Linear Methods for Classification

Based on Chapter 4 of Hastie, Tibshirani, and Friedman

Predictive Modeling

Goal: learn a mapping: $y = f(\mathbf{x};\theta)$

Need: 1. A model structure

2. A score function

3. An optimization strategy

Categorical $y \in \{c_1,\ldots,c_m\}$: classification

Real-valued y: regression

Note: usually assume $\{c_1,\ldots,c_m\}$ are mutually exclusive and exhaustive

Probabilistic Classification

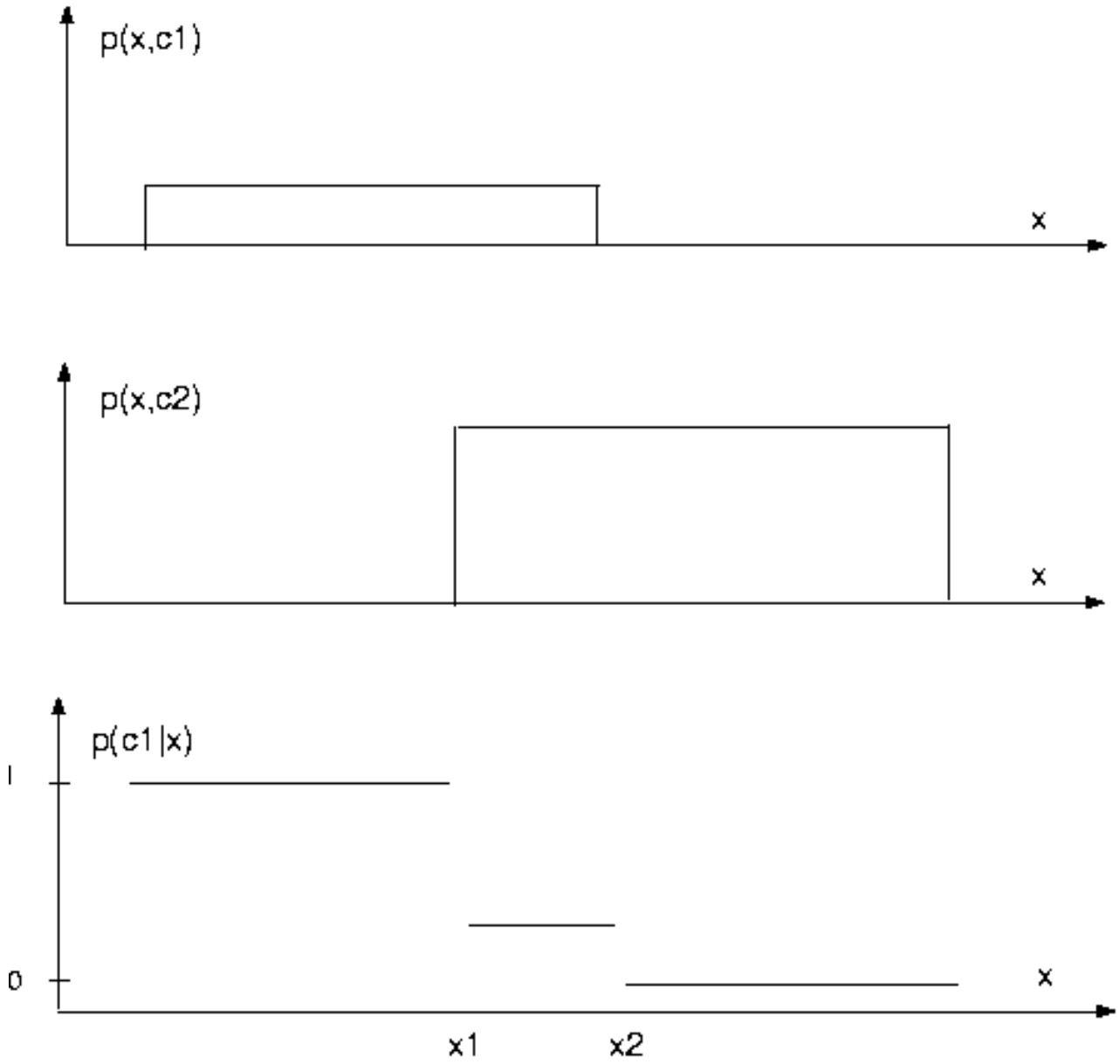
Let $p(c_k)$ = prob. that a randomly chosen object comes from c_k

Objects from c_k have: $p(\boldsymbol{x} \mid c_k, \boldsymbol{\theta}_k)$ (e.g., MVN)

Then: $p(c_k \mid \boldsymbol{x}) \propto p(\boldsymbol{x} \mid c_k, \boldsymbol{\theta}_k)\, p(c_k)$

