Logistic Regression

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About Logistic Regression

- Popularized by David Cox in 1950s
- Although a regression technique, often used for classification
- Also called **logit**
- Still very popular due to being **easy to understand and explain**, while still giving **good results**

Derivation

The logistic regression is part of the **generalized linear model (GLM)** family:

$$\begin{aligned} P(Y|X=x) &= \sigma(\beta_0 + \beta_1 x_1 + \ldots) \\ &= \sigma(\beta_0 + \beta^\intercal X) \end{aligned}$$

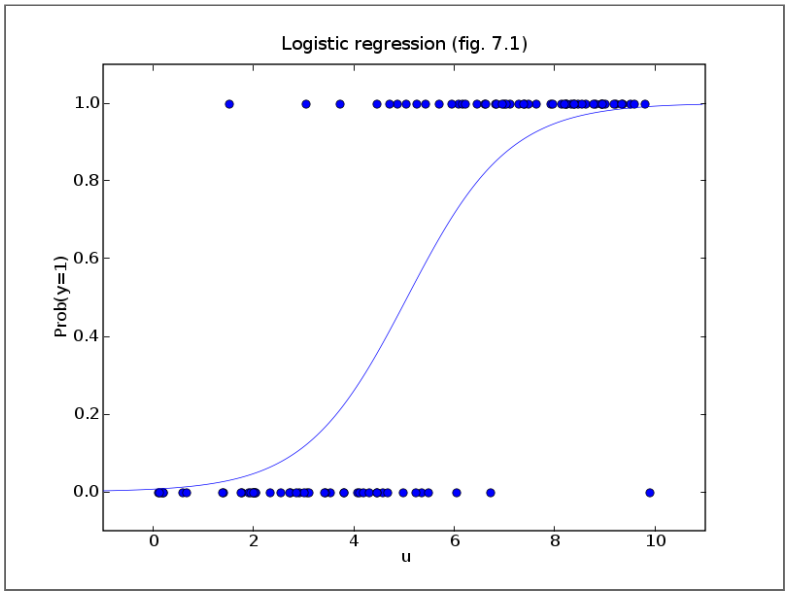
in the case of logistic regression, we have $\sigma(x) = 1/(1+e^{-x})$ to give:

$$P(Y|X=x) = \frac{1}{1+e^{-\beta^\intercal X}}$$

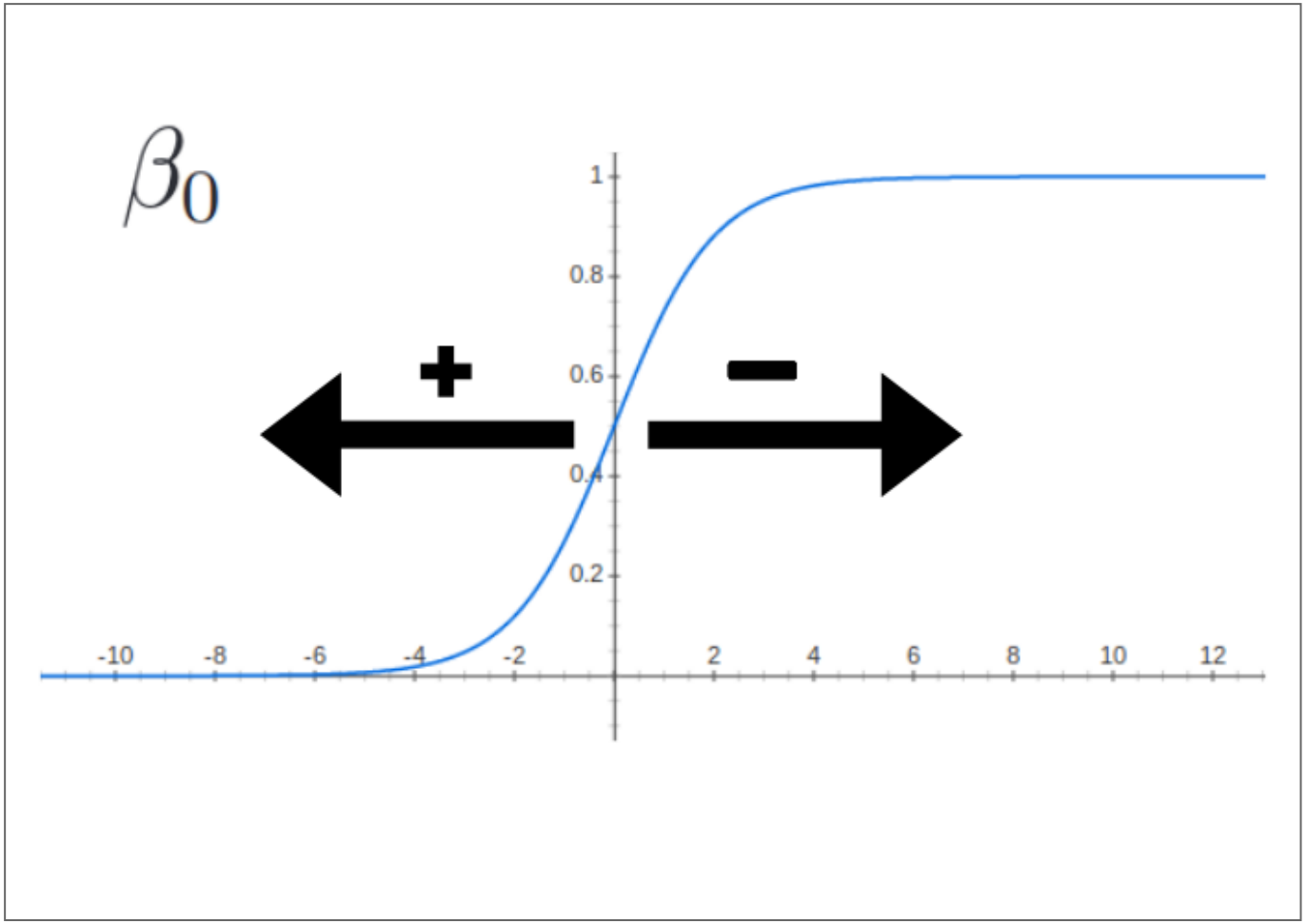
In the case of 1-dimensional X, we get

$$P(Y|X=x) = \frac{1}{1+e^{-(\beta_0+\beta_1 x)}}$$

which, when trained, looks like this



So what happens when we change the parameters β_0, β_1?


