Logistic Regression

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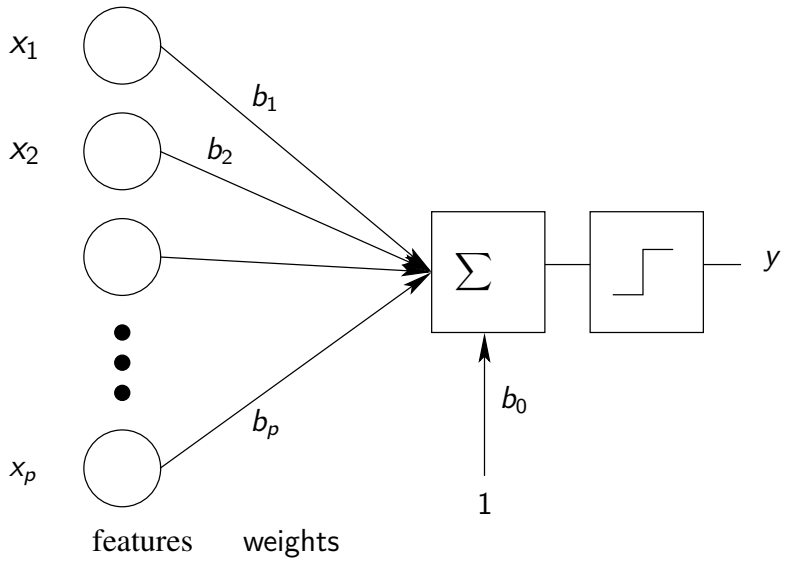
Discussion

Perdro Domingos' article

Linear classification

We started talking about classification using perceptron



$$\text{Predict} \begin{cases} \hat{Y} = 1 & \text{if } b_0 + \sum_{j=1}^{p} b_j x_j \geq 0 \\ \hat{Y} = 0 & \text{if } b_0 + \sum_{j=1}^{p} b_j x_j < 0 \end{cases}$$

How do we get probability $P(Y = 1 \mid x)$?

Logistic regression

Model for conditional distribution of Y given $X = x$

$$p_1(x; b) = P(Y = 1 \mid x; b) = \frac{\exp(b_0 + \sum_{j=1}^{p} b_j \cdot x_j)}{1 + \exp(b_0 + \sum_{j=1}^{p} b_j \cdot x_j)}$$

$$p_0(x; b) = P(Y = 0 \mid x; b) = \frac{1}{1 + \exp(b_0 + \sum_{j=1}^{p} b_j \cdot x_j)}$$

The log-odds of class 1 is a linear function of X

$$\log\left(\frac{p_1(x; b)}{p_0(x; b)}\right) = b_0 + \sum_{j=1}^{p} b_j \cdot x_j$$

Notation convention

Recall that $x = (x_1, \ldots, x_p)$ is our feature vector.

It is common to denote $x_0 = 1$ and write $x = (1, x_1, \ldots, x_p)$.

This allows us to write

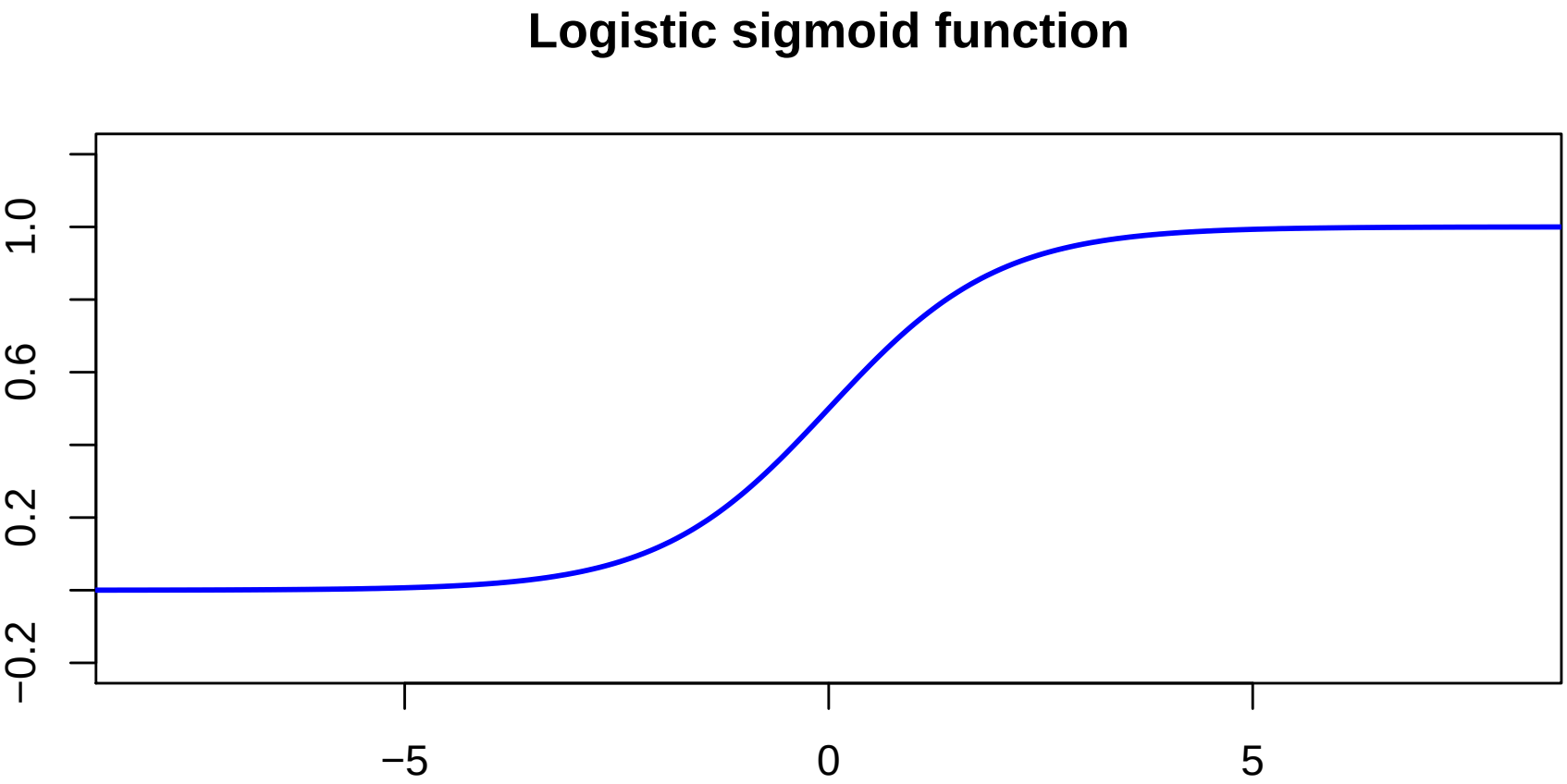
$$x^T b = \sum_{j=0}^{p} x_j \cdot b_j$$

Now we can write

$$P(Y = 1 \mid x; b) = \frac{\exp(x^T b)}{1 + \exp(x^T b)}$$

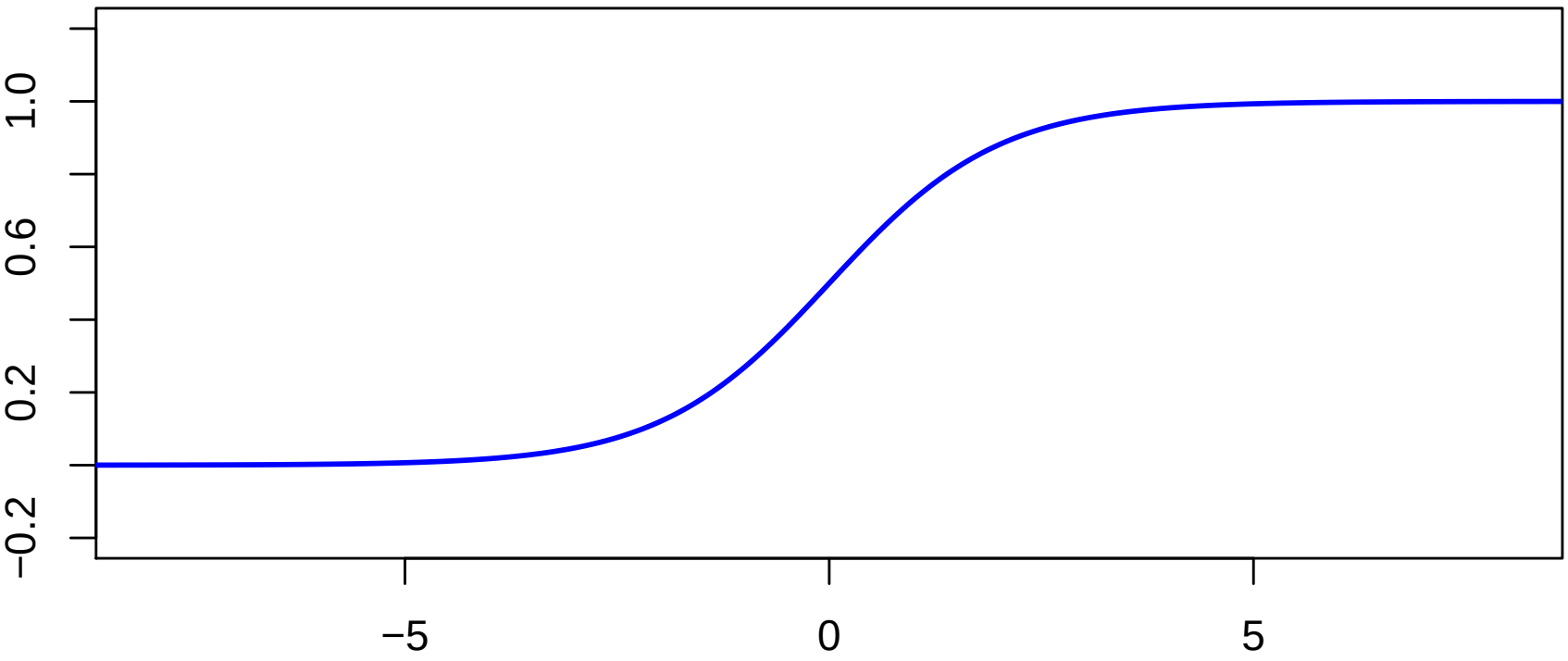
and we will also be able to present our procedures without doing anything special for our intercept term (also called bias term).

Representation with logistic regression



A linear function $x^T b$ can take values from $-\infty$ to ∞. By passing it through sigmoid, we get values in $[0, 1]$.

These values also sum to 1 to make a probability.