Bayes Error Rate: $$p_B^* = \int (1 - \max_k p(c_k \mid x))\, p(x) dx$$

- Lower bound on the best possible error rate



Bayes error rate about 6%

Classifier Types

Discriminative: model $p(c_k \mid \boldsymbol{x})$

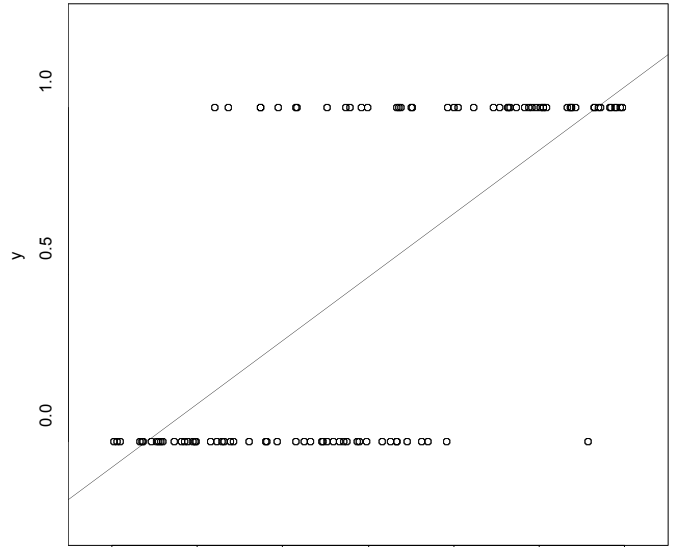
- e.g. logistic regression, CART

Generative: model $p(\boldsymbol{x} \mid c_k, \boldsymbol{\theta}_k)$

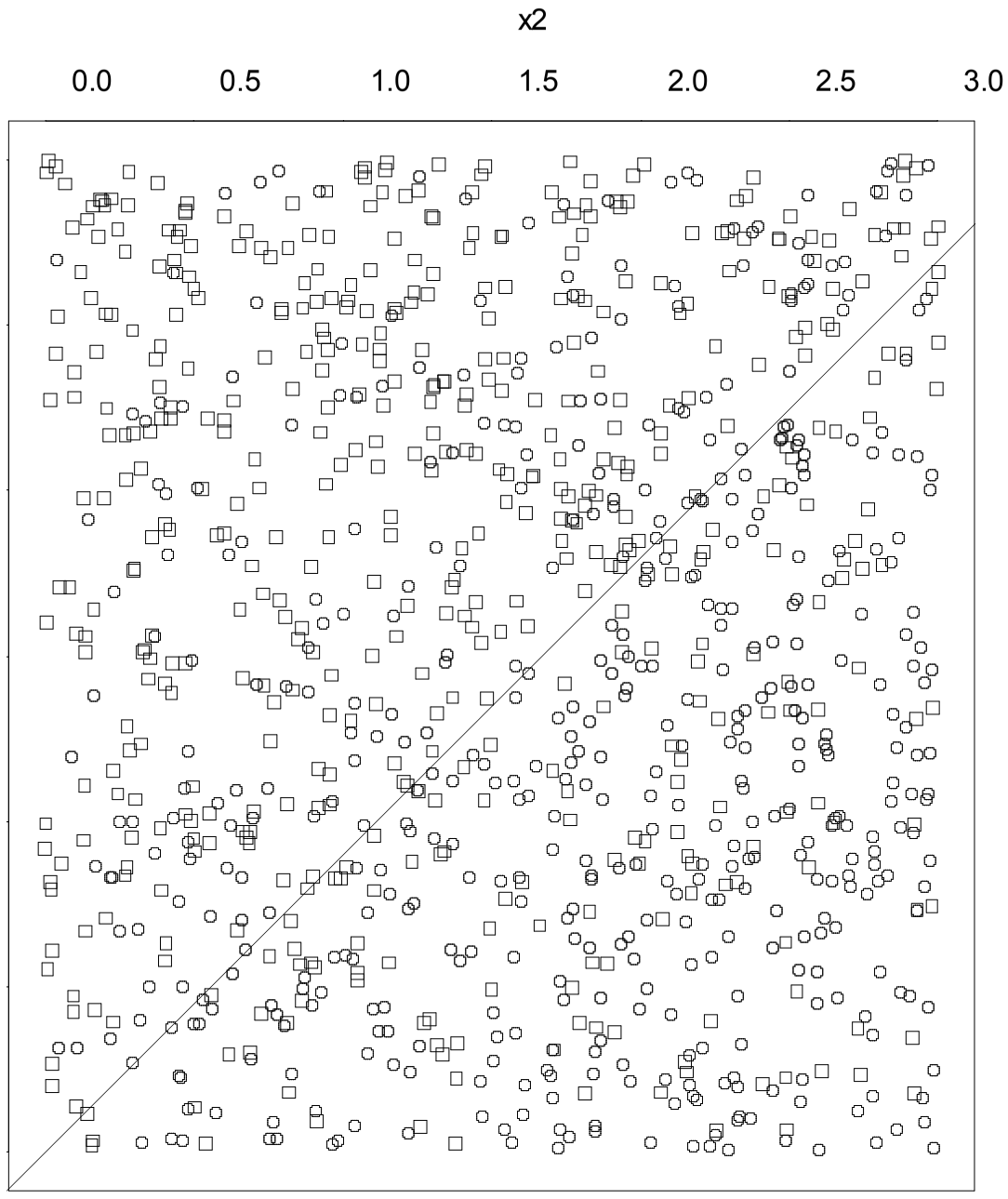
- e.g. "Bayesian classifiers", LDA

Regression for Binary Classification

- Can fit a linear regression model to a 0/1 response
- Predicted values are not necessarily between zero and one
- With p>1, the decision boundary is linear
  e.g. $0.5 = b0 + b1\ x1 + b2\ x2$



zeroOneR.txt


x2
0.0
0.5
1.0
1.5
2.0
2.5
3.0

Linear Discriminant Analysis

K classes, X $n \times p$ data matrix.

$$p(c_k \mid x) \propto p(x \mid c_k, \theta_k)\, p(c_k)$$

Could model each class density as multivariate normal:

$$p(x \mid c_k) = \frac{1}{(2\pi)^{p/2} \mid \Sigma_k \mid^{1/2}} e^{-\frac{1}{2}(x-\mu_k)^T \Sigma_k^{-1} (x-\mu_k)}$$

LDA assumes $\Sigma_k \equiv \Sigma$ for all k. Then:

$$\log \frac{p(c_k \mid x)}{p(c_l \mid x)} = \log \frac{p(c_k)}{p(c_l)} - \frac{1}{2}(\mu_k + \mu_l)^T \Sigma^{-1} (\mu_k - \mu_l) + x^T \Sigma^{-1} (\mu_k - \mu_l)$$

This is linear in x.

Linear Discriminant Analysis (cont.)

It follows that the classifier should predict: $\arg\max_k \delta_k(x)$

$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k{}^T \Sigma^{-1} \mu_k + \log p(c_k)$$

"linear discriminant function"

If we don't assume the Σ_k's are identicial, get Quadratic DA:

$$\delta_k(x) = -\frac{1}{2} \log |\Sigma_k| - \frac{1}{2} (x - \mu_k)^T \Sigma_k^{-1} (x - \mu_k) + \log p(c_k)$$

Linear Discriminant Analysis (cont.)

Can estimate the LDA parameters via maximum likelihood:

$$\hat{p}(c_k) = N_k / N$$

$$\hat{\mu}_k = \sum_{i \in k} x_i / N_k$$

$$\hat{\Sigma} = \sum_{k=1}^{K} \sum_{i \in k} (x_i - \mu_k)(x_i - \mu_k)' \ /(N - K)$$