β_0
1
0.8
0.6
0.4
0.2
-10
-8
-6
-4
-2
2
4
6
8
10
12
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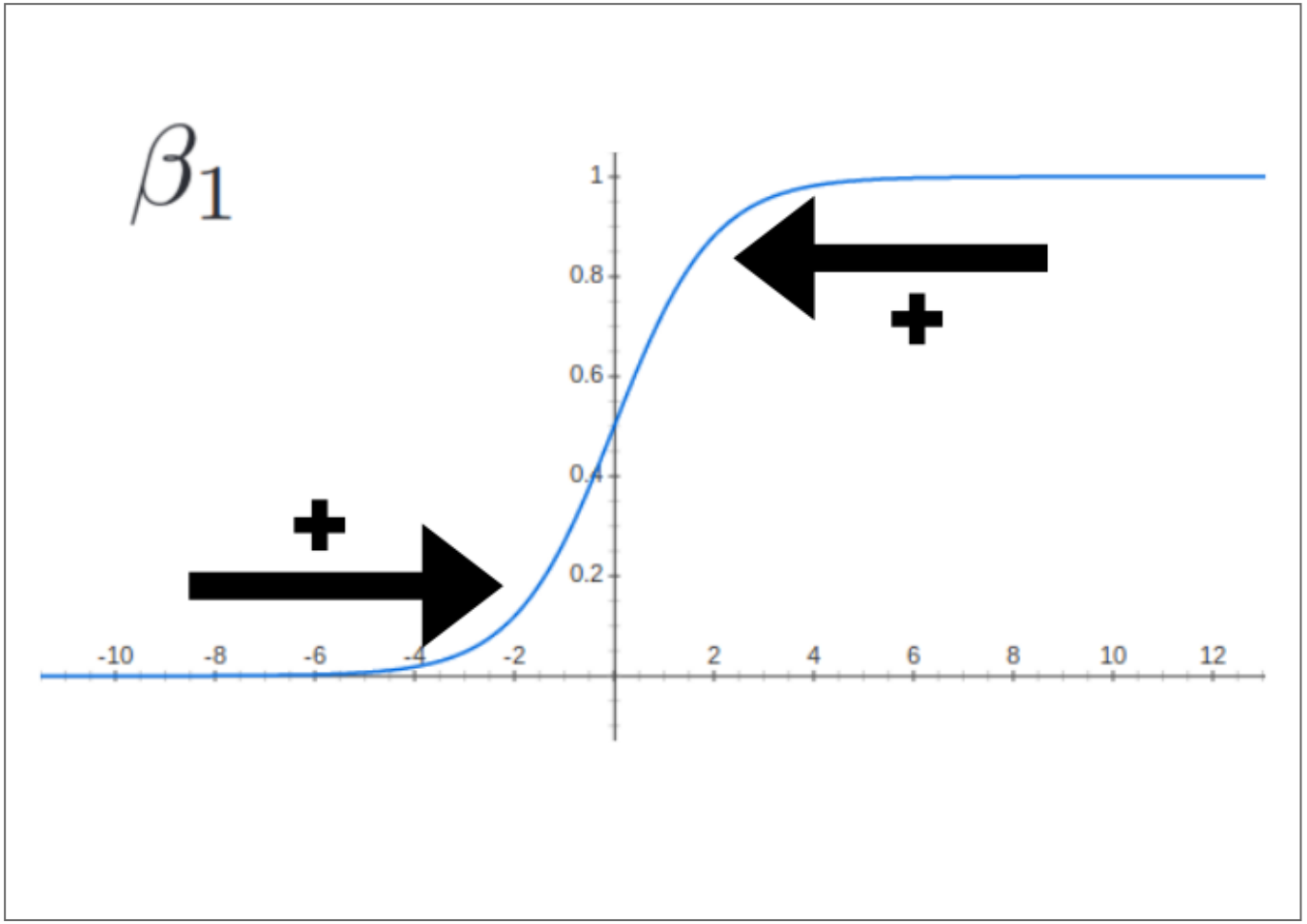
β_1
1
0.8
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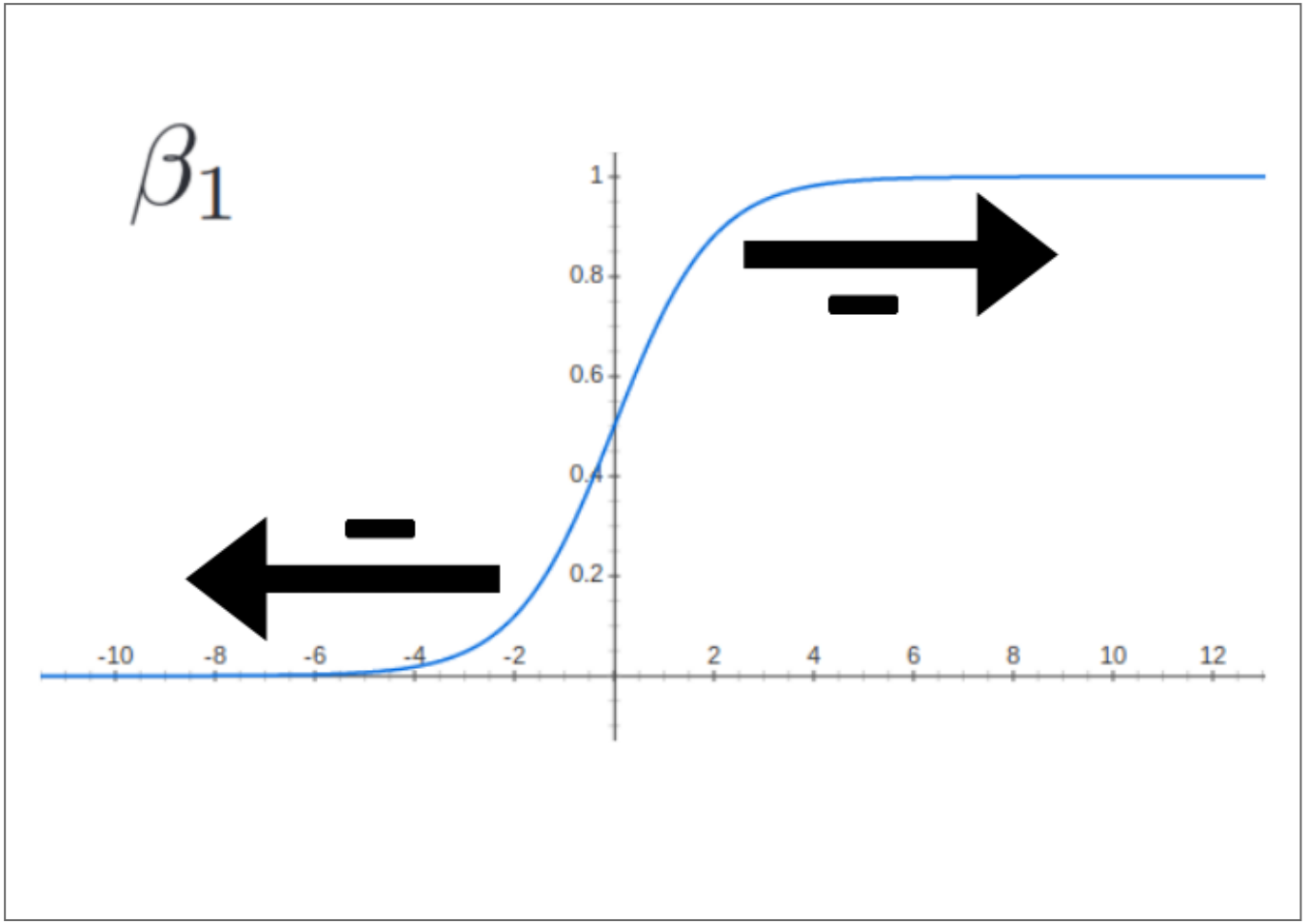

β_1
1
0.8
0.6
0.4
0.2
-10
-8
-6
-4
-2
2
4
6
8
10
12

Interpretation of weighted sum

$$P(Y=1|X=x) = \frac{1}{1+e^{-\beta^\intercal x}}$$

$$P(Y=1|X=x)\left(1+e^{-\beta^\intercal x}\right) = 1$$

$$P(Y=1|X=x) + P(Y=1|X=x)e^{-\beta^\intercal x} = 1$$

$$P(Y=1|X=x)\left(1+e^{-\beta^\intercal x}\right) = 1$$

We can write $1 - P(Y=1|X=x) = P(Y=0|X=x)$ to obtain:

$$\frac{P(Y=1|X=x)}{P(Y=0|X=x)} = e^{\beta^\intercal x}$$

$$\log\left(\frac{P(Y=1|X=x)}{P(Y=0|X=x)}\right) = \beta^\intercal x$$

This last expression

$$log\left(\frac{P(Y=1/X=x)}{P(Y=0/X=x)}\right)=\beta^{T}x$$

tells us that the weighted sum of the data can be interpreted as the **log-odds ratio**