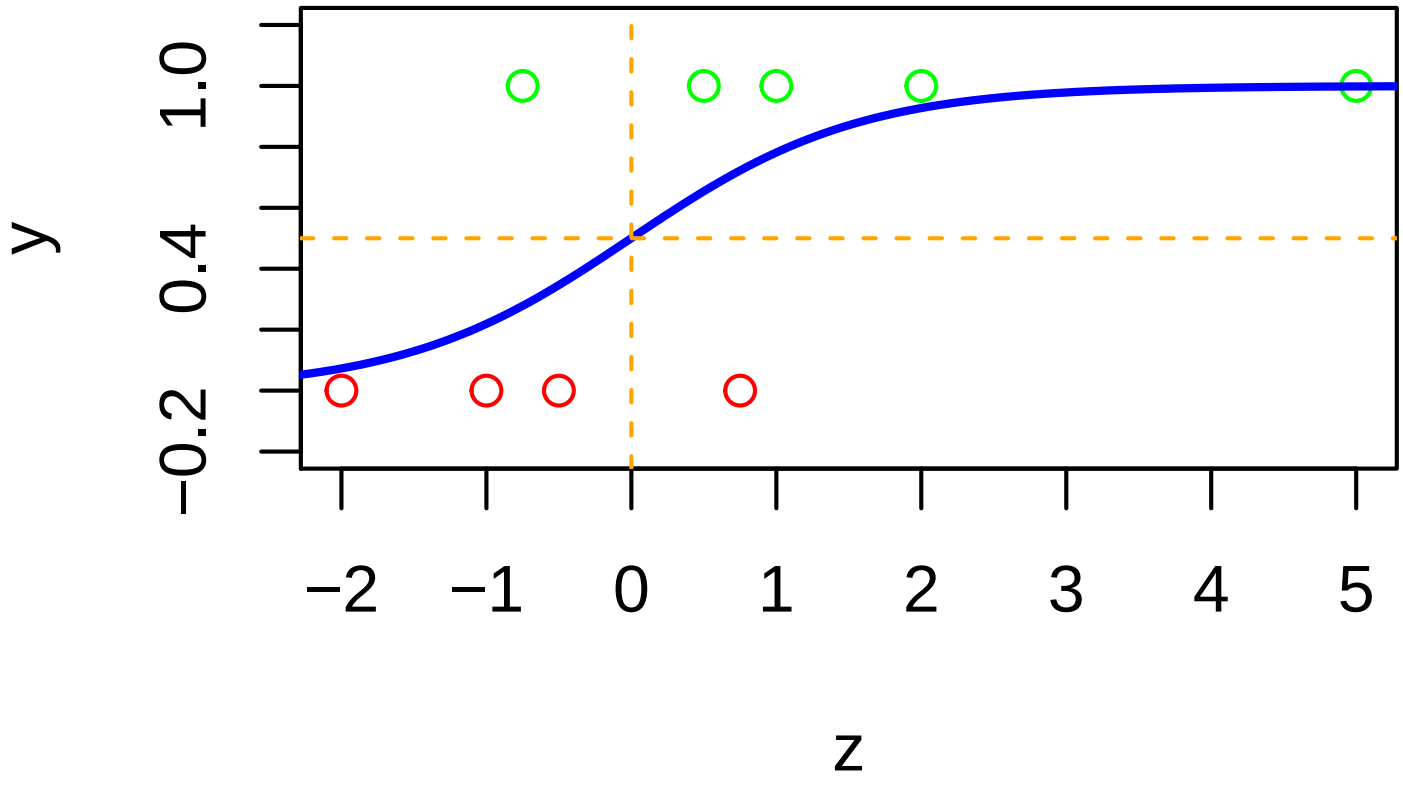
Step 1: Linear combination

$$z = x^T b$$

Step 2: Nonlinear transformation

$$P(Y = 1 \mid x; b) = F(z) = \frac{\exp(z)}{1 + \exp(z)}$$

z	$F(z)$
-3	0.05
-2	0.12
-1	0.27
0	0.5
1	0.73
2	0.88
3	0.95

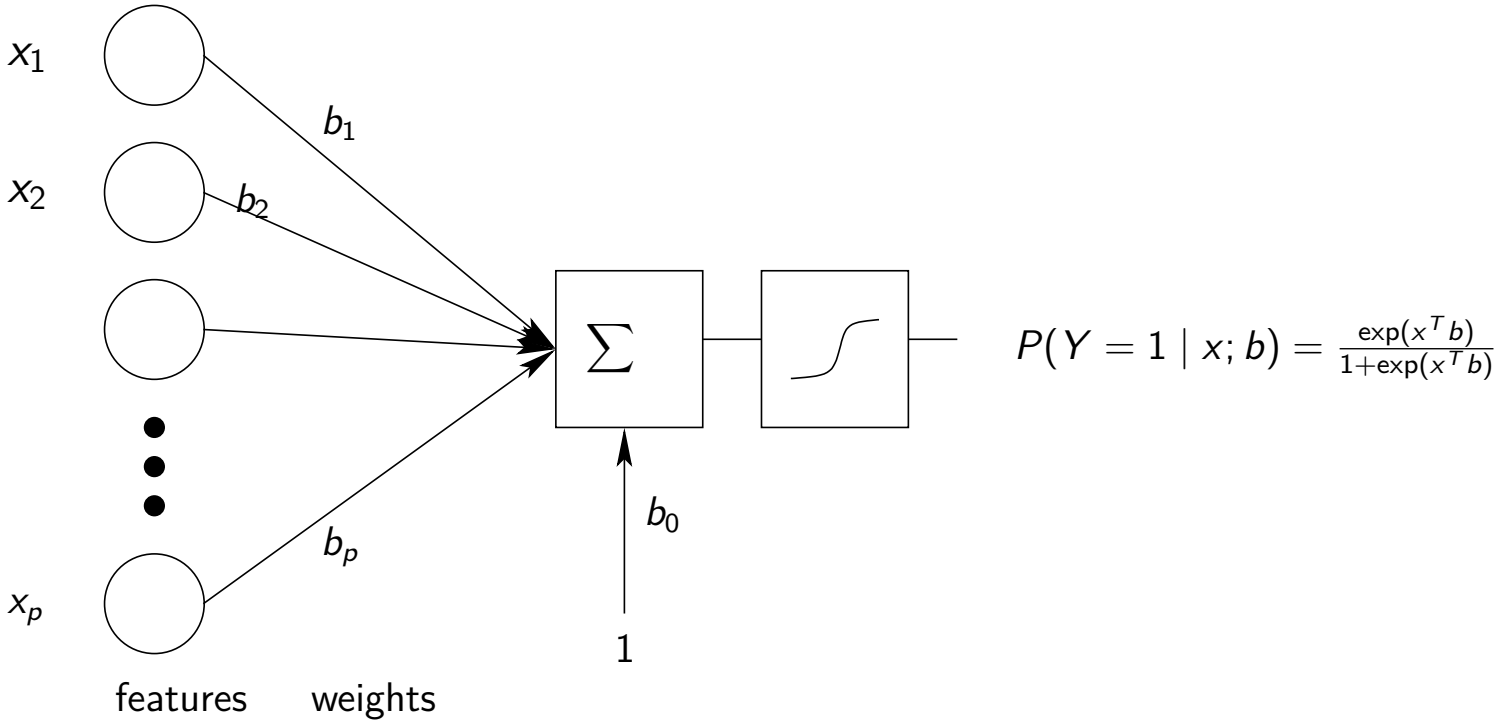


Suppose that $\hat{Y}_i = 1$ if $P(Y = 1 \mid z_i) > 0.5$ and $\hat{Y}_i = 0$ otherwise.

When do we assign a new observation to a positive class? For what values of z do we have $\hat{Y} = 1$?

What is the difference compared to perceptron?

Representation with logistic regression



A close couising to perceptron. Think about putting a rug over the threshold.

If we classify a new observation x as positive when $p_1(x; b) > 0.5$,

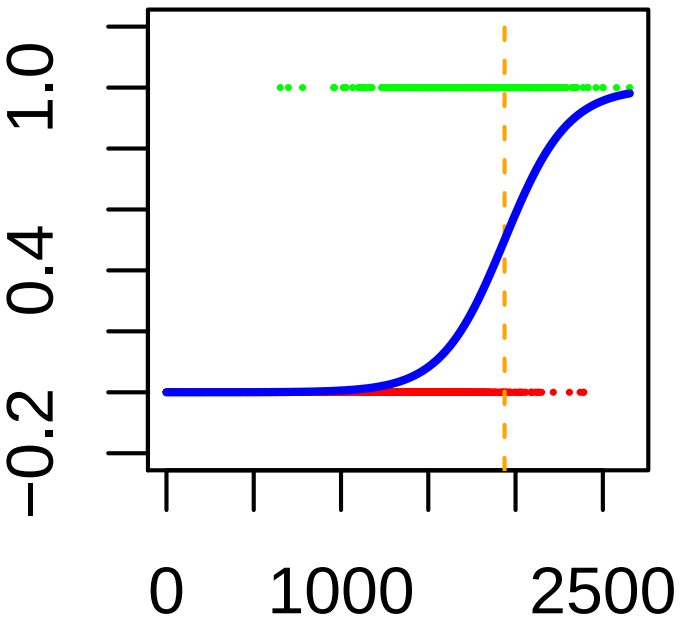
then $\begin{cases} \hat{Y} = 1 & \text{if } x^T b > 0 \\ \hat{Y} = 0 & \text{if } x^T b \leq 0 \end{cases}$

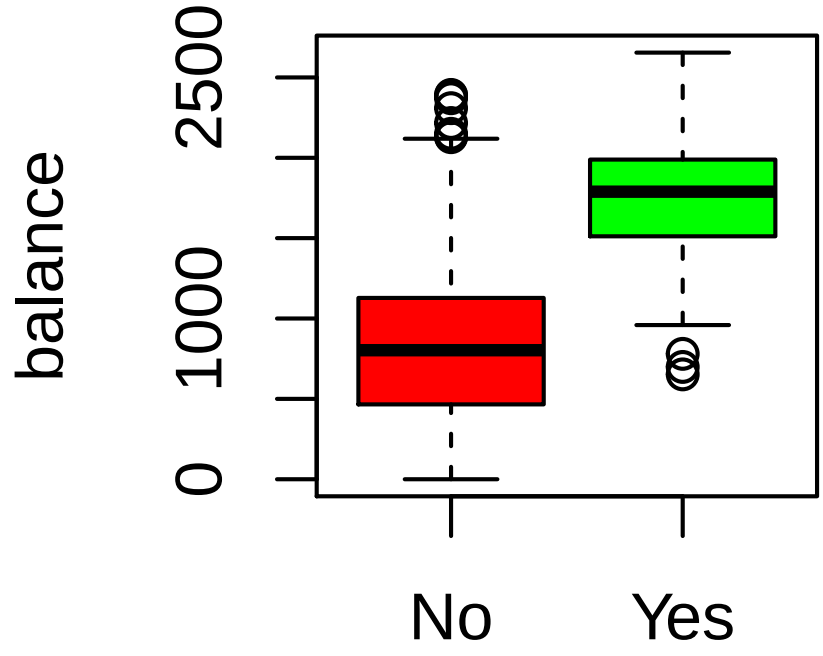
Example: Predicting default

"Default" data set from ISLR package

```
df = Default
head(df)
```

```
##   default student   balance    income
## 1      No      No  729.5265 44361.625
## 2      No     Yes  817.1804 12106.135
## 3      No      No 1073.5492 31767.139
## 4      No      No  529.2506 35704.494
## 5      No      No  785.6559 38463.496
## 6      No     Yes  919.5885  7491.559
```

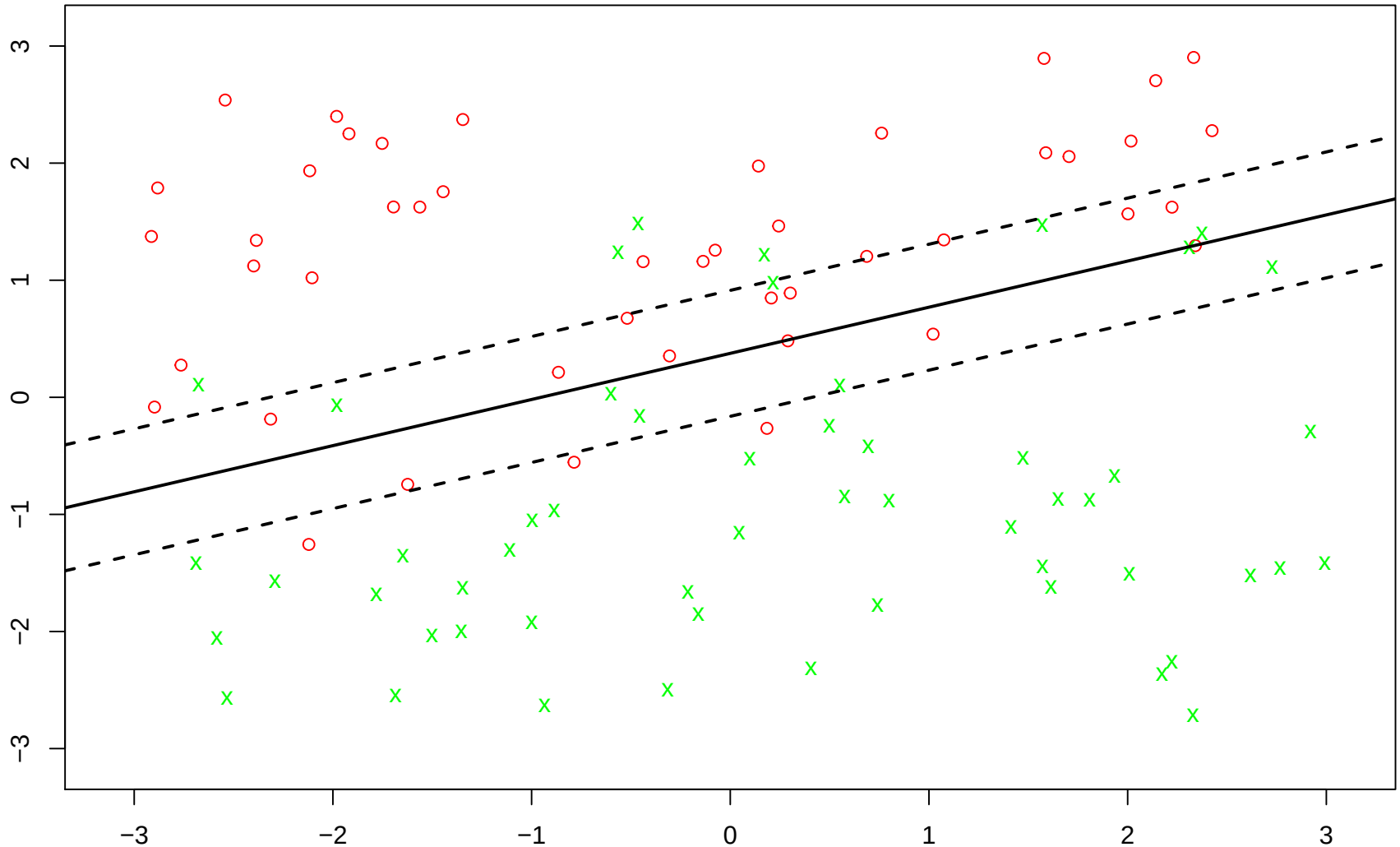





```
##   (Intercept)       balance
## -10.651330614   0.005498917
```