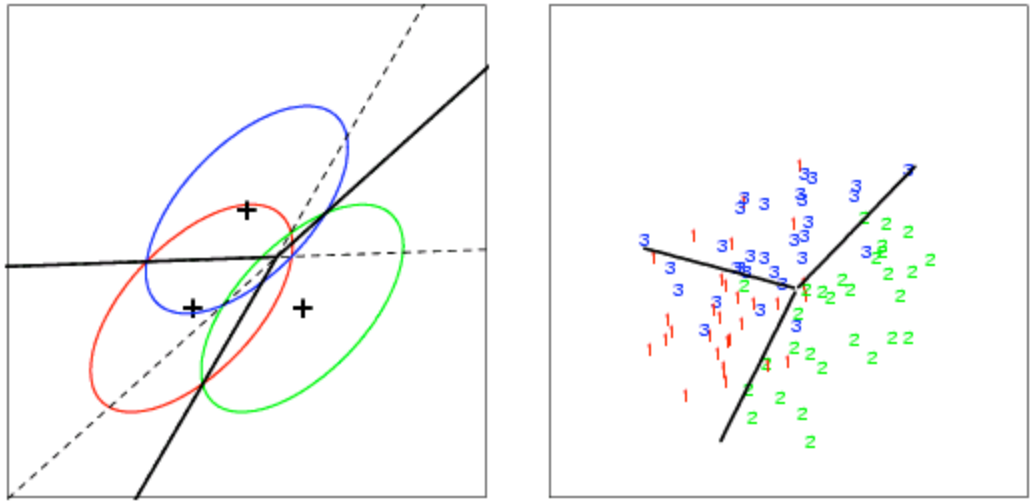
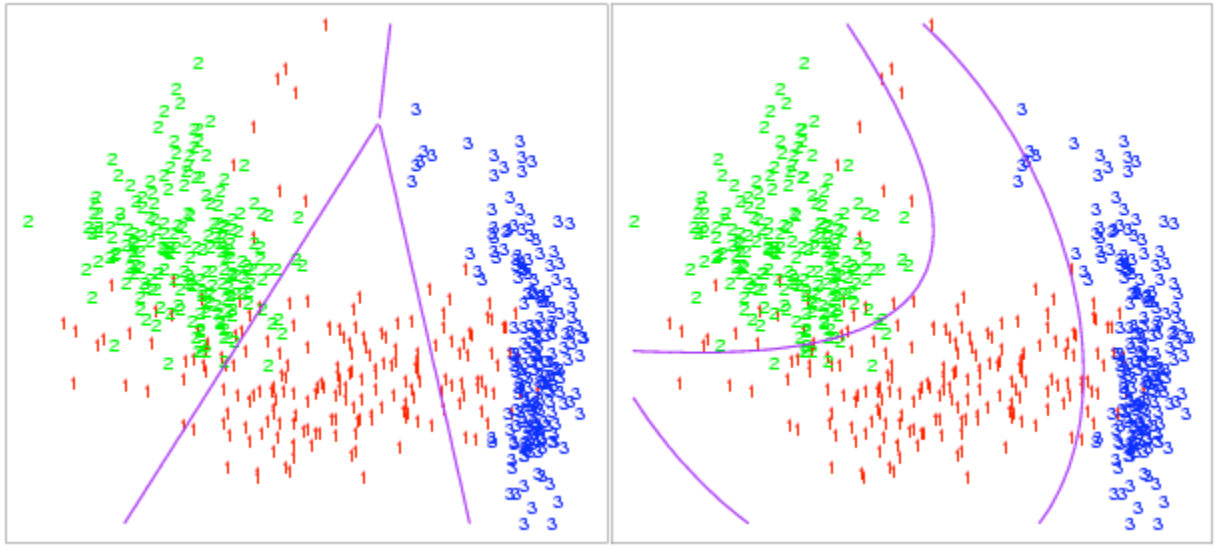


Figure 4.5: *The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density enclosing 95% of the probability in each case. The Bayes decision boundaries between each pair of classes are shown (broken straight lines), and the Bayes decision boundaries separating all three classes are the thicker solid lines (a subset of the former). On the right we see a sample of* 30 *drawn from each Gaussian distribution, and the fitted LDA decision boundaries.*



LDA QDA

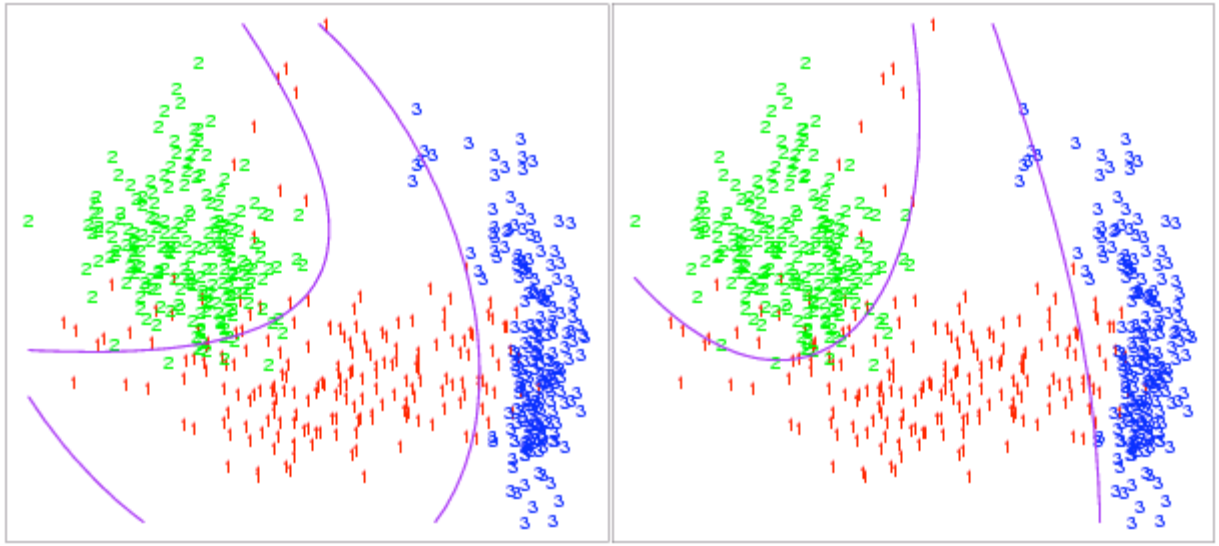


Figure 4.6: *Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space* $x_1, x_2, x_{12}, x_1^2, x_2^2$*). The right plot shows the quadratic decision boundaries found by QDA. The differences are small, as is usually the case.*

LDA (cont.)

- Fisher is optimal if the class are MVN with a common covariance matrix
- Computational complexity $O(mp^2n)$

Logistic Regression

Note that LDA is linear in x:

$$\log \frac{p(c_k \mid x)}{p(c_0 \mid x)} = \log \frac{p(c_k)}{p(c_0)} - \frac{1}{2}(\mu_k + \mu_0)^T \Sigma^{-1}(\mu_k - \mu_0) + x^T \Sigma^{-1}(\mu_k - \mu_0)$$

$$= \alpha_{k0} + \alpha_k^T x$$

Linear logistic regression looks the same:

$$\log \frac{p(c_k \mid x)}{p(c_0 \mid x)} = \beta_{k0} + \beta_k^T x$$

But the estimation procedure for the co-efficients is different. LDA maximizes joint likelihood [y,X]; logistic regression maximizes conditional likelihood [y | X]. Usually similar predictions.