Another interpretation

We can also view this as a sequence of mappings

- A function which maps the vector x to a single real number

$$\mathbb{R}^m \rightarrow \mathbb{R} : x \mapsto \beta^\intercal x$$

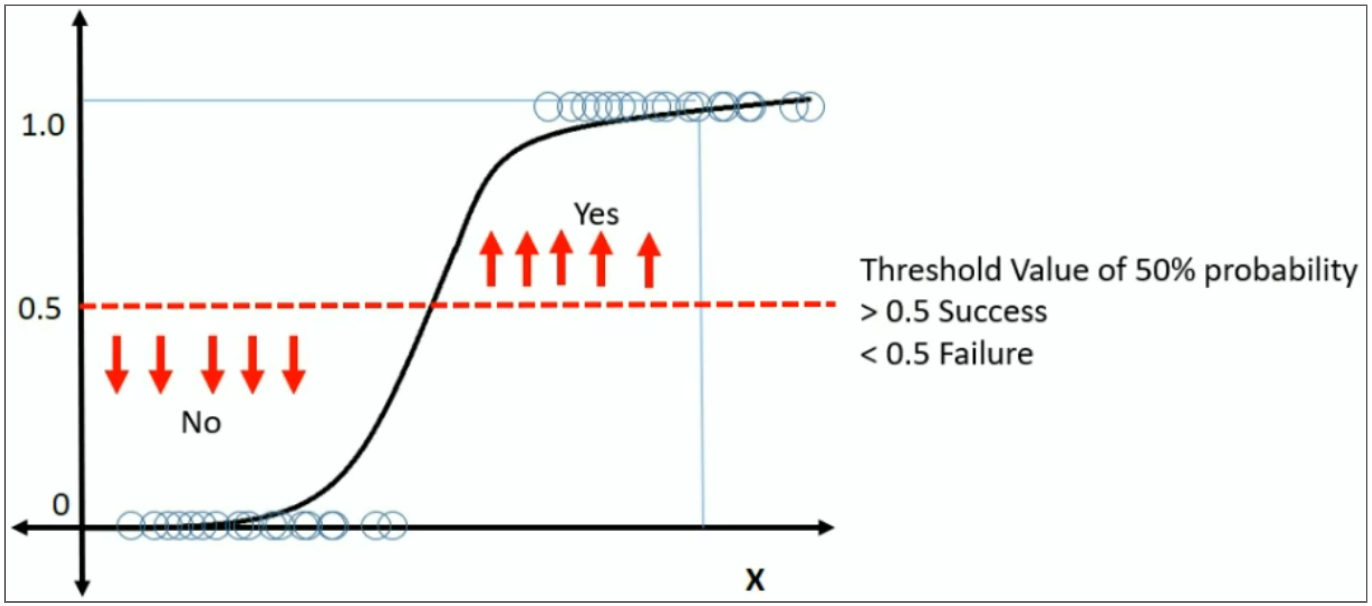
- A function which normalizes this number to a probability (monotonically):

$$\mathbb{R} \rightarrow [0, 1] : x \mapsto \frac{1}{1 + e^{-x}}$$

Decision Boundary

One problem left, we want values in $\{0, 1\}$, not $[0, 1]$.

We can solve this by introducing a **threshold** t



Finding decision boundary

Let's find the boundary in our parameter space $x \in \mathbb{R}^m$:

$$\begin{aligned} P(Y = 1 | X = x) &= \frac{1}{1 + e^{-\beta^\intercal x}} \\ &= 1/2 \end{aligned}$$

We can rewrite this as

$$\begin{aligned} \frac{1}{1 + e^{-\beta^\intercal x}} &= \frac{1}{2} \\ 1 + e^{-\beta^\intercal x} &= 2 \\ e^{-\beta^\intercal x} &= 1 \\ \beta^\intercal x &= 0 \end{aligned}$$

Finding decision boundary

The boundary is the set of points $\{x \in \mathbb{R}^m : \beta^\intercal x = 0\}$

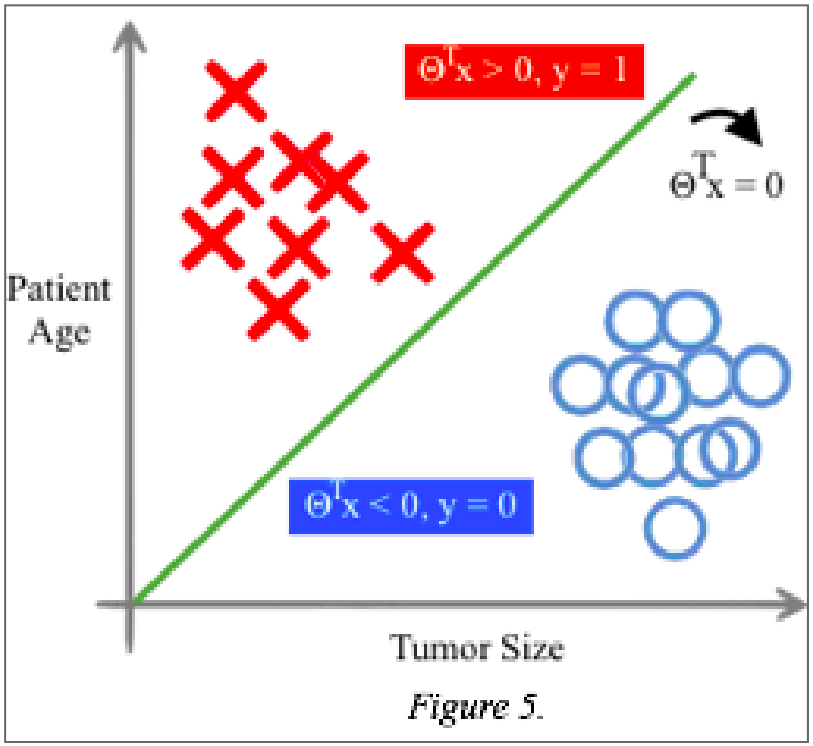


Figure 5.

Evaluating Models

So now that we've defined a model $\hat{y}_\beta$, we now have to find out how to choose the best one to fit our data.

In order to make this decision, we first need to **define what a good model is.**

*We do this with an **Loss function.***

Evaluating Models

We want a function that maps $\mathcal{L} : \mathbb{R}^{m+1} \to \mathbb{R} : \beta \mapsto \mathcal{L}(\hat{y}_\beta(x), y)$

This will allow us to, given the features x and labels y, compare two sets of parameters to see which one performs better.

Often the **log-likelihood (aka cross-entropy)** is used for this

Log-likelihood

The likelihood $\mathcal{L}$ is expressed by

$$\mathcal{L}(\beta) = \prod_{i=1}^{n} P(Y = y_i | X = x_i; \beta)$$

which is the probability of the data occuring, given the model parameter β.