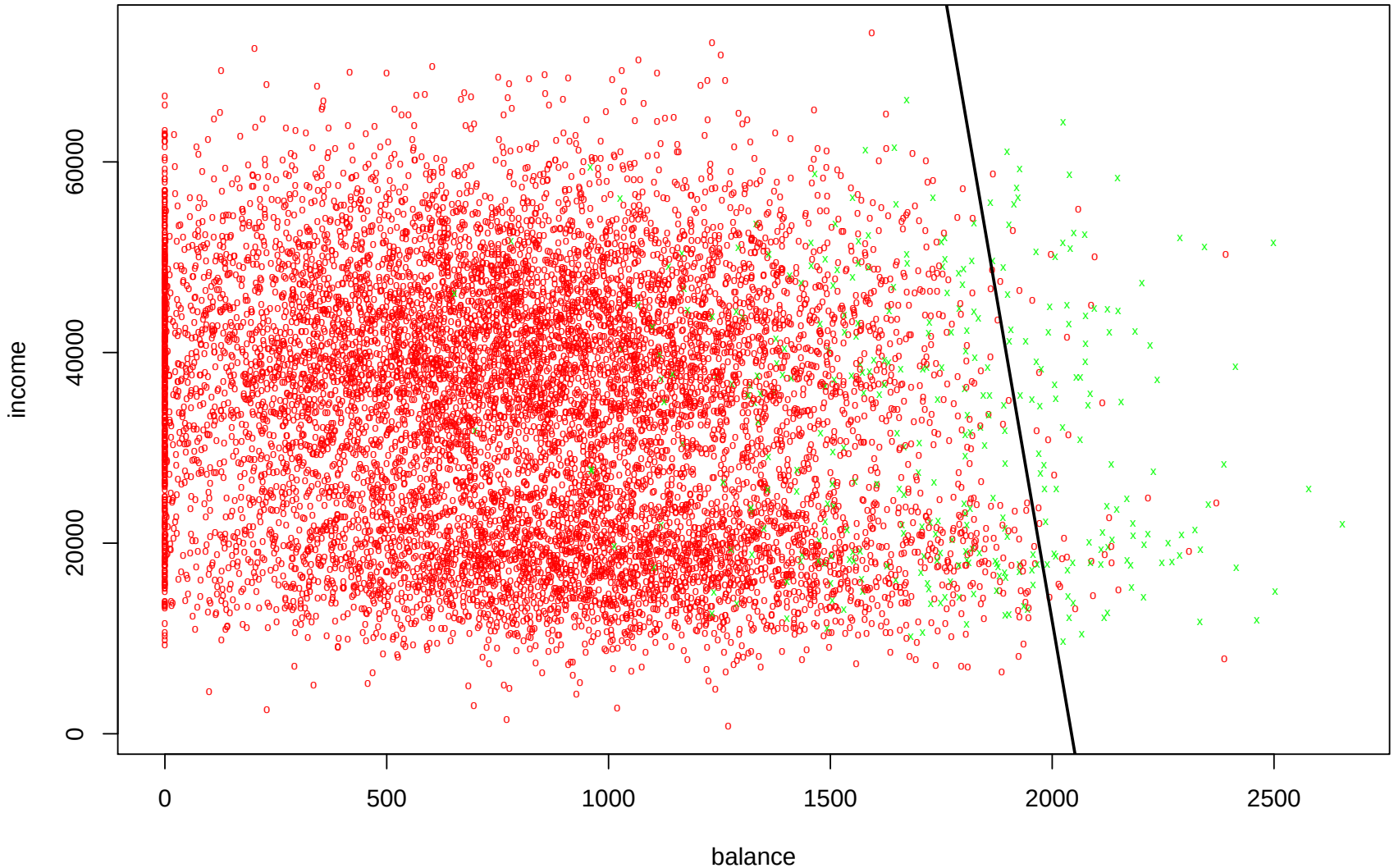
$$\hat{p}_1(x) = \frac{\exp(-10.65+x*0.0055)}{1+\exp(-10.65+x*0.0055)}$$

Simulated example in 2D



Futher away an observation is from the decision boundary, more certain its label.

Example: Predicting default



How do we learn parameters?

Our model for Y given $X = x$ is determined by the vector b.

Recall that $P(Y = 1 \mid x; b) = \frac{\exp(x^T b)}{1+\exp(x^T b)}$.

How do we find a good b?

We will minimize the deviance:

$$\hat{b} = \arg\min \sum_{i=1}^{n} -2 \times \log P(Y = y_i \mid x_i; b)$$

We need to find b that minimizes $\sum_{i=1}^{n} L(y_i, x_i; b)$.

Another way to represent the loss: (Details)

Another common way to write logistic regression objective. . .

Consider an example (x_i, y_i)

- If $y_i = 0$, then deviance is $-2 \times \log(1 - p_1(x_i; b))$
- If $y_i = 1$, then deviance is $-2 \times \log(p_1(x_i; b))$

Another way to write loss for this example

$$\begin{aligned} L(y_i, x_i; b) &= -\log(P(Y = y_i \mid x_i; b)) \\ &= -(1 - y_i) \log(1 - p_1(x_i; b)) - y_i \log p_1(x_i; b) \end{aligned}$$

Loss on training data

$$J(b) = \sum_{i=1}^{n} L(y_i, x_i; b)$$

Minimization procedures

Find b that makes the loss $J(b)$ as small as possible.

Many different numerical procedures – treat them as black boxes.

Still you need to know some high-level details.

Optimization proceedures commonly need to compute

- loss $J(b)$
- (partial) derivative of the loss $\nabla J(b) = \begin{pmatrix} \partial_1 J(b) \\ \vdots \\ \partial_p J(b) \end{pmatrix}$
- second (partial) derivative

$$\Delta J(b) = \begin{pmatrix} \partial_{11} J(b) & \partial_{12} J(b) & \dots & \partial_{1p} J(b) \\ \partial_{21} J(b) & \partial_{22} J(b) & \dots & \partial_{1p} J(b) \\ \vdots & & \ddots & \vdots \\ \partial_{p1} J(b) & \partial_{p2} J(b) & \dots & \partial_{pp} J(b) \end{pmatrix}$$

Minimization procedures

Derivative free minimization

- require $J(b)$ only
- useful when computing $\nabla J(b)$ is very expensive

Gradient descent and other first order methods

- require $J(b)$ and $\nabla J(b)$
- useful when dealing with large amounts of data
- many iterations to get high accuracy solution, but each iteration is cheap (We do not care about high accuracy. Why?)

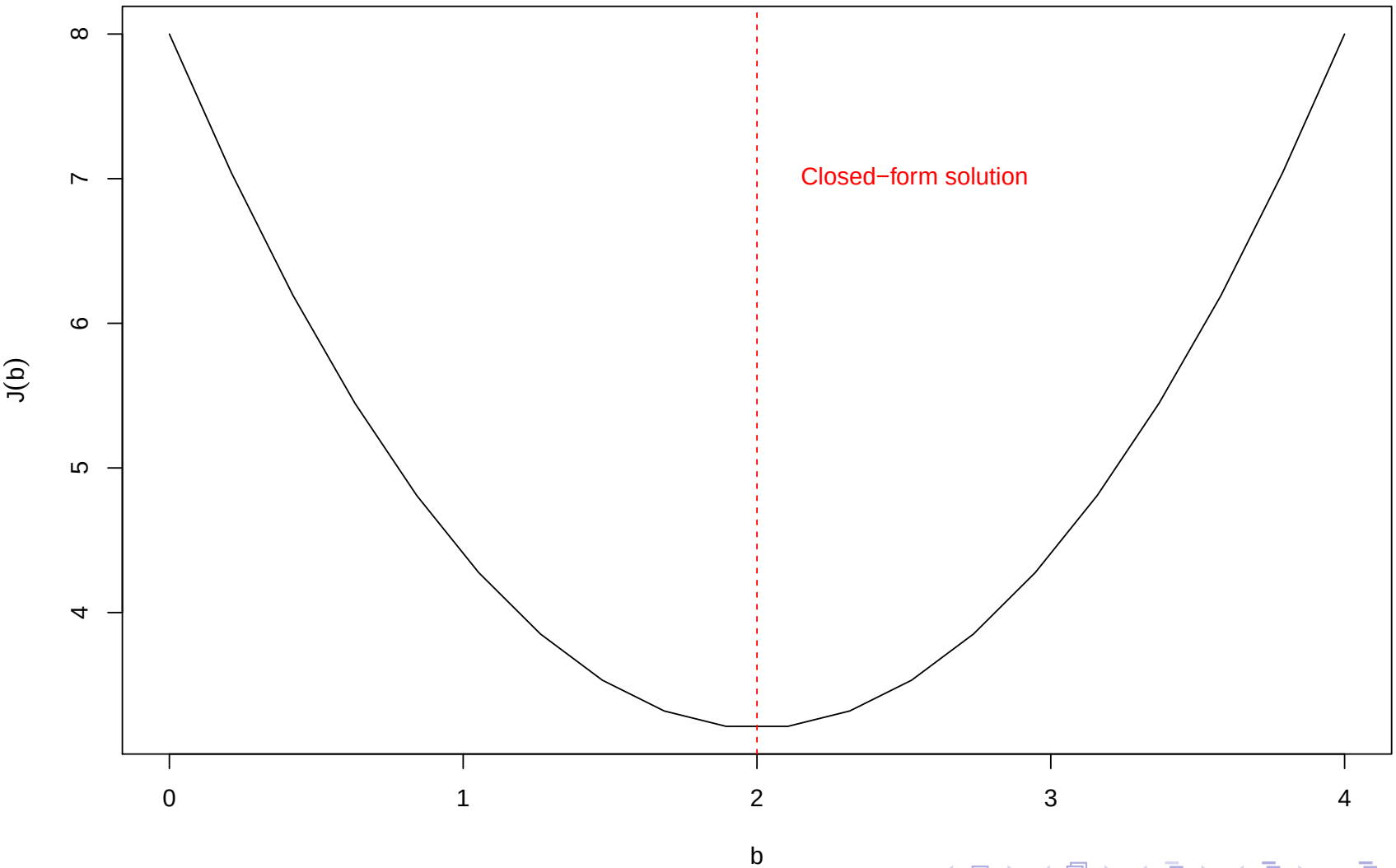
Second order methods (Newton's method)

- require $J(b)$, $\nabla J(b)$, and $\Delta J(b)$
- few iteration to find minimum, but each iteration can be expensive
- R packages (that I have seen) implement this

Gradient descent

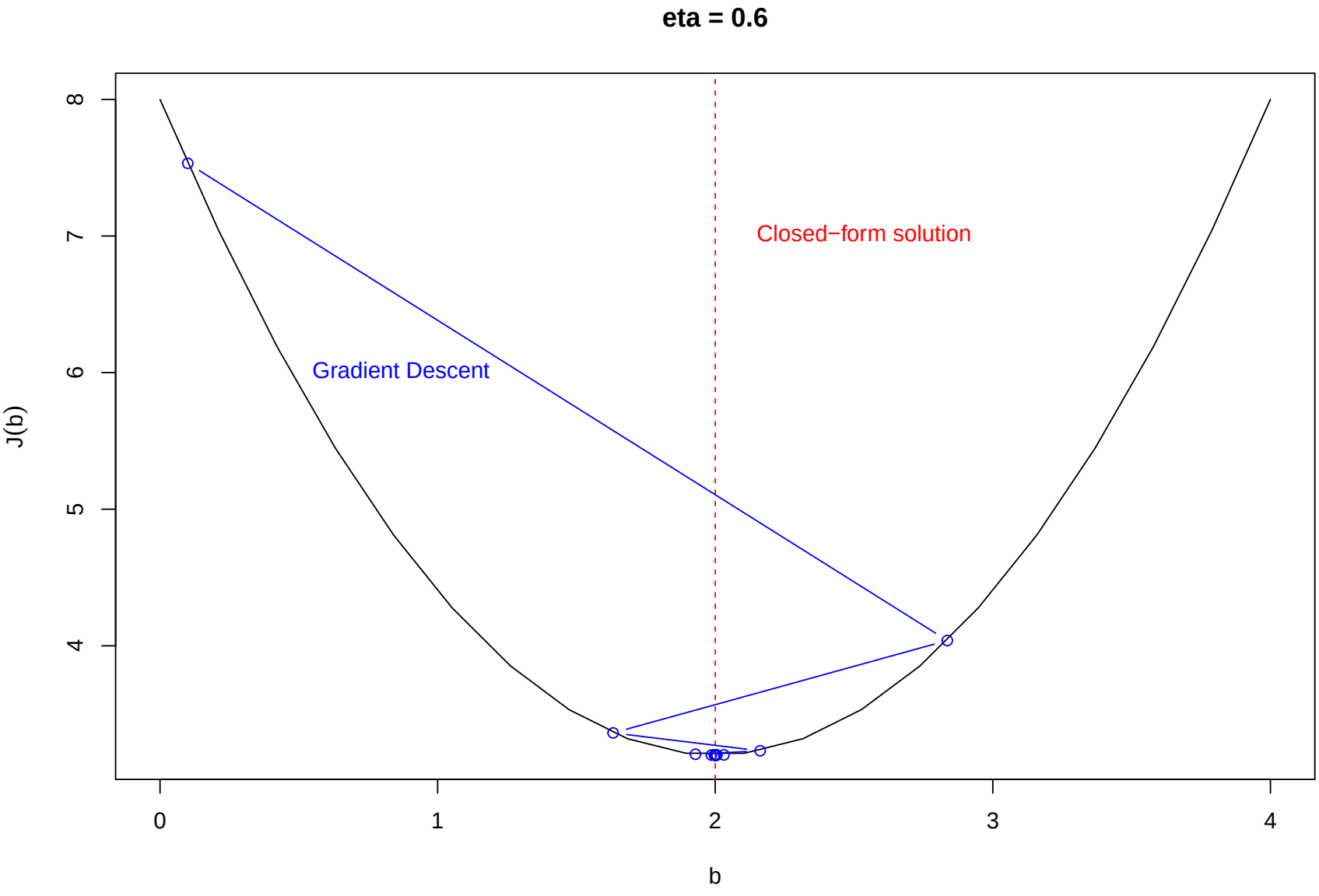
Suppose that we want to find b that minimizes the following function