Logistic Regression MLE

For the two-class case, the likelihood is:

$$l(\beta) = \sum_{i=1}^{n} \{ y_i \log p(x_i;\beta) + (1-y_i)\log(1-p(x_i;\beta)) \}$$

$$\log\left(\frac{p(x;\beta)}{1-p(x;\beta)}\right) = \beta^T x \qquad \log p(x;\beta) = \beta^T x - \log(1+\exp(\beta^T x))$$

$$\Rightarrow l(\beta) = \sum_{i=1}^{n} \{ y_i \beta^T x + \log(1+\exp(\beta^T x)) \}$$

The maximize need to solve (non-linear) score equations:

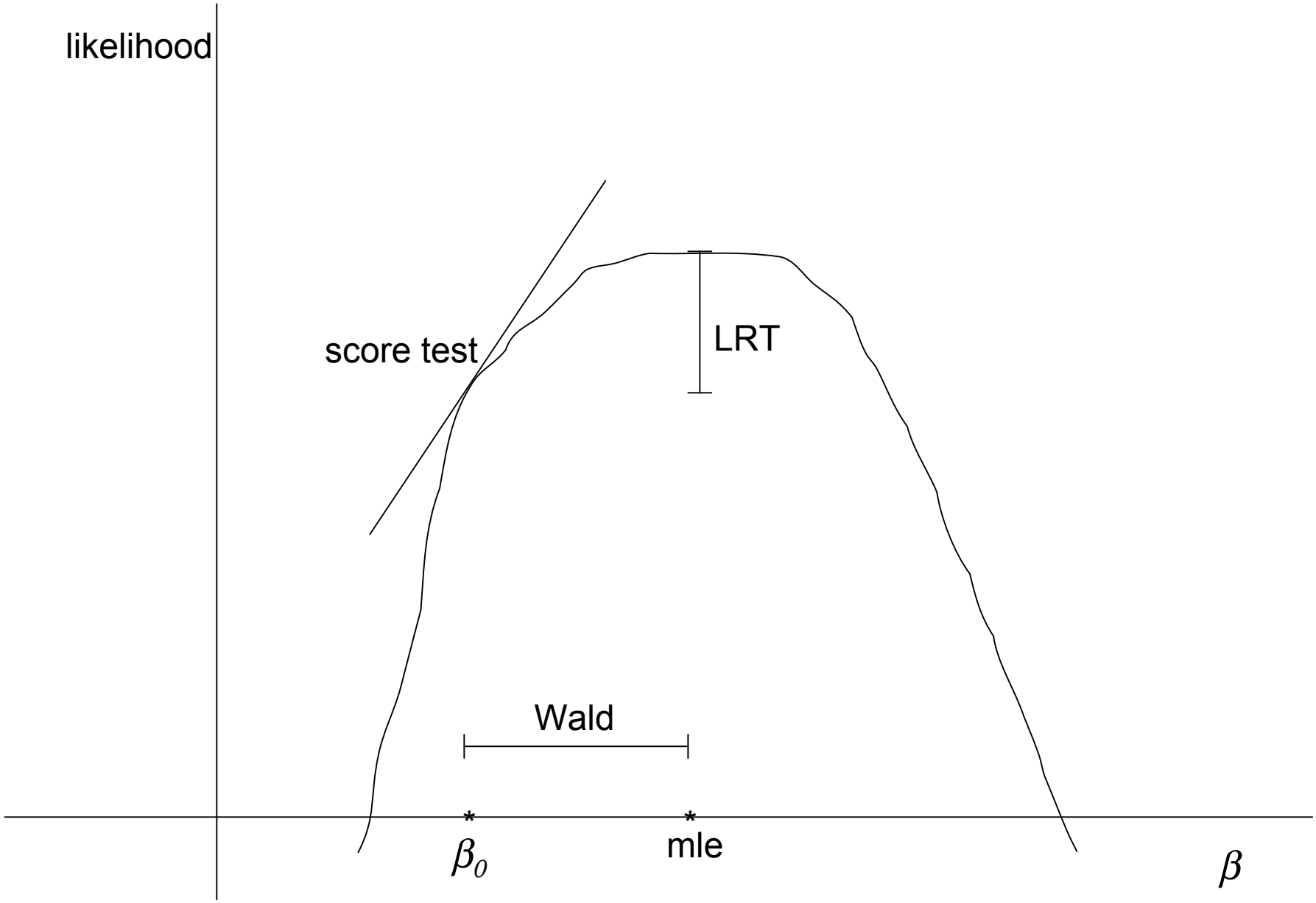
$$\frac{dl(\beta)}{d\beta} = \sum_{i=1}^{n} x_i (y_i - p(x_i;\beta)) = 0$$

Logistic Regression Modeling

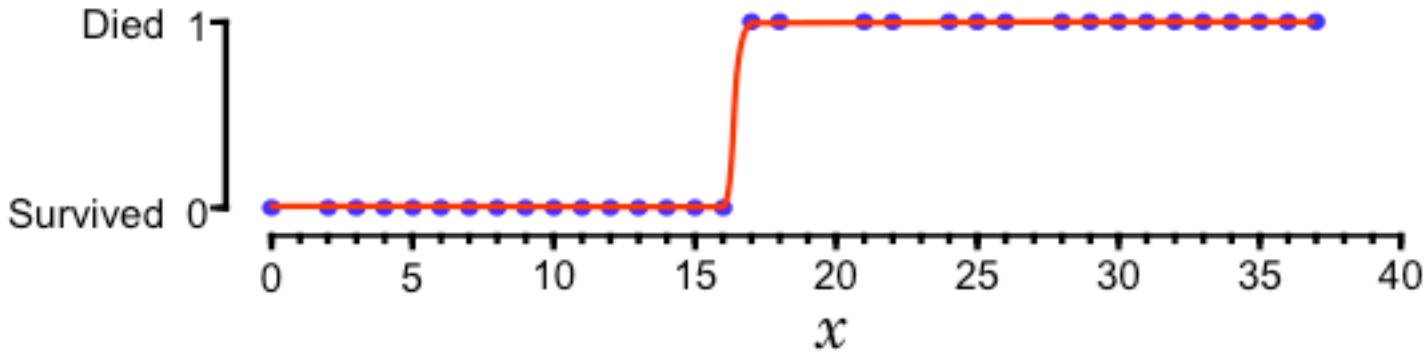
South African Heart Disease Example (y=MI)

	Coef.	S.E.	Z score
Intercept	-4.130	0.964	-4.285
sbp	0.006	0.006	1.023
Tobacco	0.080	0.026	3.034
ldl	0.185	0.057	3.219
Famhist	0.939	0.225	4.178
Obesity	-0.035	0.029	-1.187
Alcohol	0.001	0.004	0.136
Age	0.043	0.010	4.184