This is hard to work with, so we usually work with the log-likelihood

$$\log \mathcal{L}(\beta) = \sum_{i=1}^{n} \log P(Y = y_i | X = x_i; \beta)$$

Note that $\mathcal{L}$ and $\log \mathcal{L}$ have the same maximum

Log-likekelihood

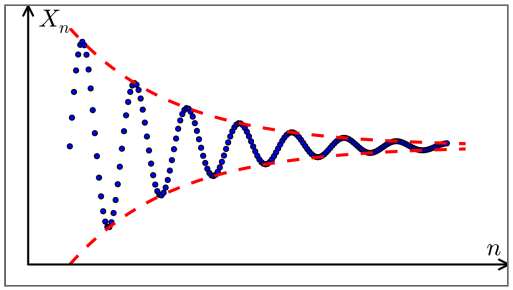
We can rewrite this to another common form using the powers of math:

$$
\begin{aligned}
\log \mathcal{L}(\beta) &= \sum_{i=1}^{n} \log P(Y = y_i | X = x_i; \beta) \\
&= \sum_{i=1}^{n} \log P(Y = 1 | X = x_i; \beta)^{y_i} + \log P(Y = 0 | X = x_i; \beta)^{(1-y_i)} \\
&= \sum_{i=1}^{n} y_i \log(\hat{y}_\beta(x)) + (1 - y_i) \log(1 - \hat{y}_\beta(x_i))
\end{aligned}
$$

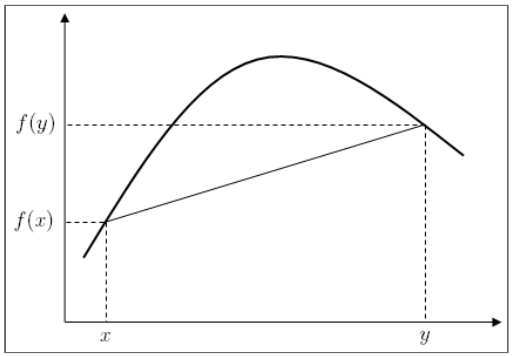
The form at the bottom is called the **cross-entropy**

Why maximum likelihood?

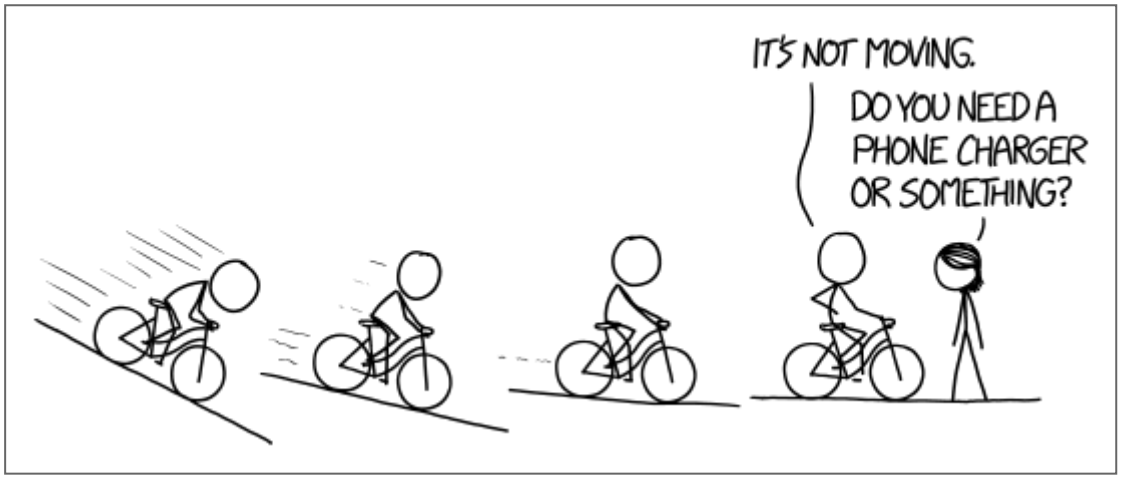
- Unbiased and consistent (under certain conditions)



- Concave function on parameter space

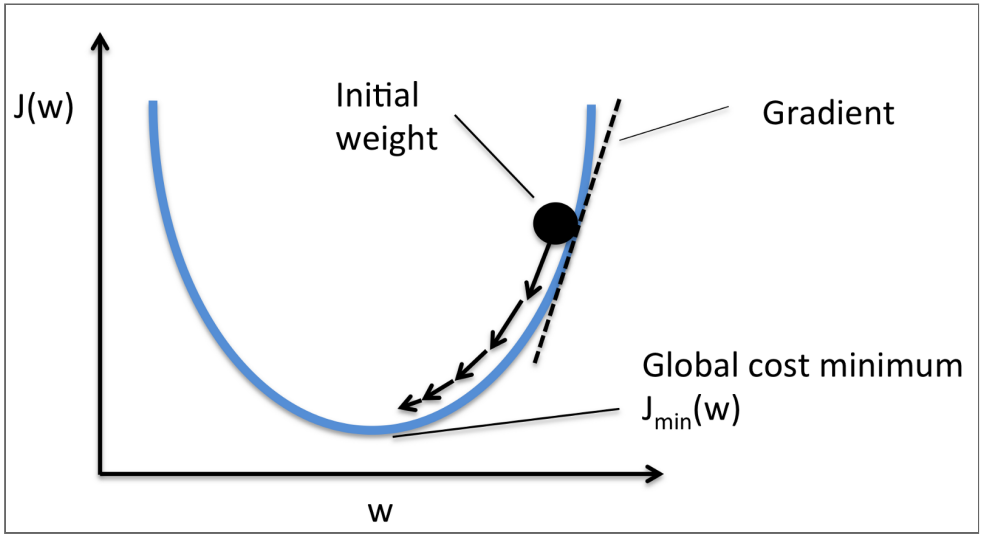


Finding the Best Model Parameters



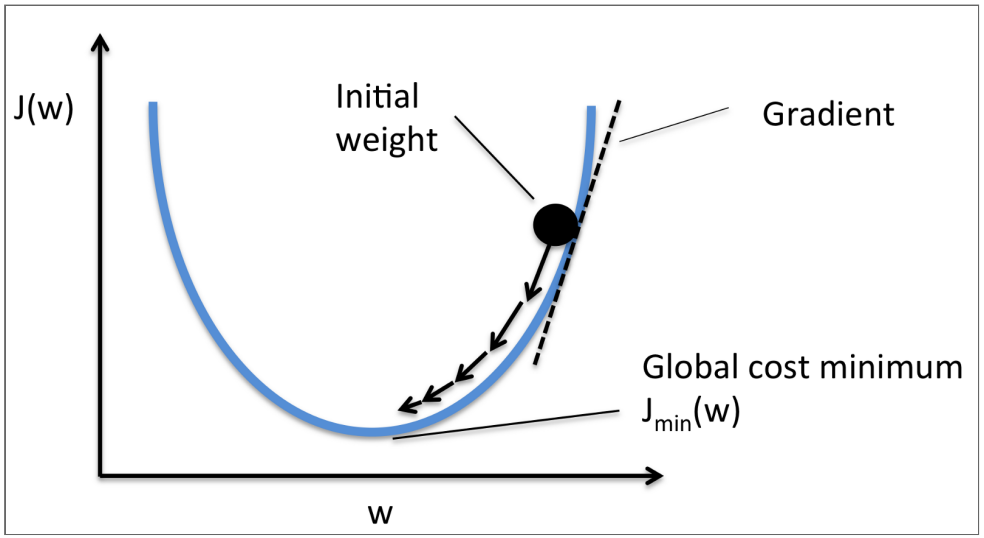
Gradient Descent Algorithm

Start at a random point, and follow the slope downwards until we stop



Gradient Descent Algorithm

1. *Set a_0 to some starting parameters (e.g. 0)*
2. *Until some condition (iterations, closeness), do:*
    - *Calculate $a_{n+1} = a_n - \gamma \nabla F(a_n)$*



Note that we need to choose the **starting point** a_0, the **learning rate** γ, and the **stopping criterion**.