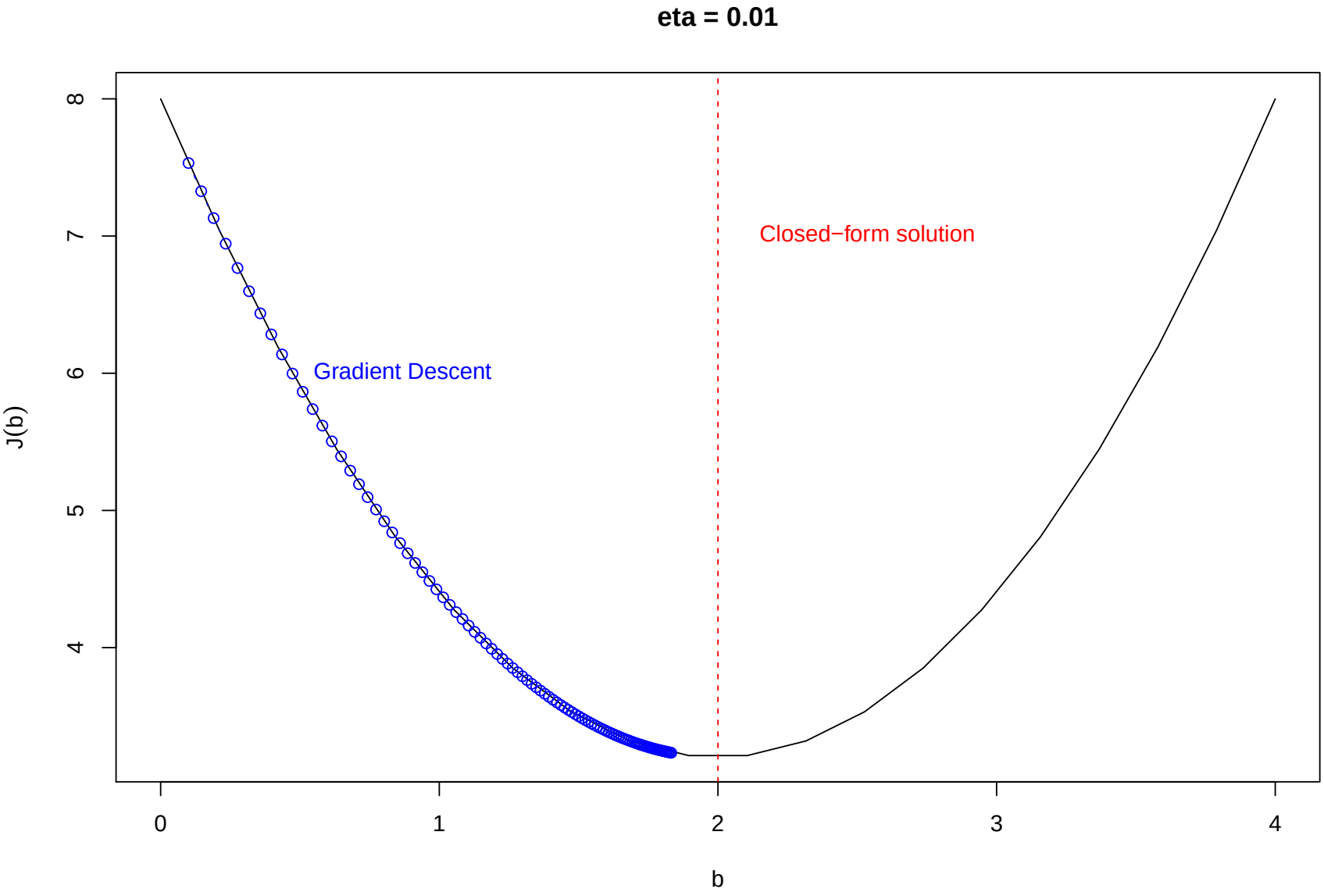
$$J(b) = 1.2(b-2)^2 + 3.2$$

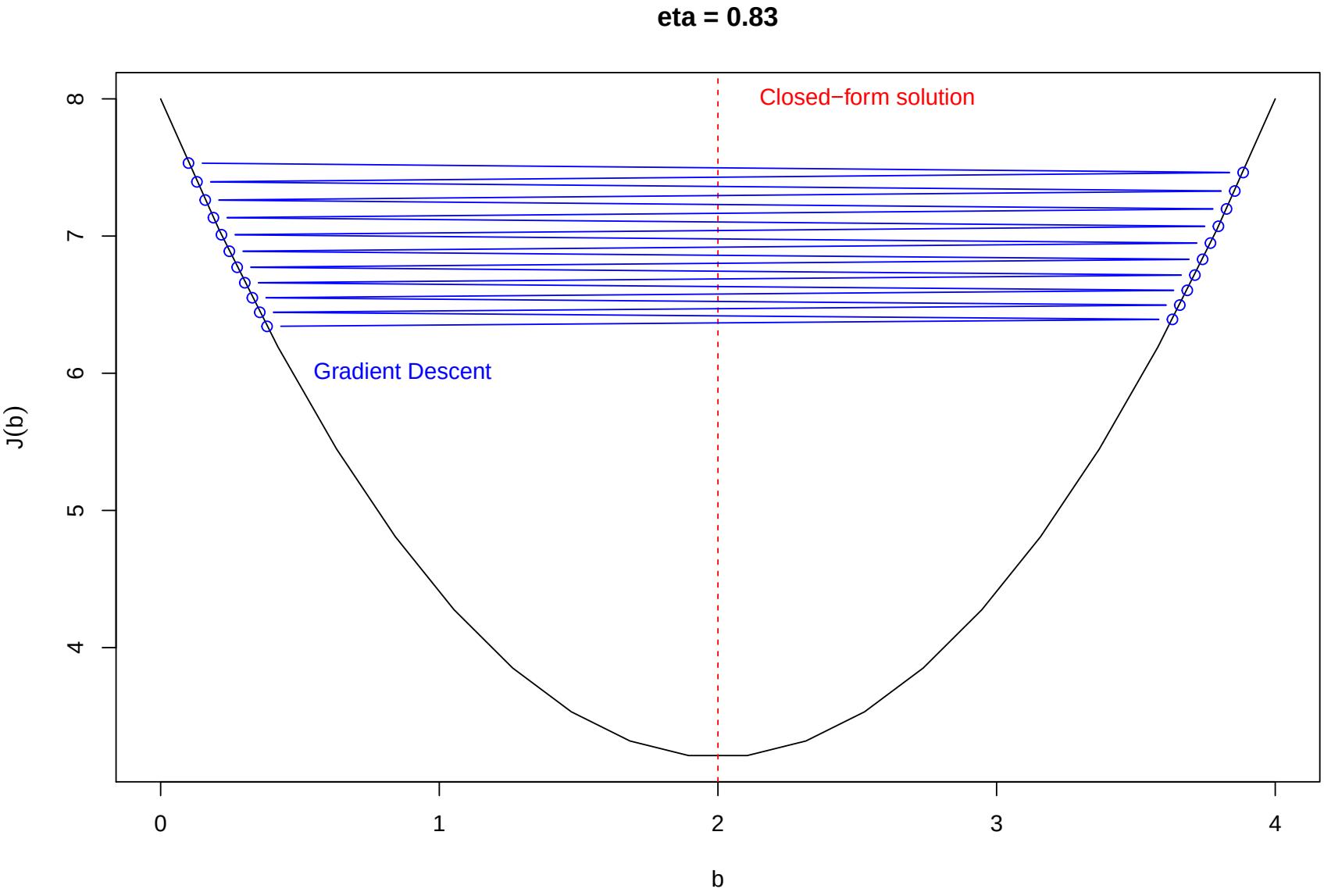


Set $b^0 = 0$. Iteratively update $b^{t+1} = b^t - \eta \partial J(b^t)$.

η is the step size. Also known as the learning rate.




eta = 0.01
Closed−form solution
Gradient Descent
J(b)
b
0
1
2
3
4
4
5
6
7
8


eta = 0.83
Closed−form solution
Gradient Descent
J(b)
b
8
7
6
5
4
0
1
2
3
4

Gradient descent

The learning rate η plays a crucial role in convergence.

For multivariate problems, where $b = (b_0, b_1, \ldots, b_p)$, the gradient descent takes the following form:

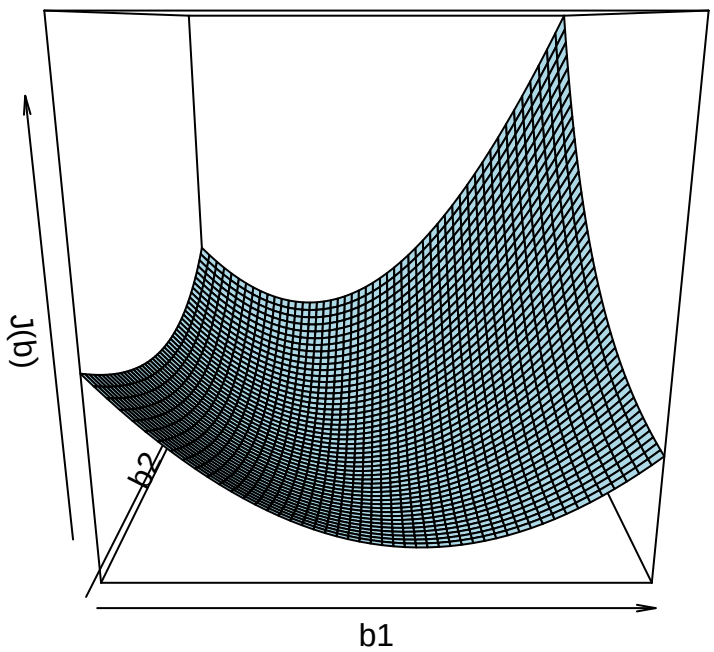
- Start with $b^0 = (0, \ldots, 0)$.
- In each iteration, $t = 1, 2, \ldots$ update

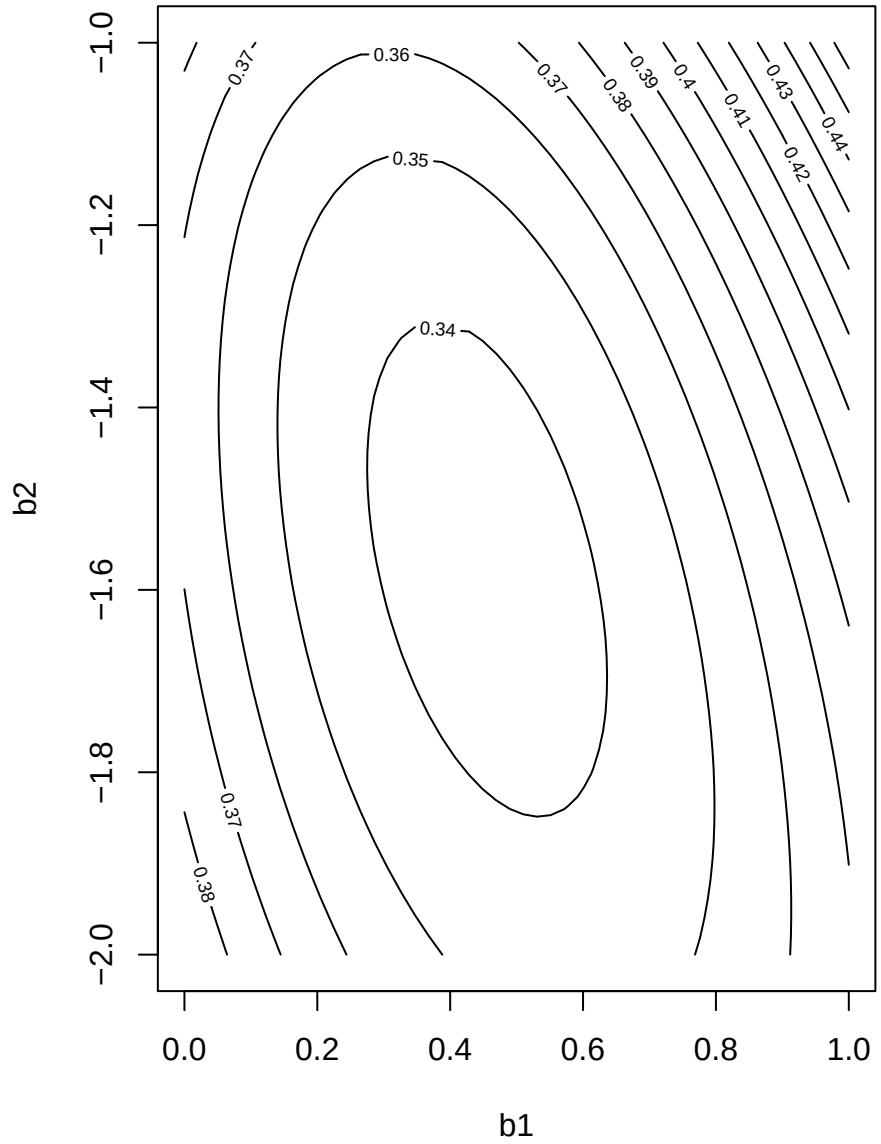
$$b_j^{t+1} = b_j^t - \eta \partial_j J(b^t), \qquad \text{for all } j = 0, 1, \ldots, p$$

When to stop?