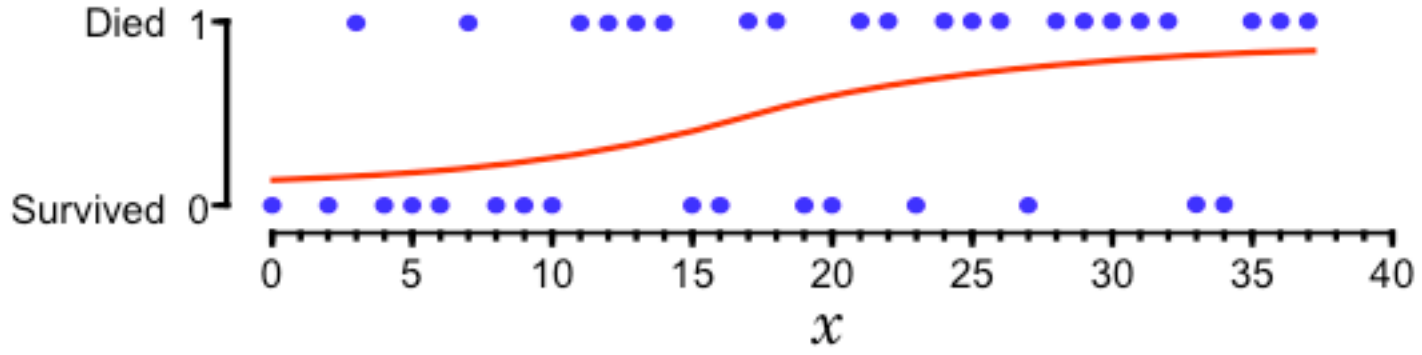
Wald


likelihood
score test
LRT
Wald
β_0
mle
β

Data that has a sharp survival cut off point between patients who live or die should have a large value of β.



Data with a lengthy transition from survival to death should have a low value of β.



Regularized Logistic Regression

- Ridge/LASSO logistic regression

$$\hat{w} = \arg\inf_{w} \frac{1}{n} \sum_{i=1}^{n} \ln(1 + \exp(-w^T x_i y_i)) + \lambda w^2$$

$$\hat{w} = \arg\inf \frac{1}{n} \sum_{i=1}^{N} \log(1 + \exp(-w^T x_i y_i)) + \lambda \sum_j |w_j|$$

- Successful implementation with over 100,000 predictor variables
- Can also regularize discriminant analysis

Simple Two-Class Perceptron

Define: $h(x) = \sum w_j x_j,\ 1 \le j \le p$

Classify as class 1 if $h(x)>0$, class 2 otherwise

Score function: # misclassification errors on training data

For training, replace class 2 x_j's by $-x_j$; now need $h(x)>0$

Initialize weight vector

Repeat one or more times:

For each training data point $\boldsymbol{x}_i$

If point correctly classified, do nothing

Else $w \leftarrow w + \lambda x_i$

Guaranteed to converge to a separating hyperplane (if exists)

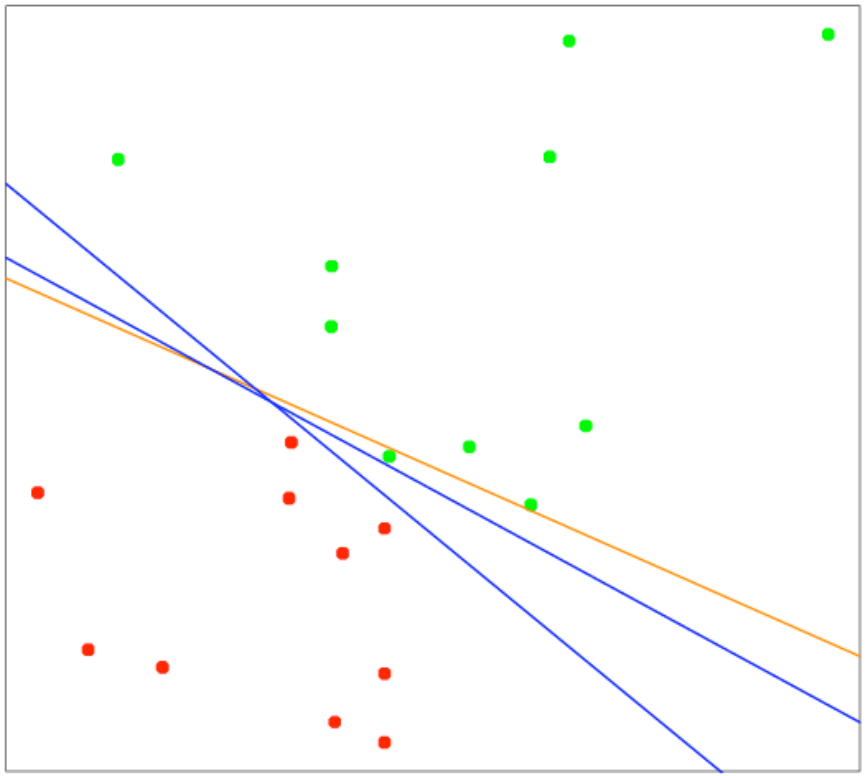


Figure 4.13: *A toy example with two classes separable by a hyperplane. The orange line is the least squares solution, which misclassifies one of the training points. Also shown are two blue separating hyperplanes found by the* perceptron learning algorithm *with different random starts.*

“Optimal” Hyperplane

The “optimal” hyperplane separates the two classes and maximizes the distance to the closest point from either class.

Finding this hyperplane is a convex optimization problem.