Calculating Gradient $\nabla F(a_n)$

$$\nabla f := \left(\frac{\partial f}{\partial x_1}, \ldots, \frac{\partial f}{\partial x_m} \right)$$

With some math and the chain rule we can show that

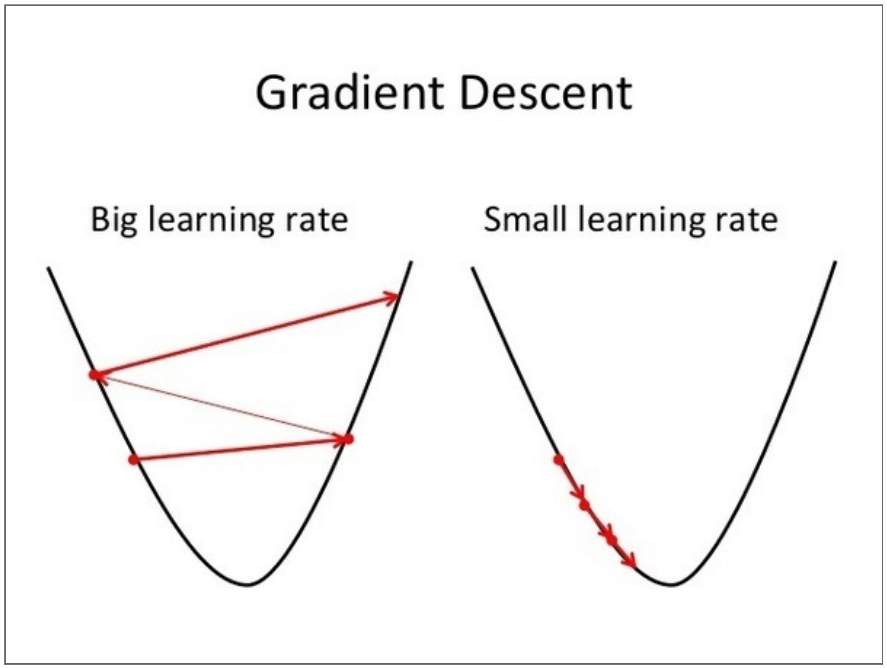
$$\frac{\partial \log \mathcal{L}}{\partial \beta_j} = \sum_{i=1}^{n} \left(\hat{y}_\beta(x^i) - y^i \right) x_j^i$$

We can vectorize this to:

$$\nabla \log \mathcal{L} = x^\intercal \left(\hat{y}_\beta(x) - y \right)$$

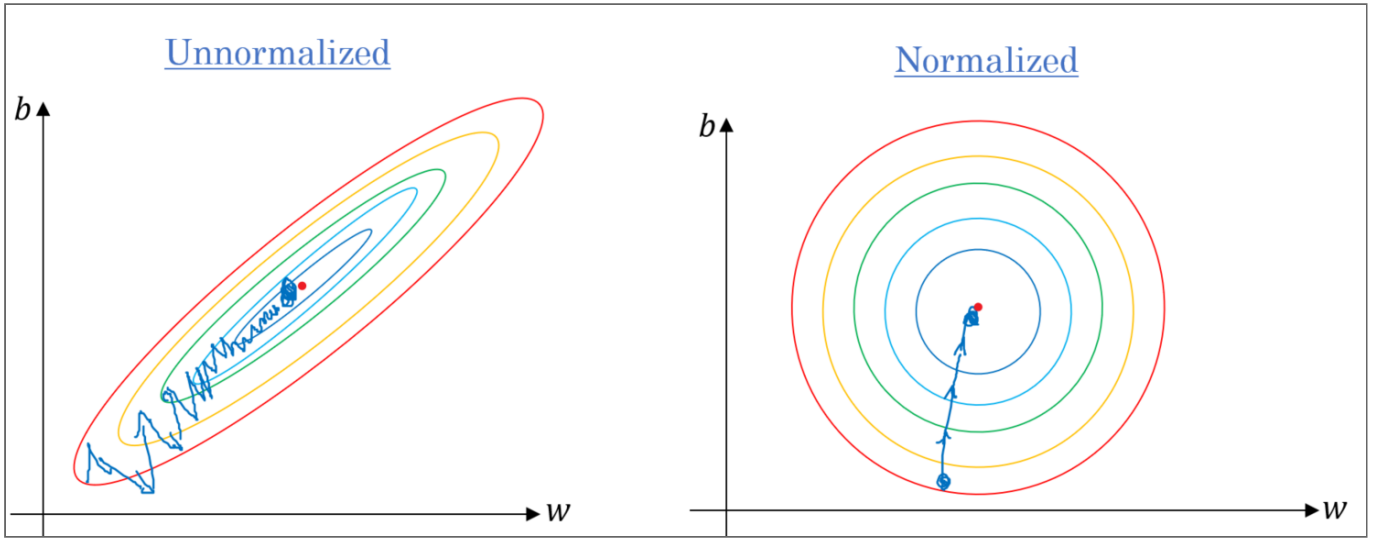
Choosing γ

Watch out what learning rate is chosen:



There are dynamic learning rates γ_n which calculate the optimal rate

Normalizing features



Normalizing features can make convergence faster

Gradient Descent Algorithm

Some limitations:

1. Slow converge (there are faster methods)
2. Only finds global maximum on convex functions
3. Our objective function must be differentiable to find gradient

Stochastic Gradient Descent

Often Stochastic Gradient Descent is used instead of plan GD

Instead of calculating the gradient $\nabla log \mathcal{L}$ on all rows of data:

- *randomly pick a row x_i*
- *update β with the gradient for the loss at x_i*
- *if stopping criterion is fulfilled, stop*

Mini-batch gradient descent uses a batch $\{x_i, \ldots, x_j\}$ for updating β

Newton's Method

1. *Initialize at starting point a_0*
2. *Calculate 2nd order taylor approximation T of F at a_0*
3. *Find minimum of T, and set a_{n+1} to this minimum*

The step can be calculated with

$$x_{n+1} = x_n - \gamma_n [\mathbf{H} f(x_n)]^{-1} \nabla f(x_n)$$

where H is the Hessian operator, which gives the matrix of all second order derivatives

