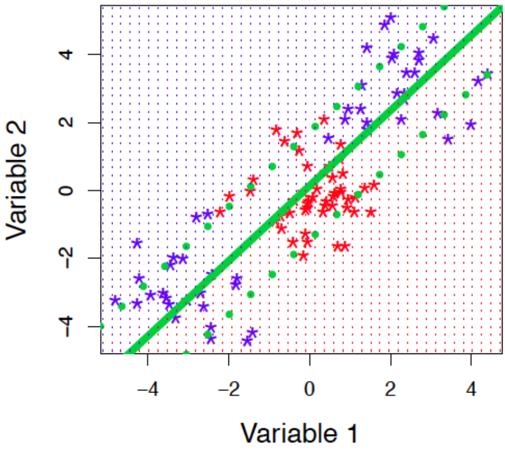
- However, linear regression, logistic regression, and other classical statistical approaches can also be applied to non-linear functions of the variables.
- For historical reasons, SVMs are more frequently used with non-linear expansions as compared to other statistical approaches.

Non-Linear Class Structure



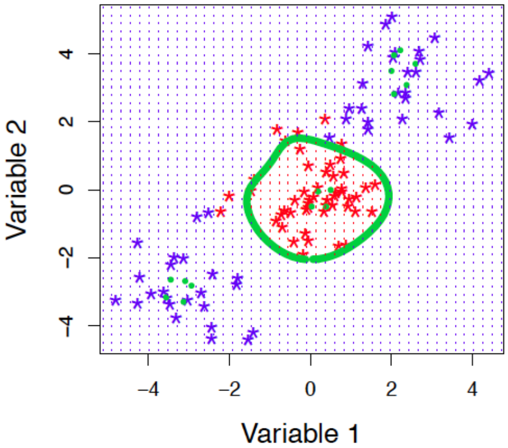
This will be hard for a linear classifier!

Try a Support Vector Classifier



Uh-oh!!

Support Vector Machine



Much Better.

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- Yes, if the true decision boundary between the classes is non-linear, and you have enough observations (relative to the number of features) to accurately estimate the decision boundary.
- No, if you are in a very high-dimensional setting such that estimating a non-linear decision boundary is hopeless.

SVM vs Other Classification Methods

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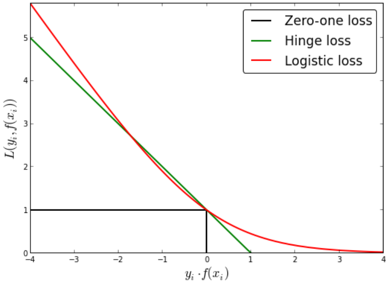

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- One of the disadvantages of SVM (compared to some of the other methods) is that it does not provide a measure of uncertainty: cases are "classified" to belong to one of the two classes.
- Both SVM and logistic regression are not well-suited for problems with $H > 2$ categories; LDA/QDA may be a better choice in that setting.

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- Can get a sparse SVM using a lasso penalty; this yields a decision rule involving only a subset of the features.
- Logistic regression and other classical statistical approaches could be used with non-linear expansions of features. But this makes high-dimensionality issues worse.

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- The misclassification error, which is what is used in Bayes classifier, is one way to combine FP and FN

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- We can obtain different classifiers by changing the "cutoff"...the ROC plot measures the performance of classifiers

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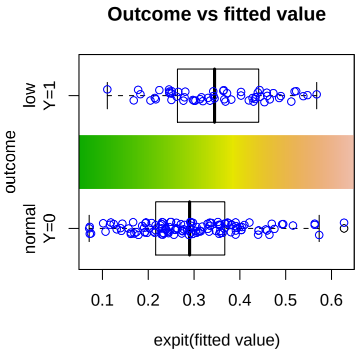

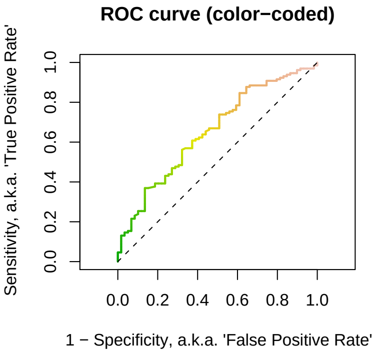

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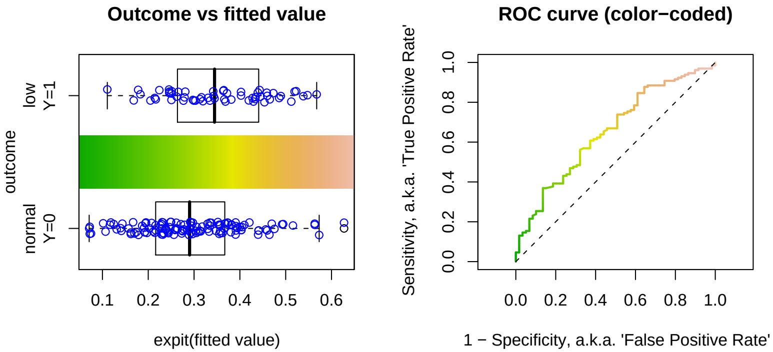

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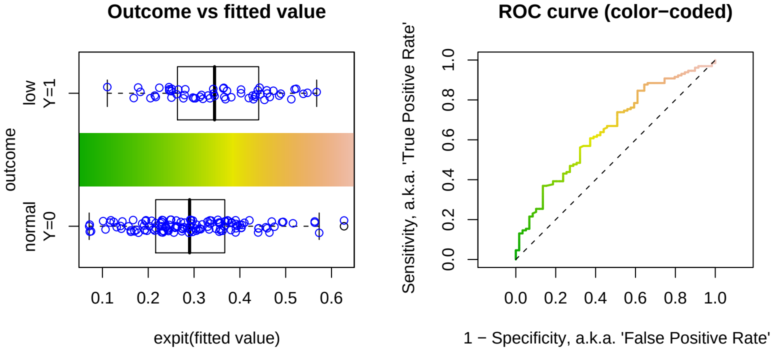

- Each point on the ROC curve corresponds to a single decision (i.e. cutoff)
- The area under the ROC curve (AUC) measures the overall performance of a classifier (over the range of cutoffs)

Next Lecture

- Tree-based methods