This notion plays an important role in support vector machines

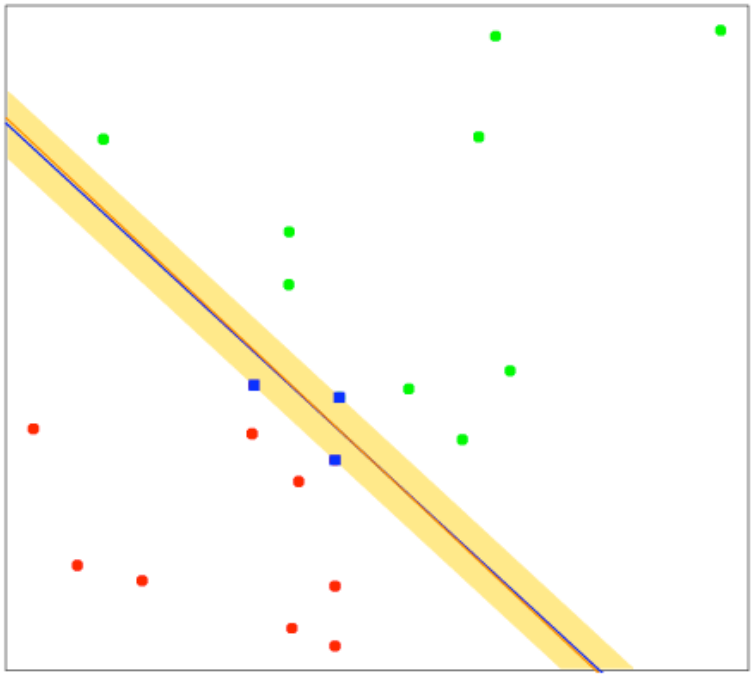
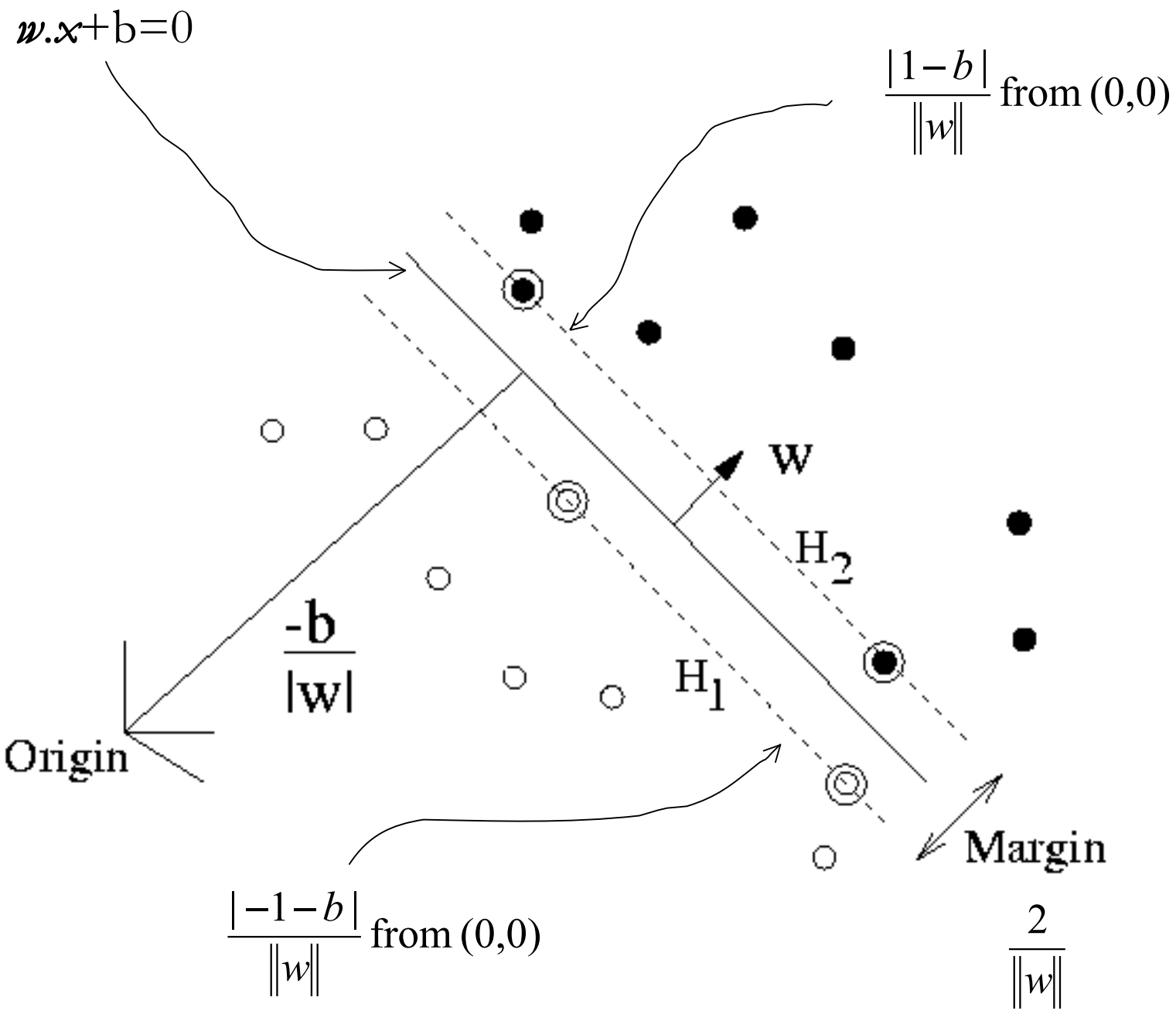
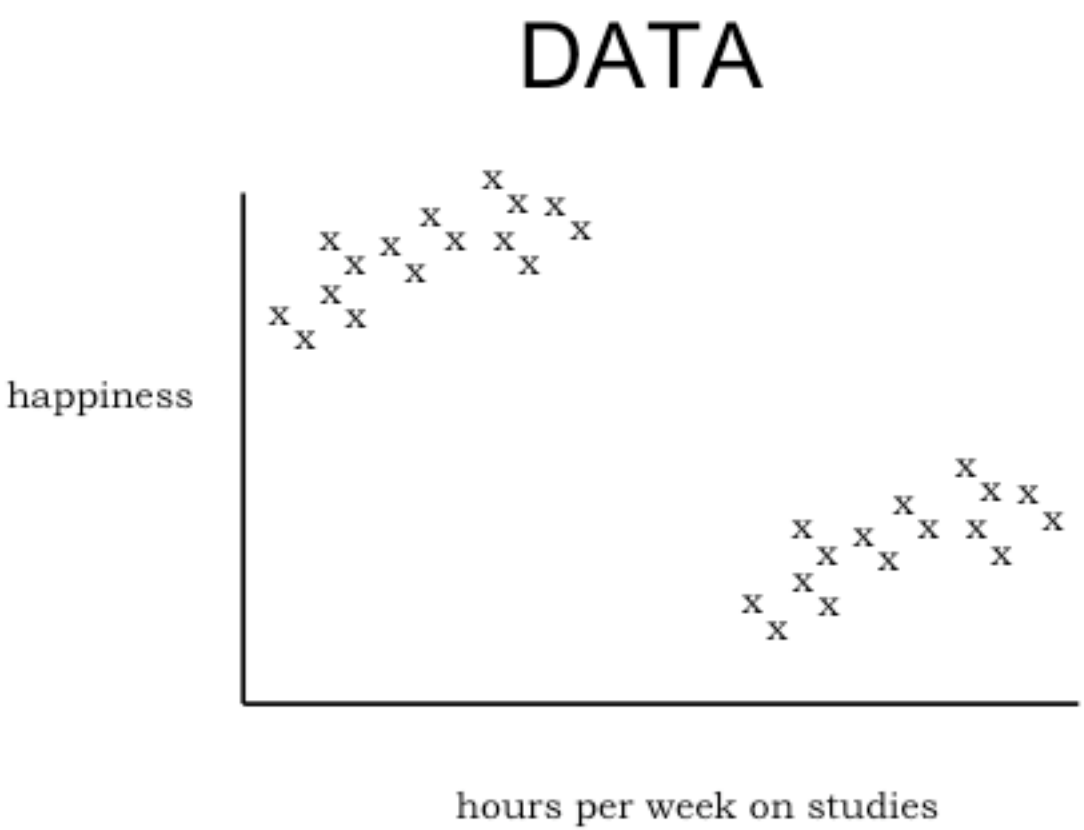