Problem with Newton's Method

If we have lots of features, the **Hessian becomes expensive to compute**

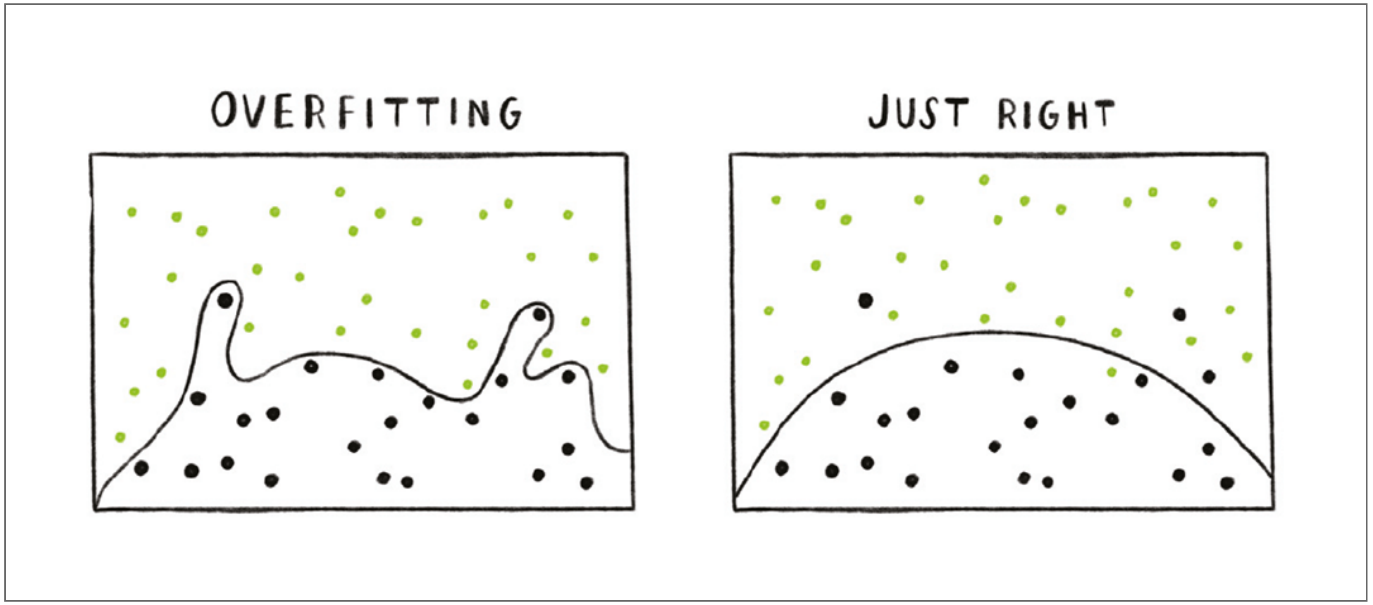
Quasi-Newton methods approximate the Hessian matrix to speed things up

Enter Quasi-Newton methods

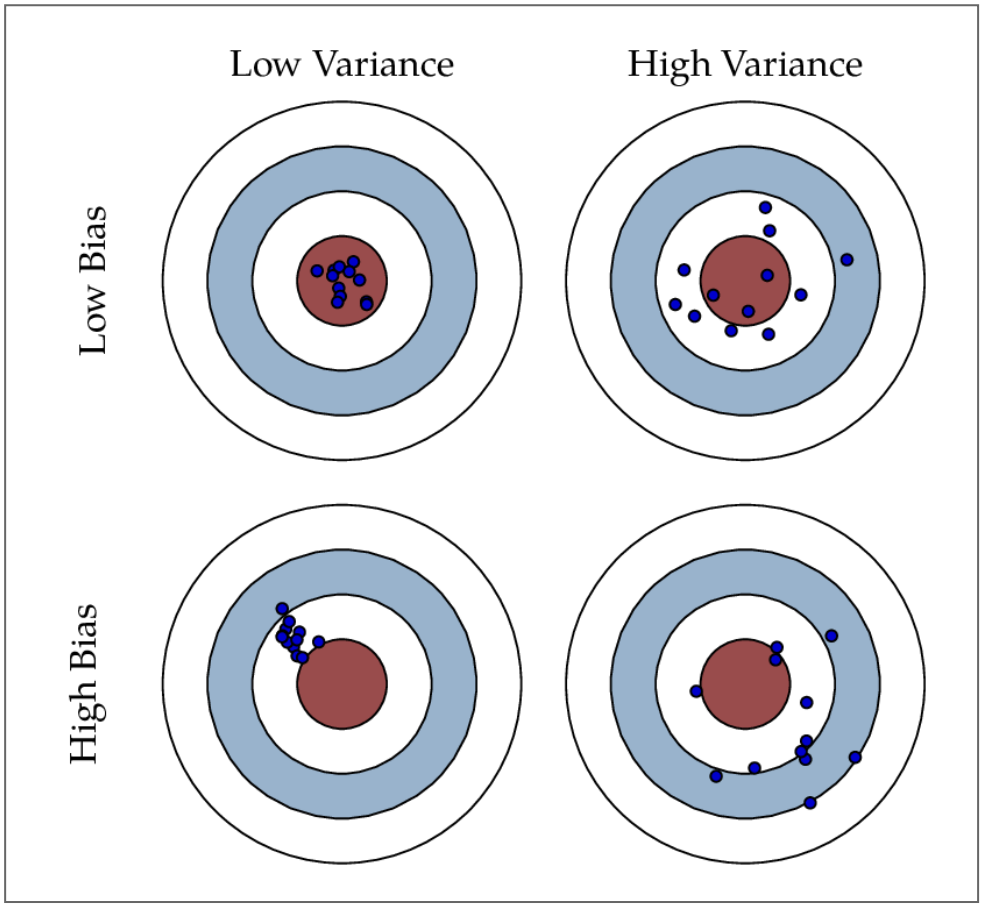
Instead of the inverse Hessian, we can work with an **approximation** of H^{-1}

1. Most used is **BFGS** which iteratively approximates the Hessian $\{h_0, h_1, \ldots\}$
2. Storing the approximation h_i takes a lot of memory, so **L-BFGS** only stores the minimal information needed to compute h_i.

Reducing Overfitting

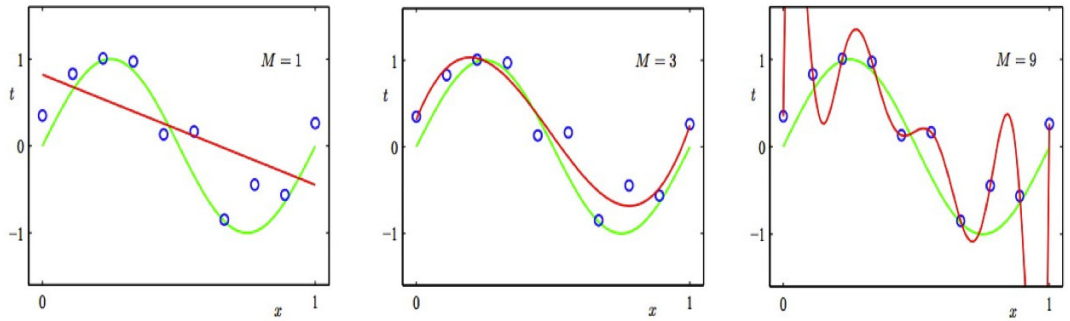


What are Bias and Variance



The bias-variance tradeoff (signal vs noise)

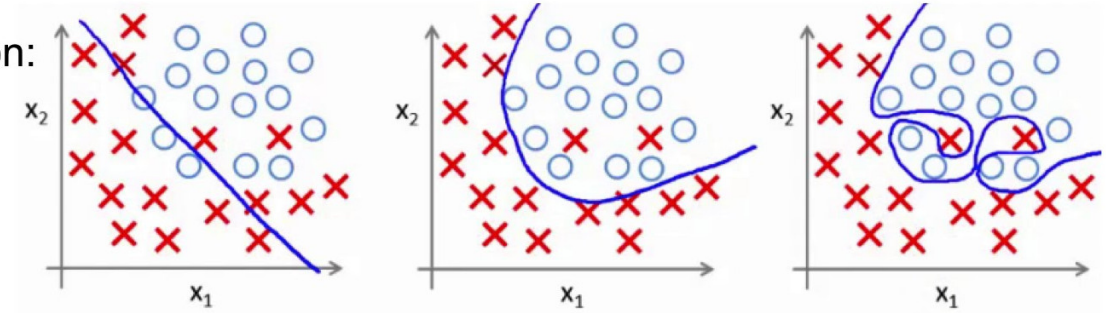
Regression:



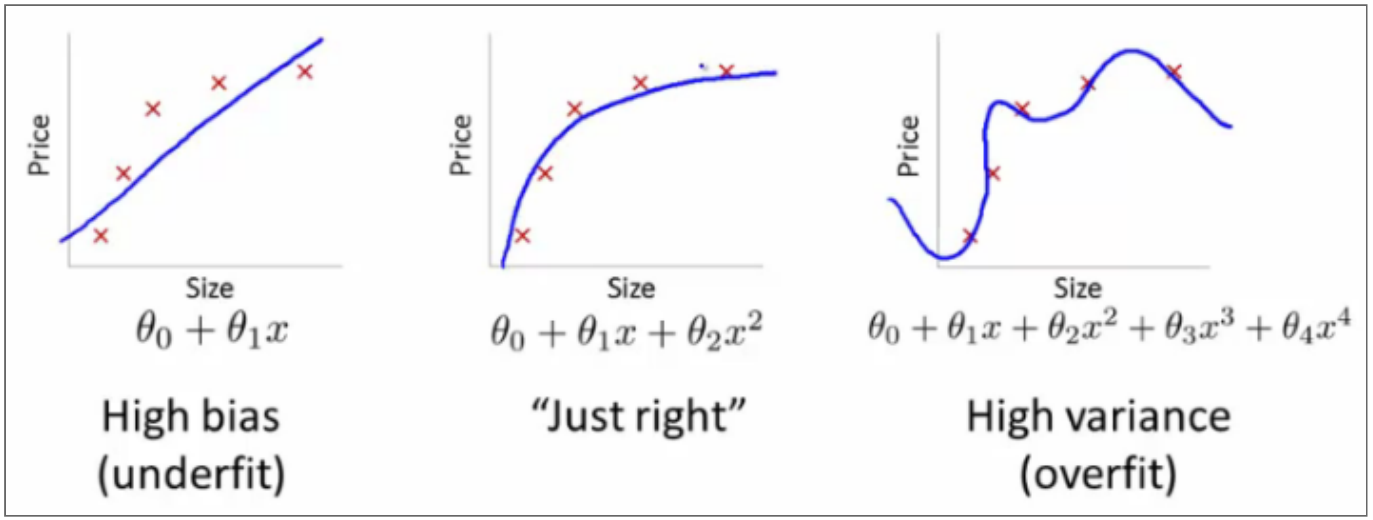
predictor too inflexible:
cannot capture pattern

predictor too flexible:
fits noise in the data

Classification:



How do we solve this?



We need to adjust the complexity of our model

Reducing Overfitting

There are two often used techniques for reducing overfitting:

1. L2 Regularization (Ridge Regression)
2. L1 Regularization (Lasso Regression)

They both **add bias to the model to reduce variance**

Regularizaton

Originally we were minimizing the error:

$$\sum_{i=1}^{n} L(\beta, x_i) = \sum_{i=1}^{n} y_i \log(\hat{y}_\beta(x)) + (1 - y_i) \log(1 - \hat{y}_\beta(x_i))$$

If we add a constant term *(bias)* to the error, we get:

$$\min_{\beta} \sum_{i=1}^{n} L(\beta, x_i) + \lambda \|\beta\|$$

where $\|\beta\|$ is the "size" of β

L2 Regularization (aka Ridge)

In the case of L2 regularization, we have $||\beta||_2 = \sum_i \beta_i^2$, or

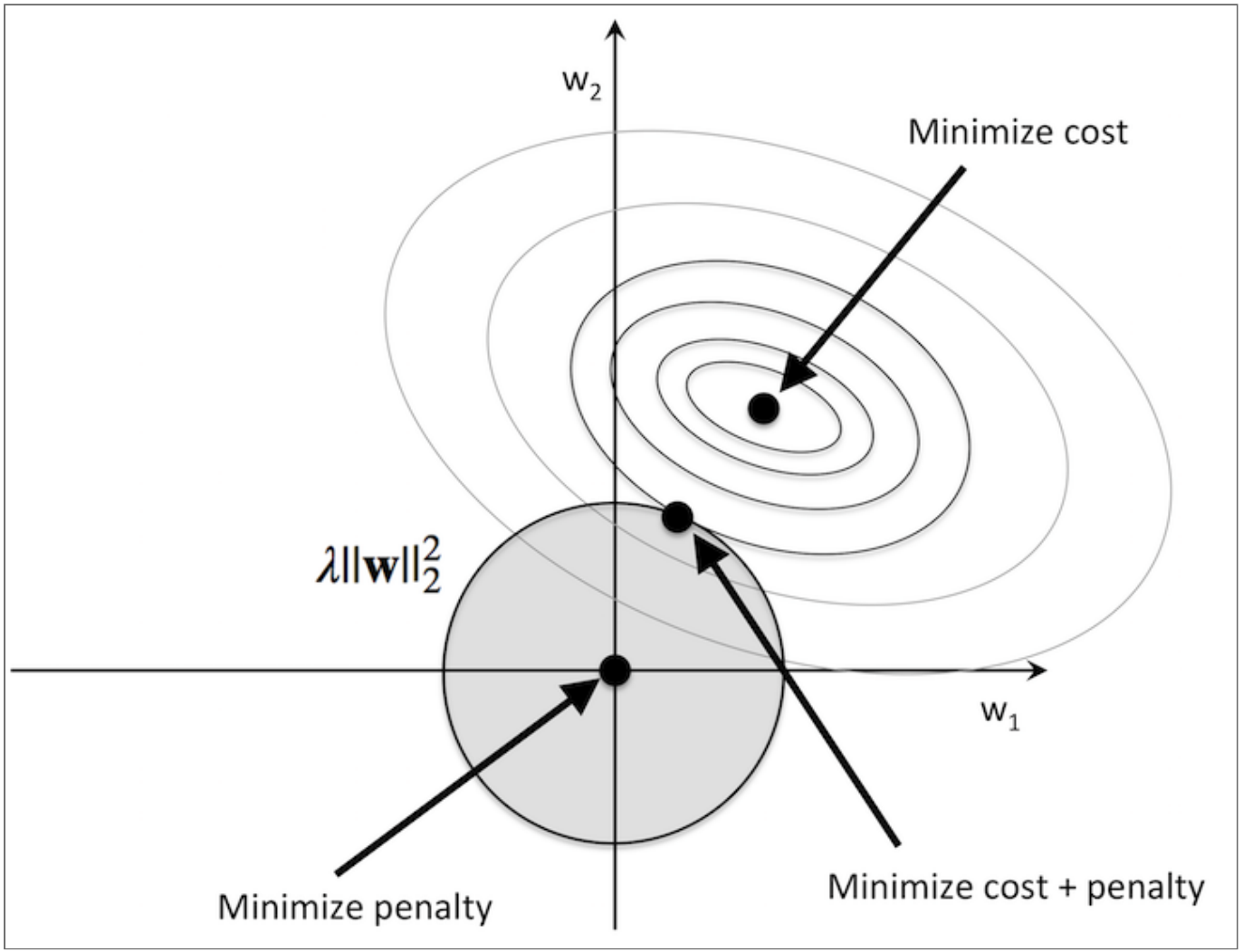
$$\min_{\beta} \sum_{i=1}^{n} L(\beta, x_i) + \lambda \sum_{j=1}^{M} \beta_j^2$$