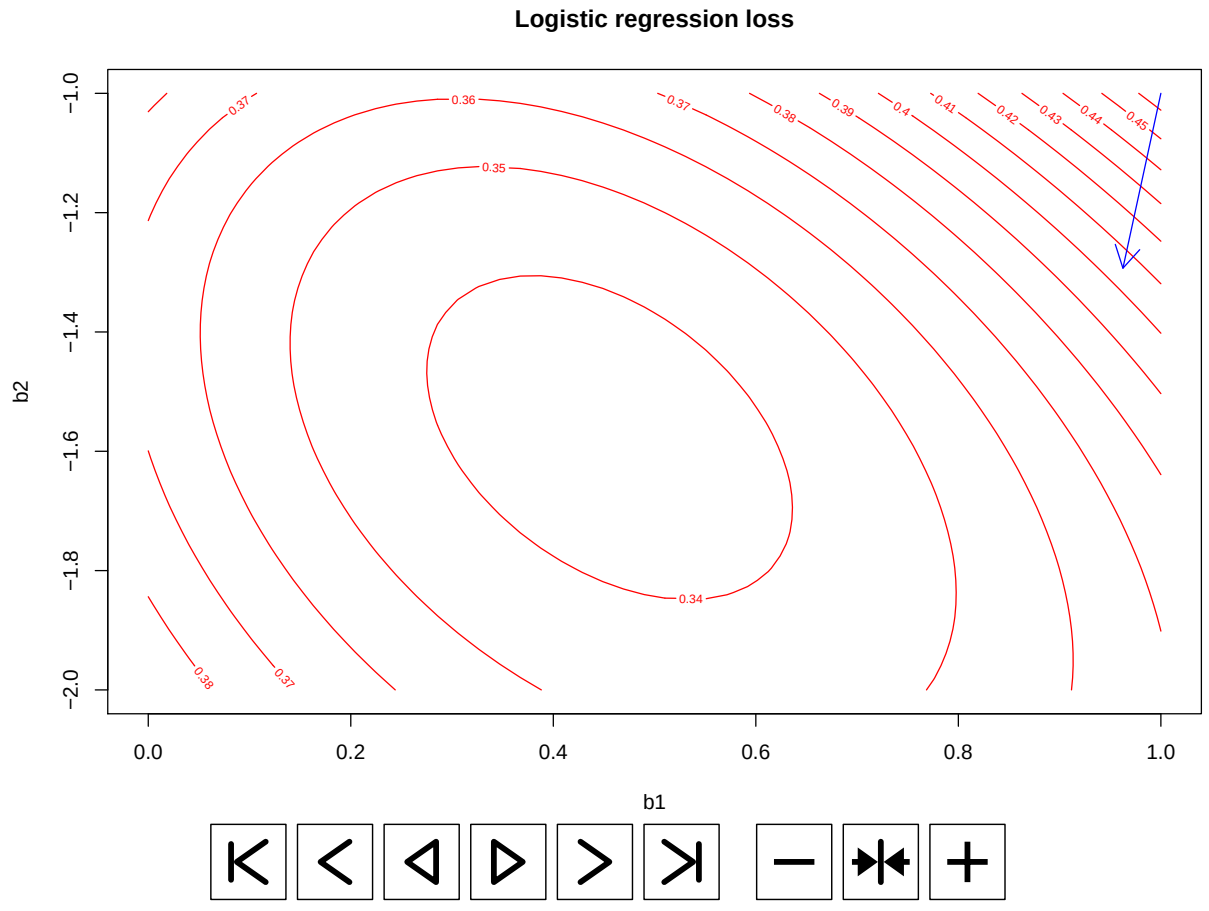
- $|J(b^t) - J(b^{t-1})|$ is small
- $|b^t - b^{t-1}|$ is small
- $\|\nabla J(b^t)\|$ is small
- ...

Gradient descent





Gradient descent



Gradient descent for logistic regression

Logistic regression loss per example

$$L(y_i, x_i; b) = -(1 - y_i) \log(1 - p_1(x_i; b)) - y_i \log p_1(x_i; b)$$

Gradient of the loss per example

$$\partial_j L(y_i, x_i; b) = (p_1(x_i; b) - y_i) x_{ij}$$

The overall gradient

$$\partial_j J(b) = \sum_{i=1}^{n} (p_1(x_i; b) - y_i) x_{ij}$$

Gradient descent for logistic regression

Initialize $b = (0, \ldots, 0)$
repeat
  Let $g = (0, \ldots, 0)$ be the gradient vector
  for *i = 1:n* **do**
    $p_i = \exp(x_i^T b)/(1 + \exp(x_i^T b))$
    $\text{error}_i = p_i - y_i$
    $g = g + \text{error}_i \cdot x_i$
  end
  $b = b - \eta \cdot g/n$
until *until convergence*;

Note that algorithm uses all observations to compute the gradient.

This approach is called batch gradient descent.

Stochastic gradient descent for logistic regression

Initialize $b = (0, \ldots, 0)$
repeat
  Pick observation i
  $p_i = \exp(x_i^T b)/(1 + \exp(x_i^T b))$
  $\text{error}_i = p_i - y_i$
  $b = b - \eta(\text{error}_i \cdot x_i)$
until *until convergence*;

Coefficient b is updated after each observation.

In practice, mini batch is often used.

- Compute gradient based on a small subset of observations
- Make update to coefficient vector

Extending logistic regression to $K > 2$ classes

Choose class K to be the reference class

Represent each of the other classes as a logistic function of the odds of class k versus class K

$$\log\left(\frac{P(Y=1 \mid x)}{P(Y=K \mid x)}\right) = x^T b_1$$
$$\log\left(\frac{P(Y=2 \mid x)}{P(Y=K \mid x)}\right) = x^T b_2$$
$$\vdots$$
$$\log\left(\frac{P(Y=K-1 \mid x)}{P(Y=K \mid x)}\right) = x^T b_{K-1}$$

Extending logistic regression to $K > 2$ classes

The conditional probability for class $k \neq K$

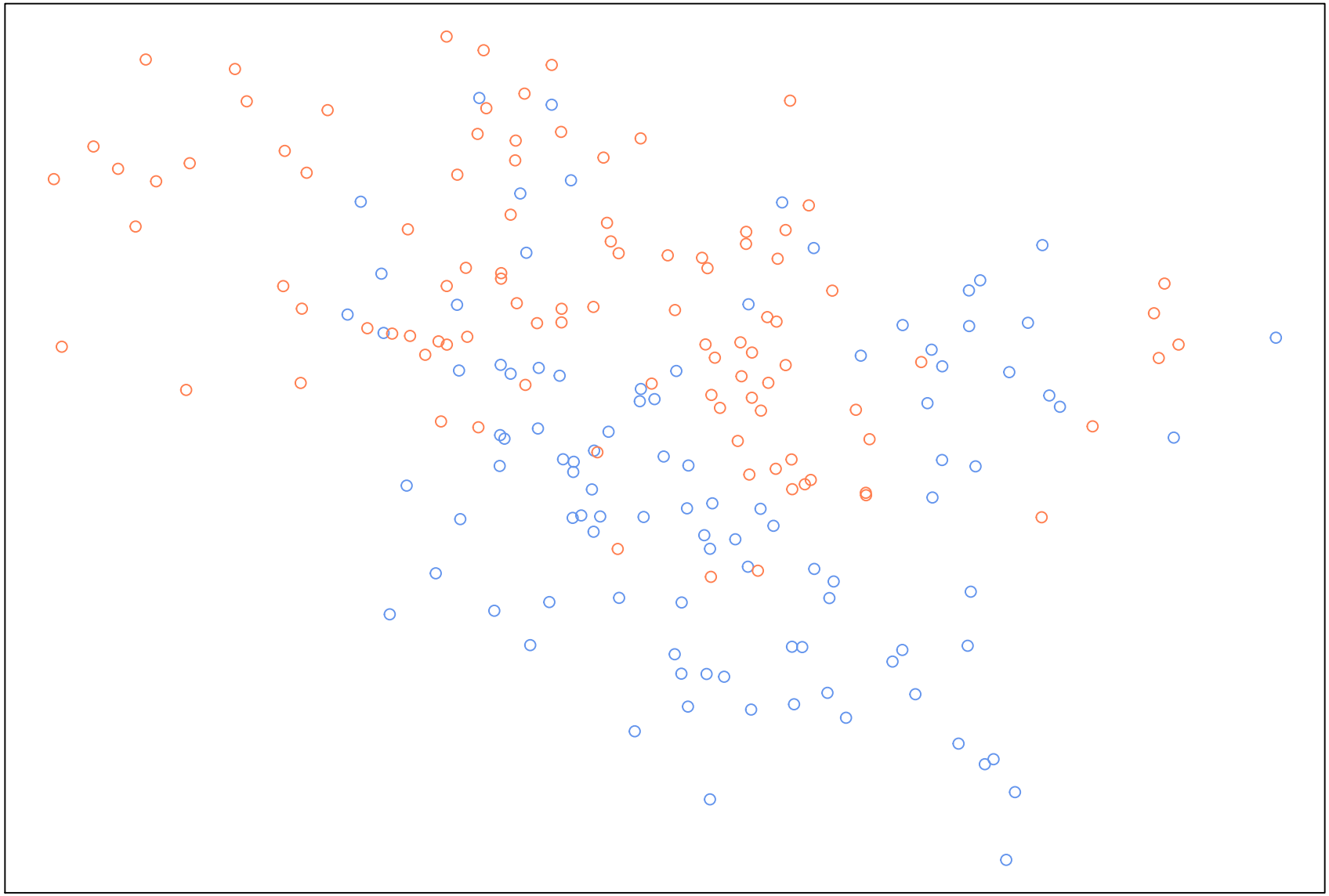
$$P(Y = k \mid x) = \frac{\exp(x^T b_k)}{1 + \sum_{l=1}^{K-1} \exp(x^T b_l}$$

The conditional probability for class K

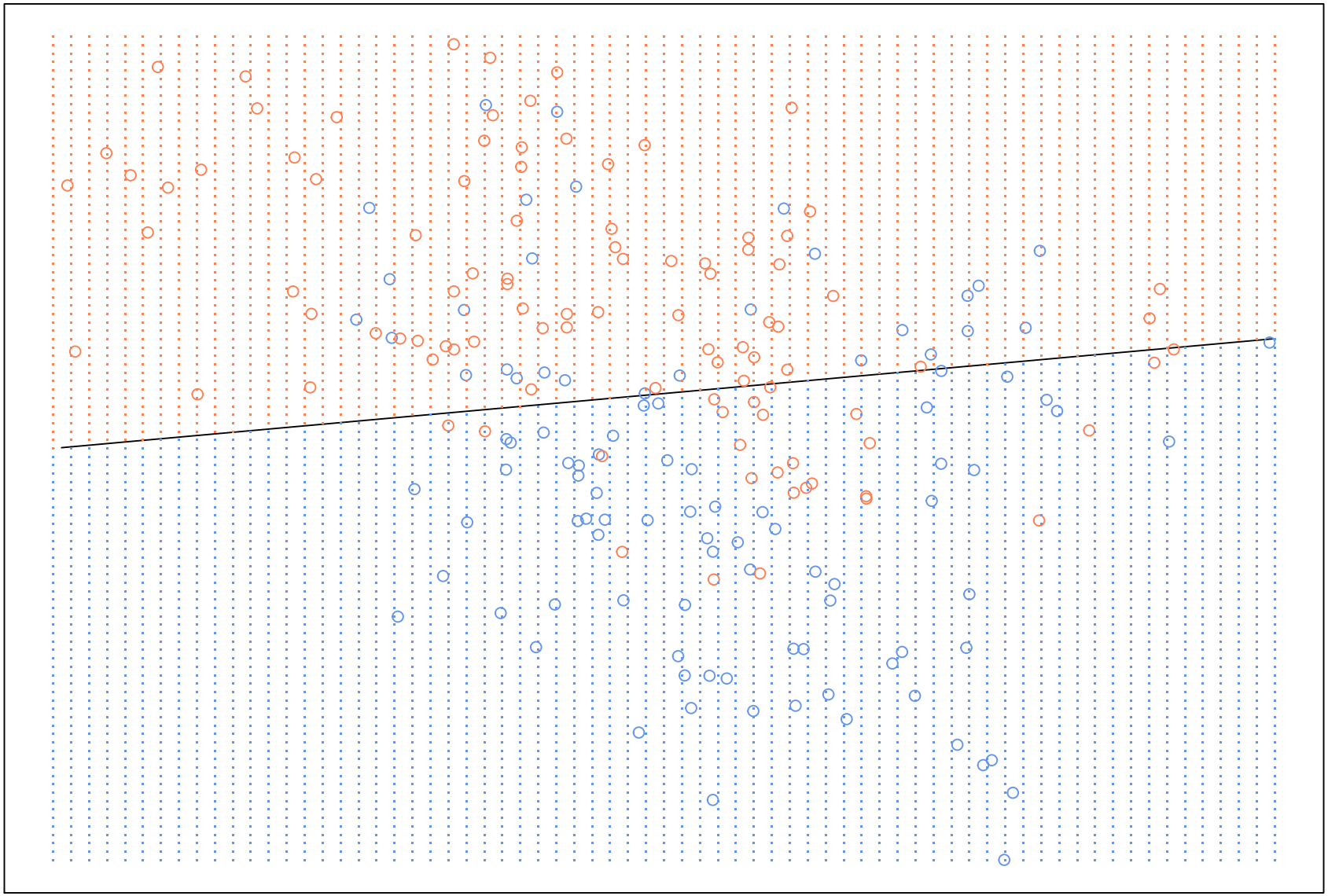
$$P(Y = k \mid x) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp(x^T b_l}$$