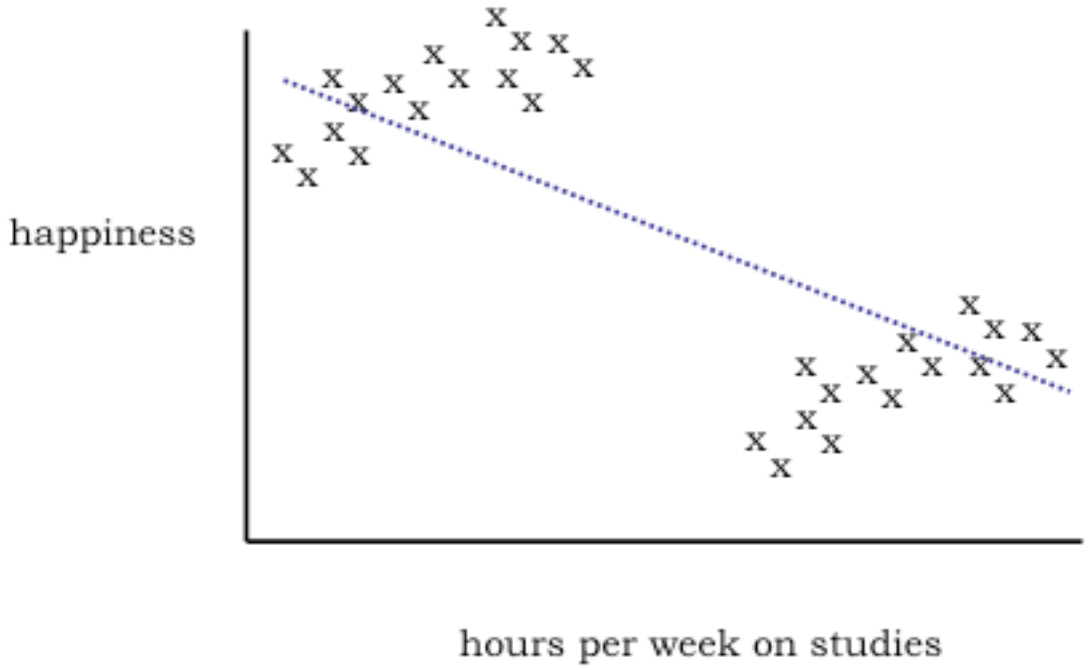
Figure 4.15: *The same data as in Figure 4.13. The shaded region delineates the maximum margin separating the two classes. There are three support points indicated, which lie on the boundary of the margin, and the optimal separating hyperplane (blue line) bisects the slab. Included in the figure is the boundary found using logistic regression (red line), which is very close to the optimal separating hyperplane (see Section 12.3.3).*


w.x+b=0
$\frac{|1-b|}{\|w\|}$ from (0,0)
w
H_2
H_1
$\frac{-b}{|w|}$
Origin
Margin
$\frac{|-1-b|}{\|w\|}$ from (0,0)
$\frac{2}{\|w\|}$