Fitting can be again done using a number of procedures that will simultaneously obtain coefficients for each class $b_1, \ldots, b_{K-1}$

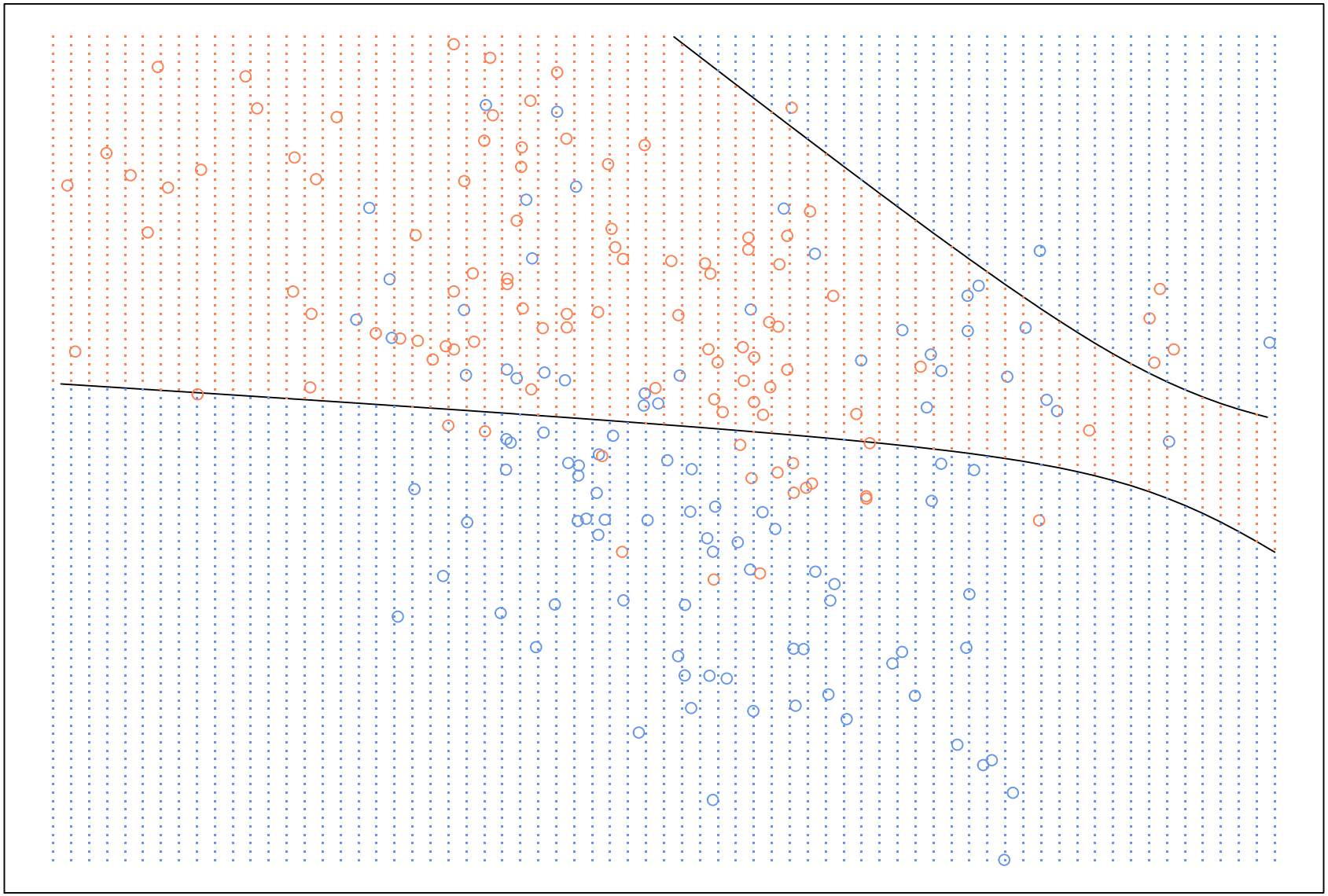
Avoiding overfitting



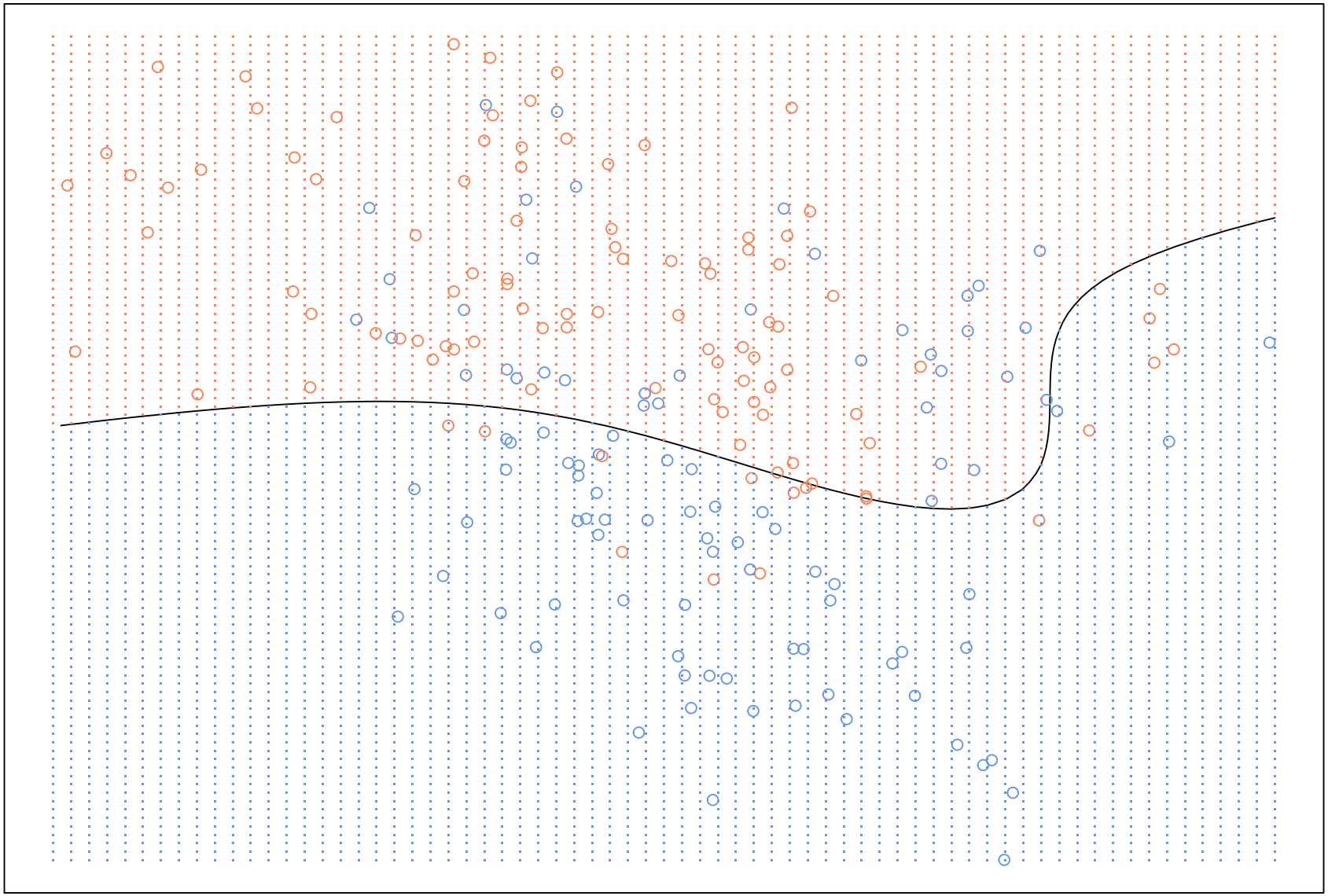
logistic regression



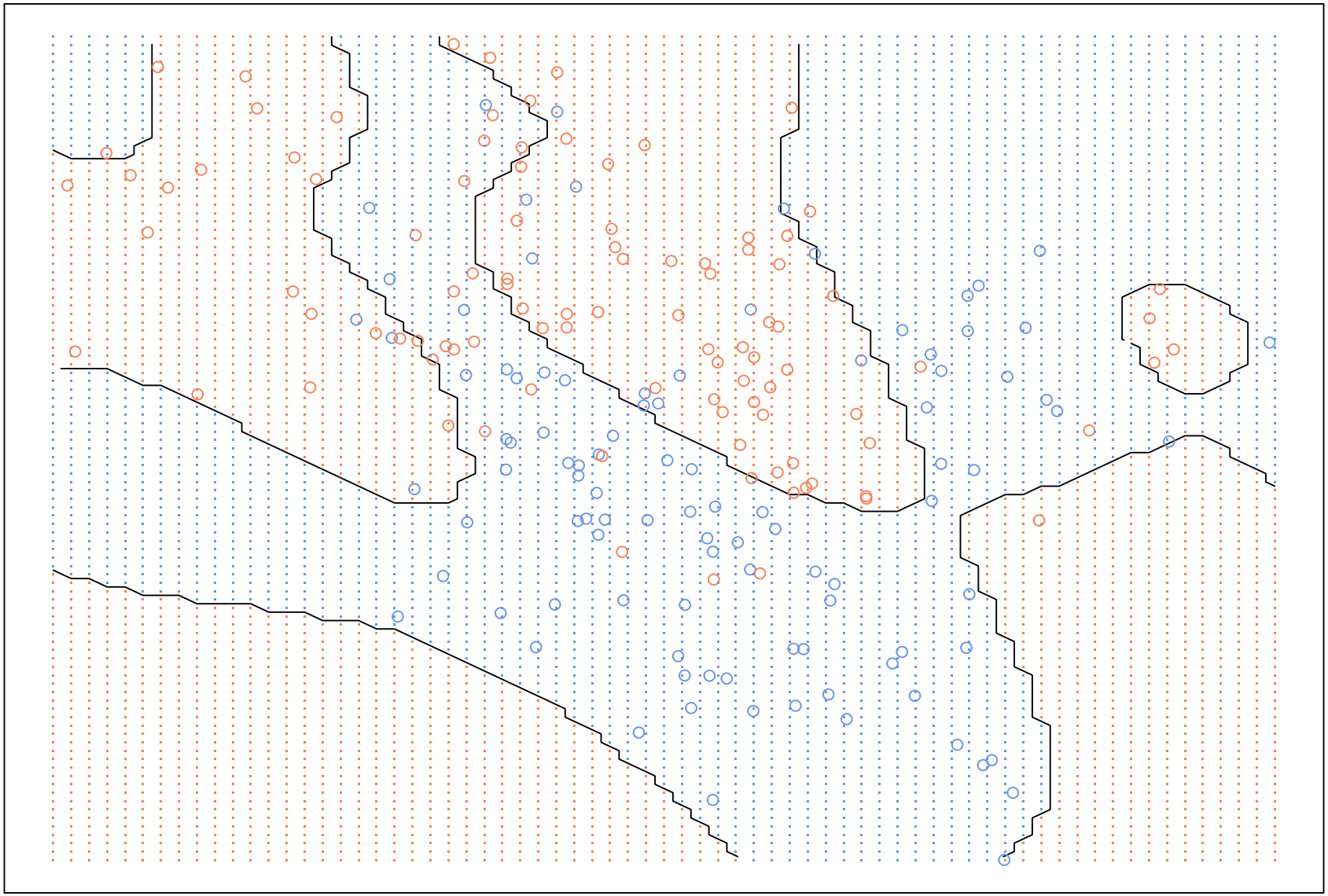
logistic regression −− quadratic with interactions



logistic regression −− cubic with interactions



logistic regression −− 7th degree polynomial



```
lr_fit_7$coefficients[1:10]
```

```
##   (Intercept)          x.1.0          x.2.0
## -1.100958e+15 -1.733179e+15 -9.387873e+13
##          x.3.0          x.4.0          x.5.0
##  3.202179e+15 -1.736921e+15 -2.390935e+13
##          x.6.0          x.7.0          x.0.1
##  1.699264e+14 -2.496843e+13  1.283042e+15
##          x.1.1
## -7.430262e+15
```