Bad Things Can Happen…

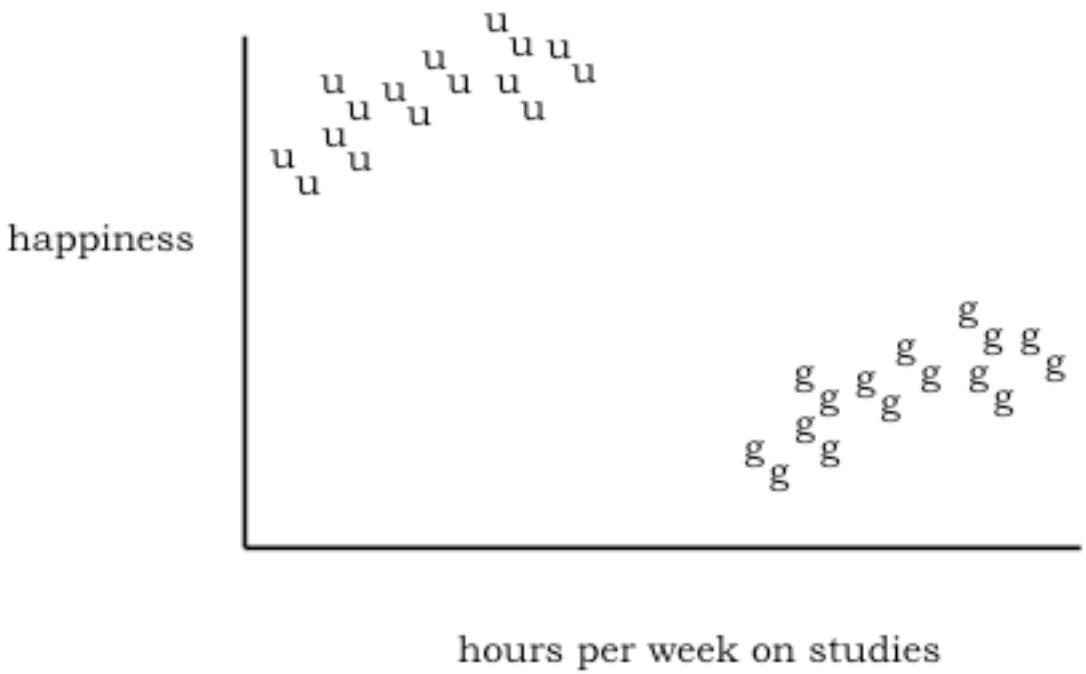


simple regression line

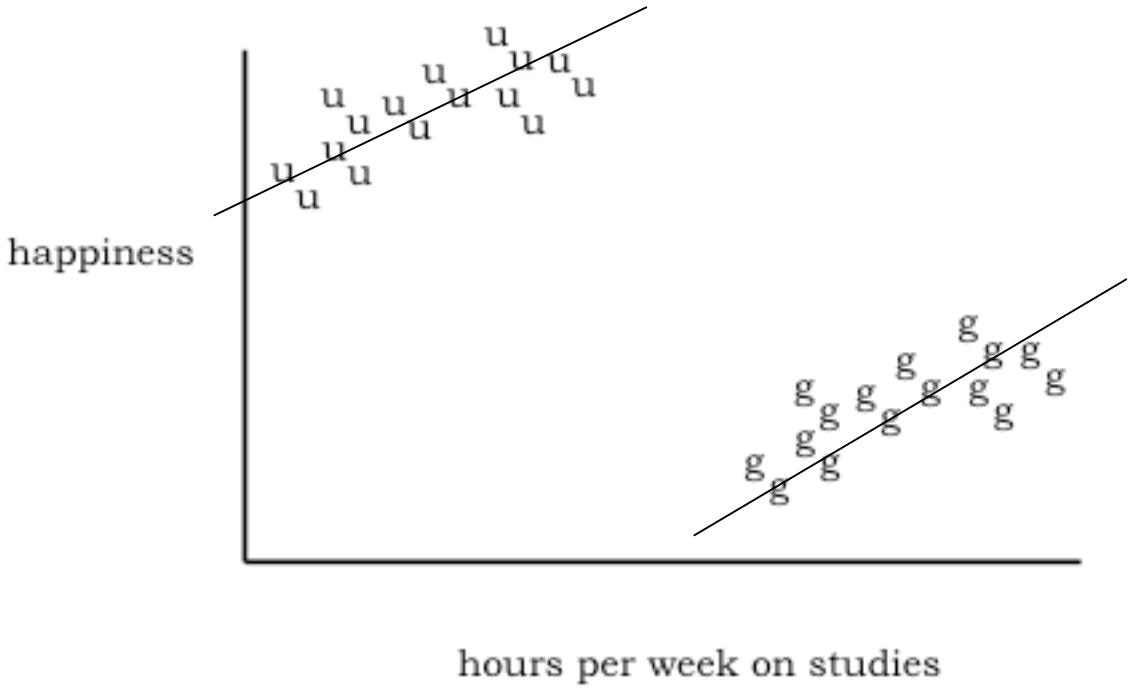


HAP = β_0 + β_1 x HOURS, β_1 will be estimated to be negative

A 2nd Look at the DATA

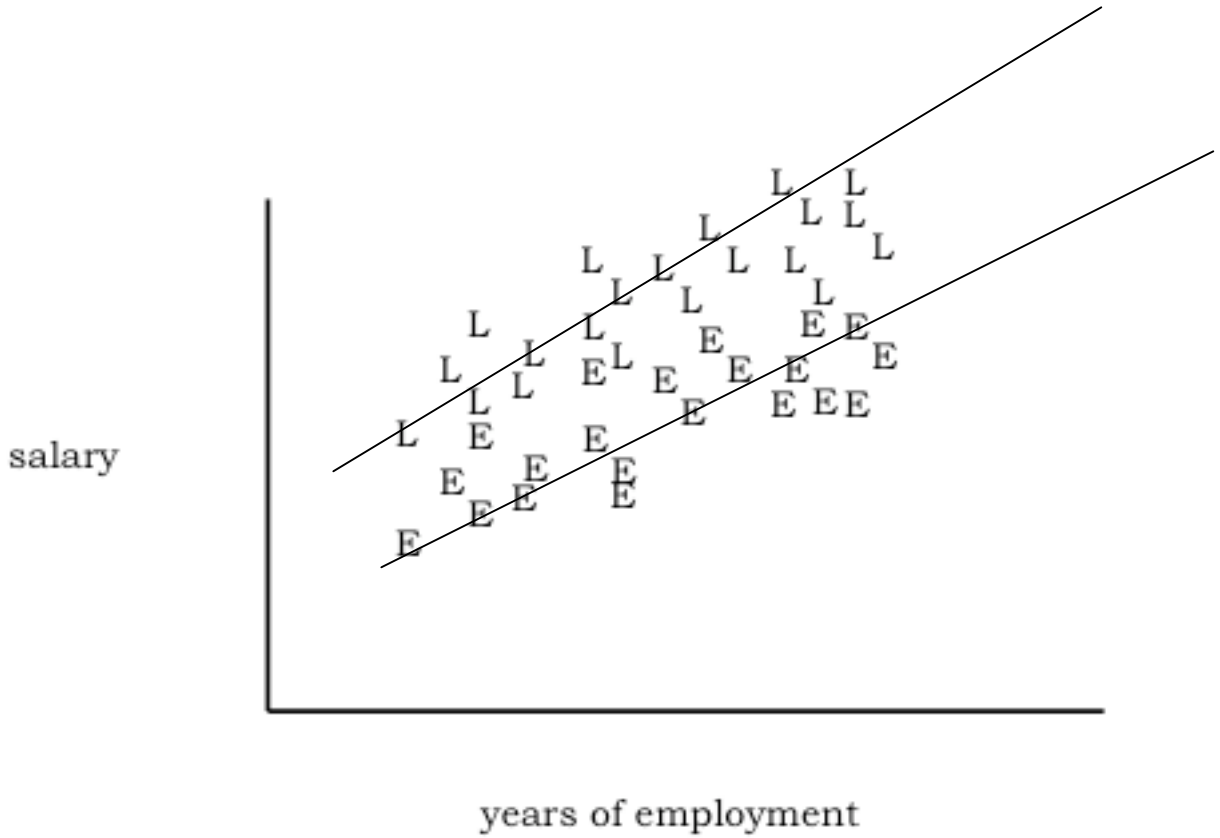


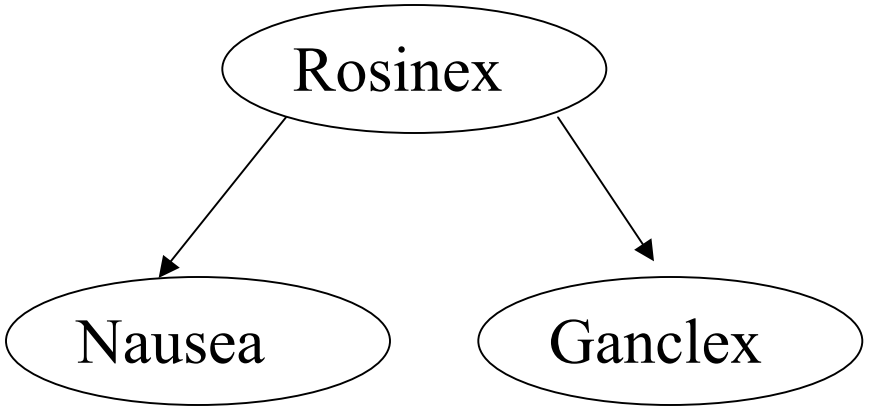
A 2nd Look at the DATA



Other Odd Things Can Happen…

Other Odd Things Can Happen…


salary
years of employment



		Nausea	*No Nausea*
Rosinex	Ganclex	81	9
Rosinex	No Ganclex	9	1
No Rosinex	Ganclex	1	9
No Rosinex	No Ganclex	90	810

```
Call:
glm(formula = N ~ G, family = binomial(link = logit), data = d)

Deviance Residuals:
    Min       1Q   Median       3Q      Max
-1.8519  -0.4800  -0.4800  -0.4800   2.1063

Coefficients:
            Estimate Std. Error z value Pr(>|z|)
(Intercept)  -2.1031     0.1065  -19.76   <2e-16 ***
G             3.6195     0.2812   12.87   <2e-16 ***
---
Signif. codes:  0 `***' 0.001 `**' 0.01 `*' 0.05 `.' 0.1 ` ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 949.78  on 1009  degrees of freedom
Residual deviance: 720.32  on 1008  degrees of freedom
AIC: 724.32
```