Avoiding overfitting using L1/L2 penalization

Find b that minimizes

$$J(b) + \lambda \left(\frac{1-\alpha}{2} \sum_{j=1}^{p} b_j^2 + \alpha \sum_{j=1}^{p} |b_j| \right)$$

This is known as an elastic net penalty (see glmnet package)

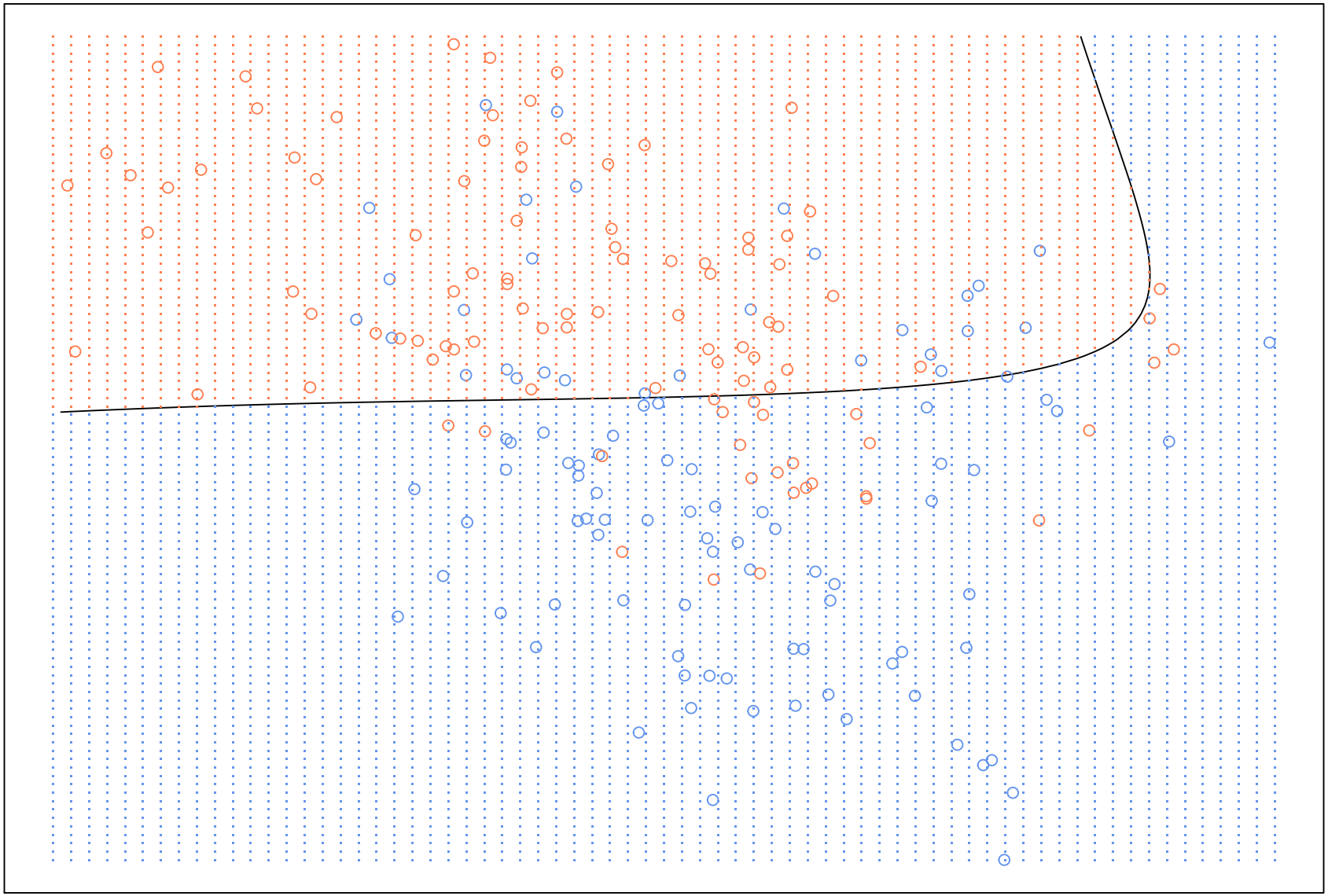
λ is the penalty parameter

- large value: prefer simple models
- small value: prefer complex models (no regularization)

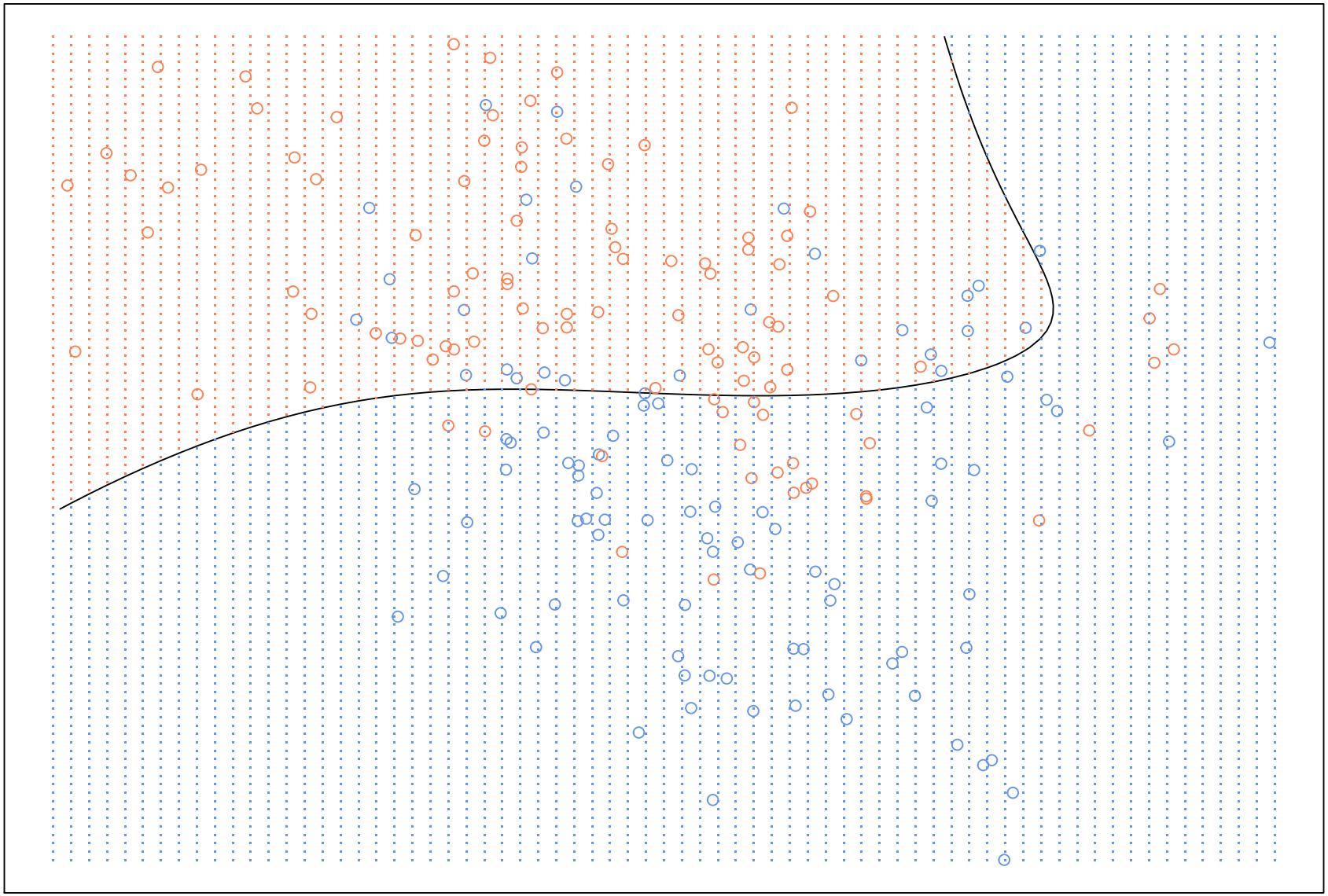
α is the elasticnet mixing parameter

- $\alpha = 0$: ridge penalty
- $\alpha = 1$: lasso penalty

logistic regression −− lasso



logistic regression −− ridge penalty



Example: Predicting quality of restaurant

Can we predict quality of a restaurant based on a review?

```
# data from textir package
data(we8there)
dim(we8thereCounts)
```

Data are very high dimensional.

But fortunately not many words per document.

See code in *we8there.R*

An example of a positive review

```
we8thereCounts[1, we8thereCounts[1, ]!=0]
```

```
##  even though larg portion  mouth water
##            1            1            1
##     red sauc    babi back     back rib
##            1            1            1
## chocol mouss veri satisfi
##            1            1
```

An example of a negative review

```
we8thereCounts[6100, we8thereCounts[6100, ]!=0]
```

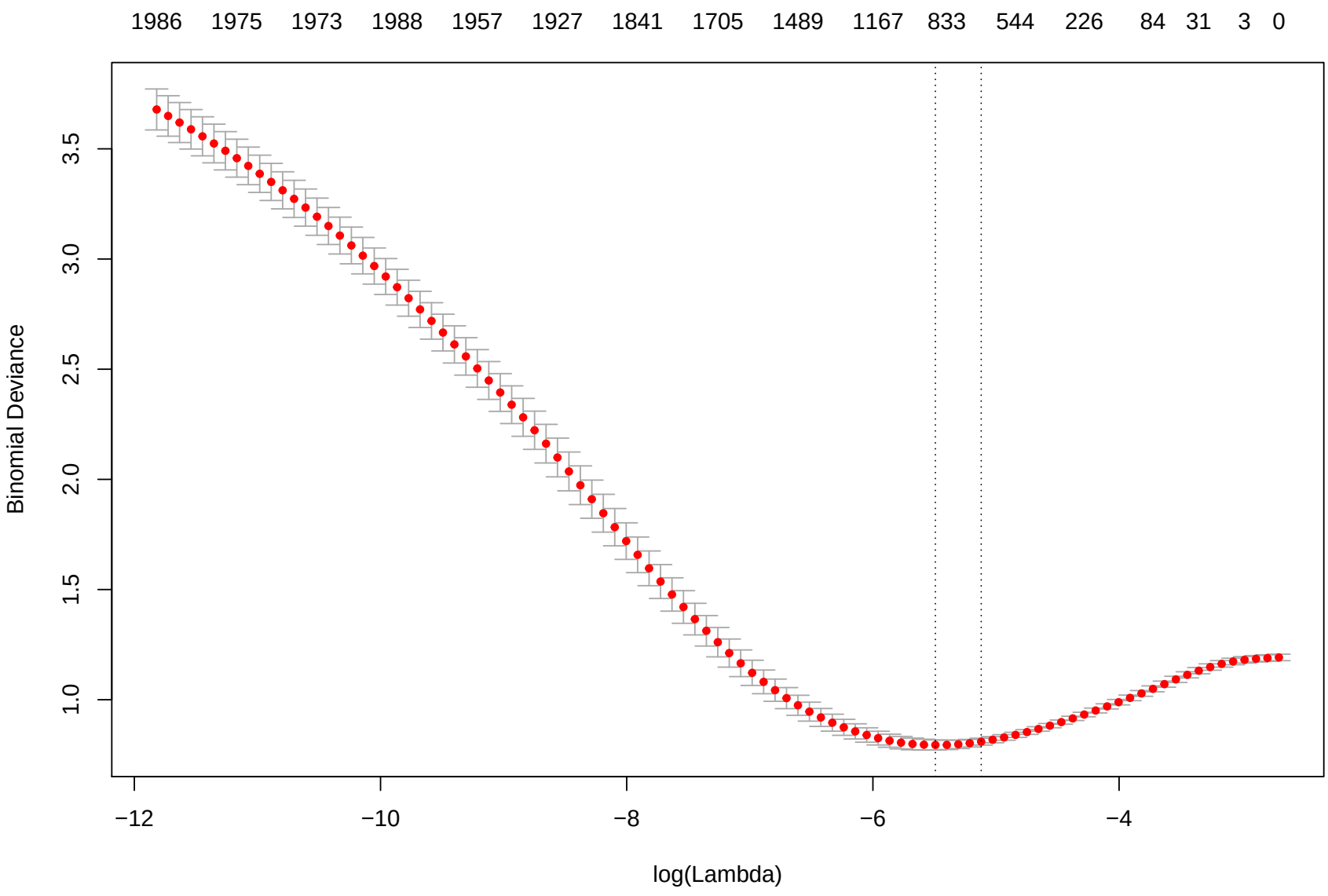
```
## never return      just few      one side
##            1             1             1
##     tri make        go box  order wrong
##            1             1             1
##  place clean   order just      seat one
##            1             1             1
##   side build
##            1
```

```
we8thereRatings[1:3,]
```

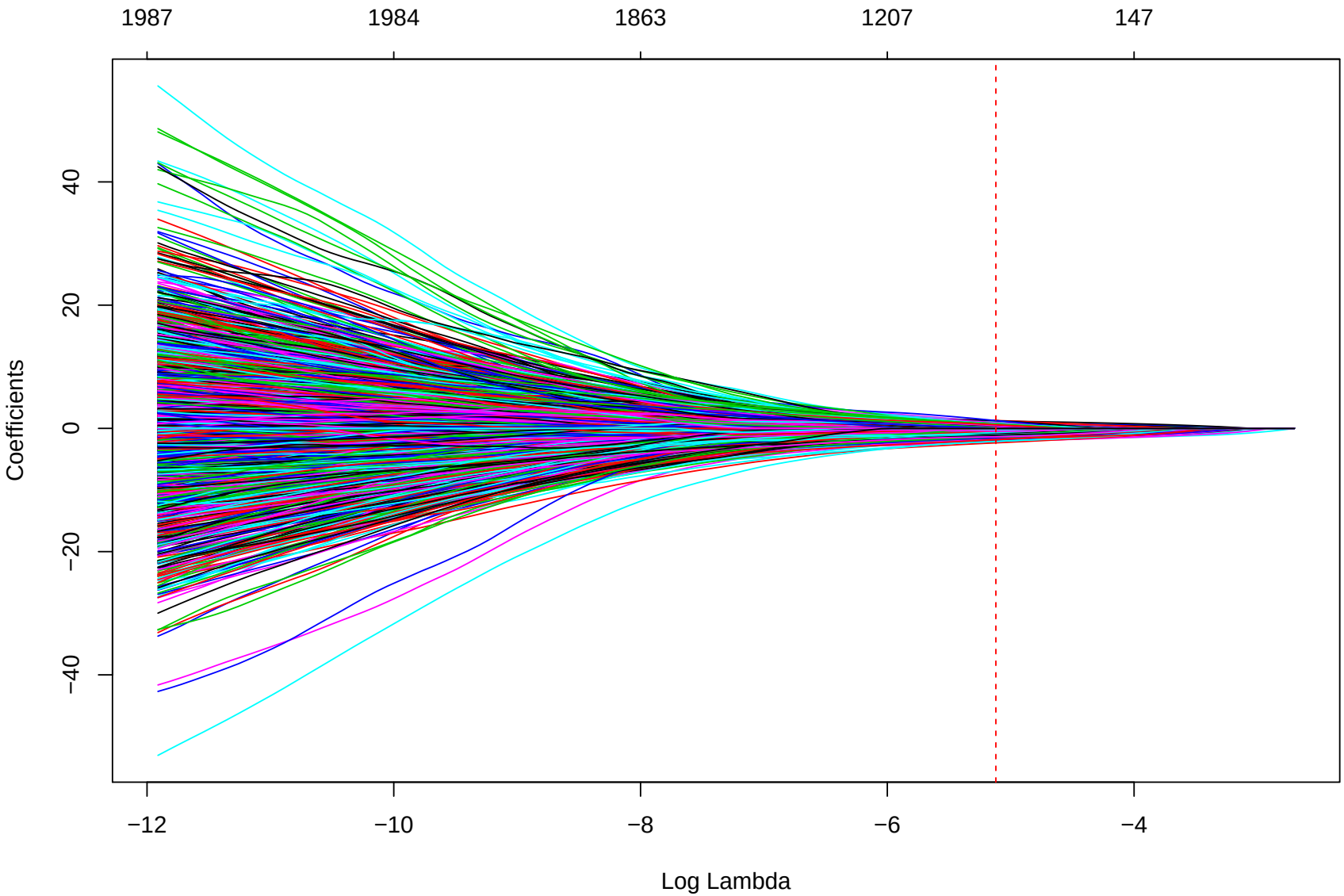
```
##   Food Service Value Atmosphere Overall
## 1    5       5     5          5       5
## 2    5       5     5          5       5
## 5    5       5     4          4       5
```

```
# transform rating into {0, 1}
y = ifelse(we8thereRatings$Overall>3, 1, 0)
y = as.factor(y)
glm_fit = cv.glmnet(x = we8thereCounts, y = y,
                    family = "binomial",
                    # lasso - 1, ridge - 0
                    alpha = 1,
                    nfold = 5
                   )
```

Cross validation for Lasso



Coefficients for Lasso



```
glm.coef = coef(glm_fit$glmnet.fit, s=glm_fit$lambda.1se)
o = order( glm.coef, decreasing = TRUE )
```

```
# positive coefficients
glm.coef@Dimnames[[1]][o[1:10]]
```

```
##  [1] "can wait"        "between two"
##  [3] "beef sandwich"   "high recommend"
##  [5] "friend help"     "best meal"
##  [7] "food delici"     "(Intercept)"
##  [9] "melt mouth"      "wonder experi"
```

```
glm.coef[o[1:10]]
```

```
##  [1] 1.2741278 1.2633252 1.2482930 1.2121773
##  [5] 1.0930038 1.0704775 1.0245261 1.0169857
##  [9] 1.0118636 0.9496681
```

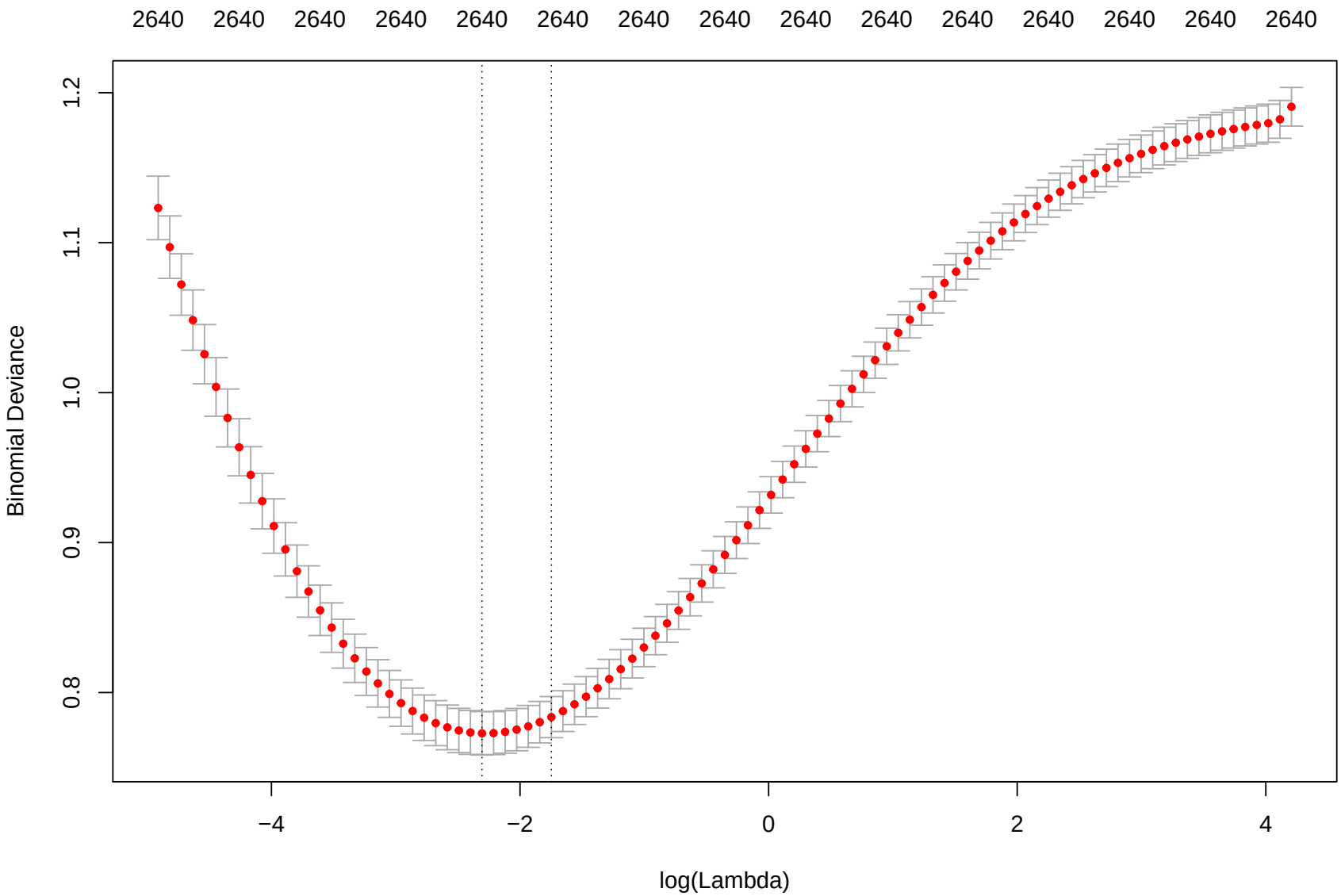
```
# negative coefficients
glm.coef@Dimnames[[1]][tail(o,10)]
```

```
##  [1] "gone down"       "never go"
##  [3] "servic terribl" "food terribl"
##  [5] "stay away"       "never return"
##  [7] "far better"      "mediocr best"
##  [9] "veri rude"       "extrem rude"
```

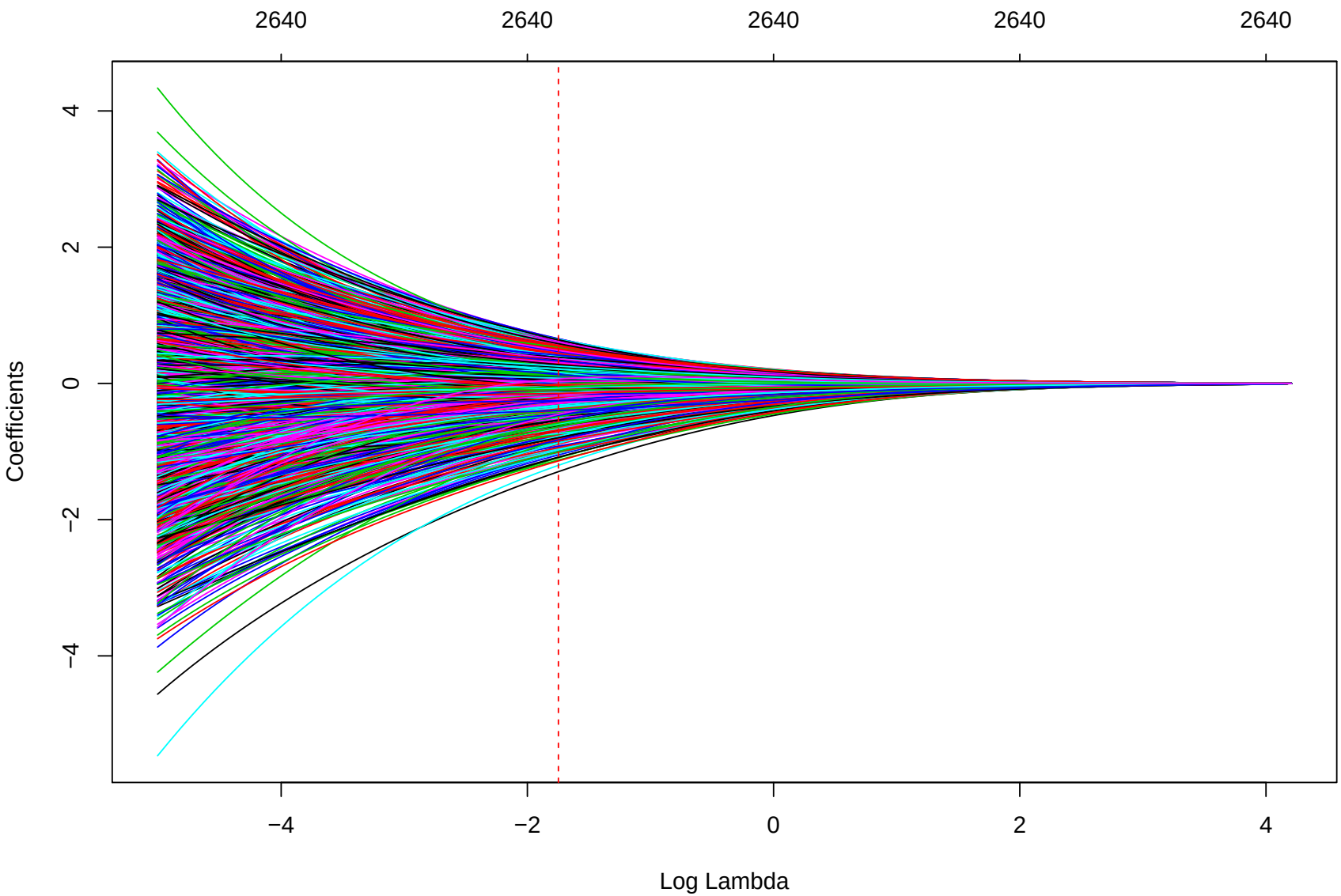
```
glm.coef[tail(o,10)]
```

```
##  [1] -1.842253 -1.875542 -1.892049 -1.939003
##  [5] -1.949946 -2.025724 -2.107226 -2.109239
##  [9] -2.191691 -2.348292
```

Cross validation for Ridge regression



Coefficients for Ridge



Avoiding overfitting using early stopping

Common practice is to stop gradient descent before it reaches optimum

One monitors peformance of the current solution on the validation data

If the performance starts to deteriorate, stop the descent

Why should this work?

Summary: Logistic regression

Learns conditional probability distribution

Linear desicion boundary. We can craft non-linear features (feature engineering), but the decision is going to be linear in the non-linear features.

Gradient descent starts with an initial vector and modifies it to find best parameter.