this is the same as

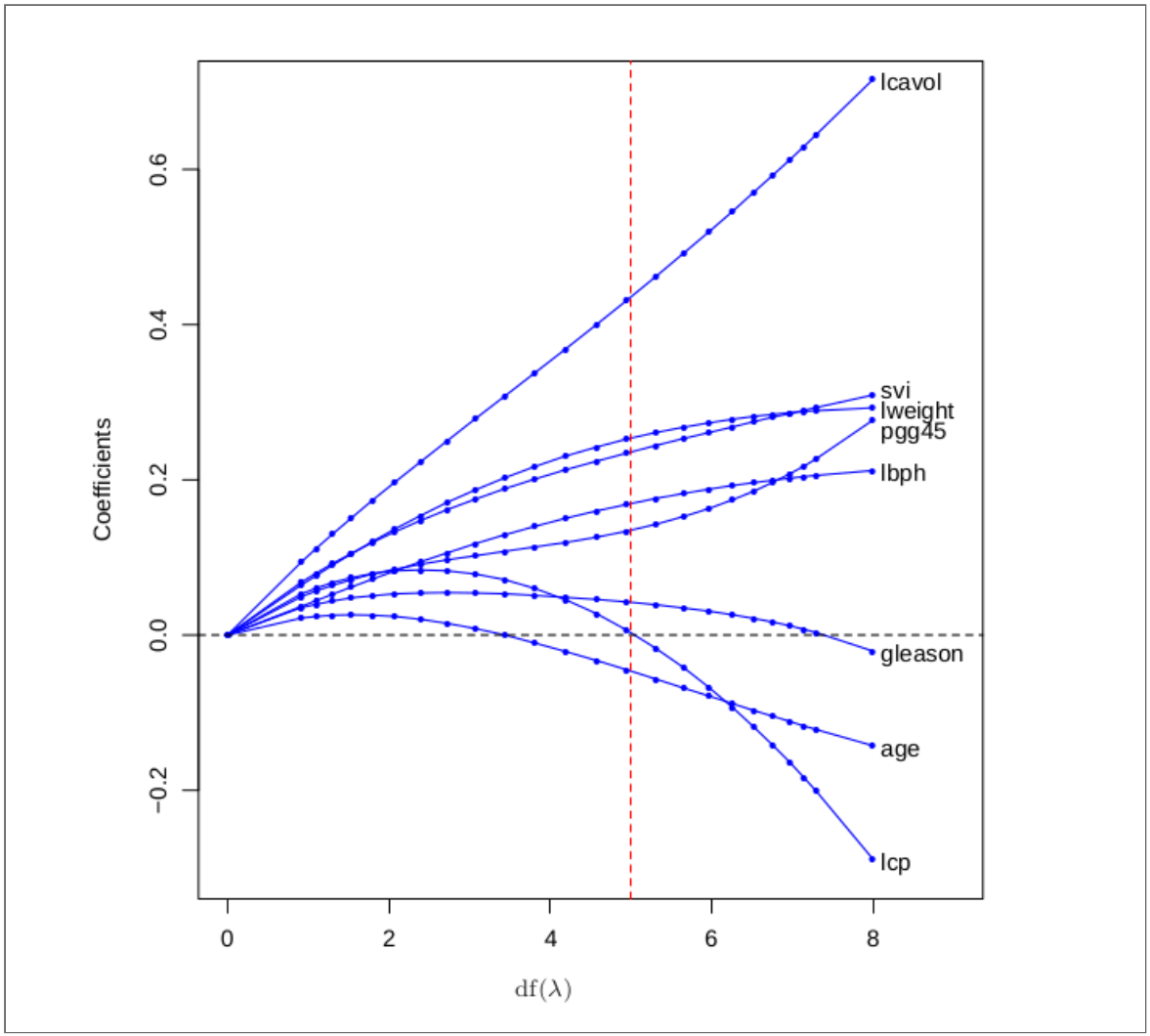
$$\min_{\beta} \sum_{i=1}^{n} L(\beta, x_i)$$

with the constraint that $\sum_{j=1}^{M} \beta_j^2 < \lambda$

L2 Visual Aid



Controlling Regularization with λ



L1 Regularization (aka Lasso)

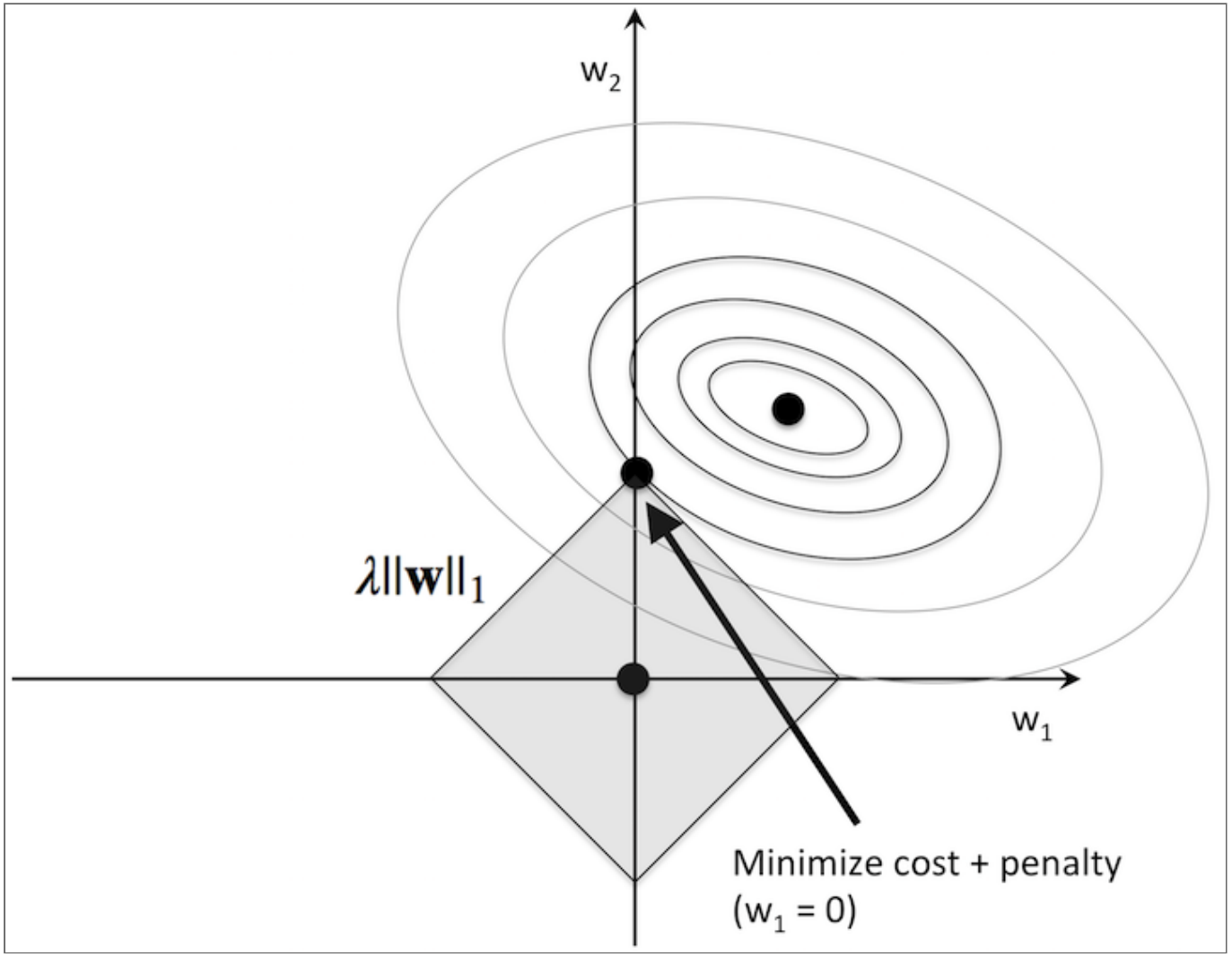
With lasso we use the L1 norm $\|\beta\|_1 = \sum_j |\beta_j|$, which gives:

$$\min_{\beta} \sum_{i=1}^{n} L(\beta, x_i)$$

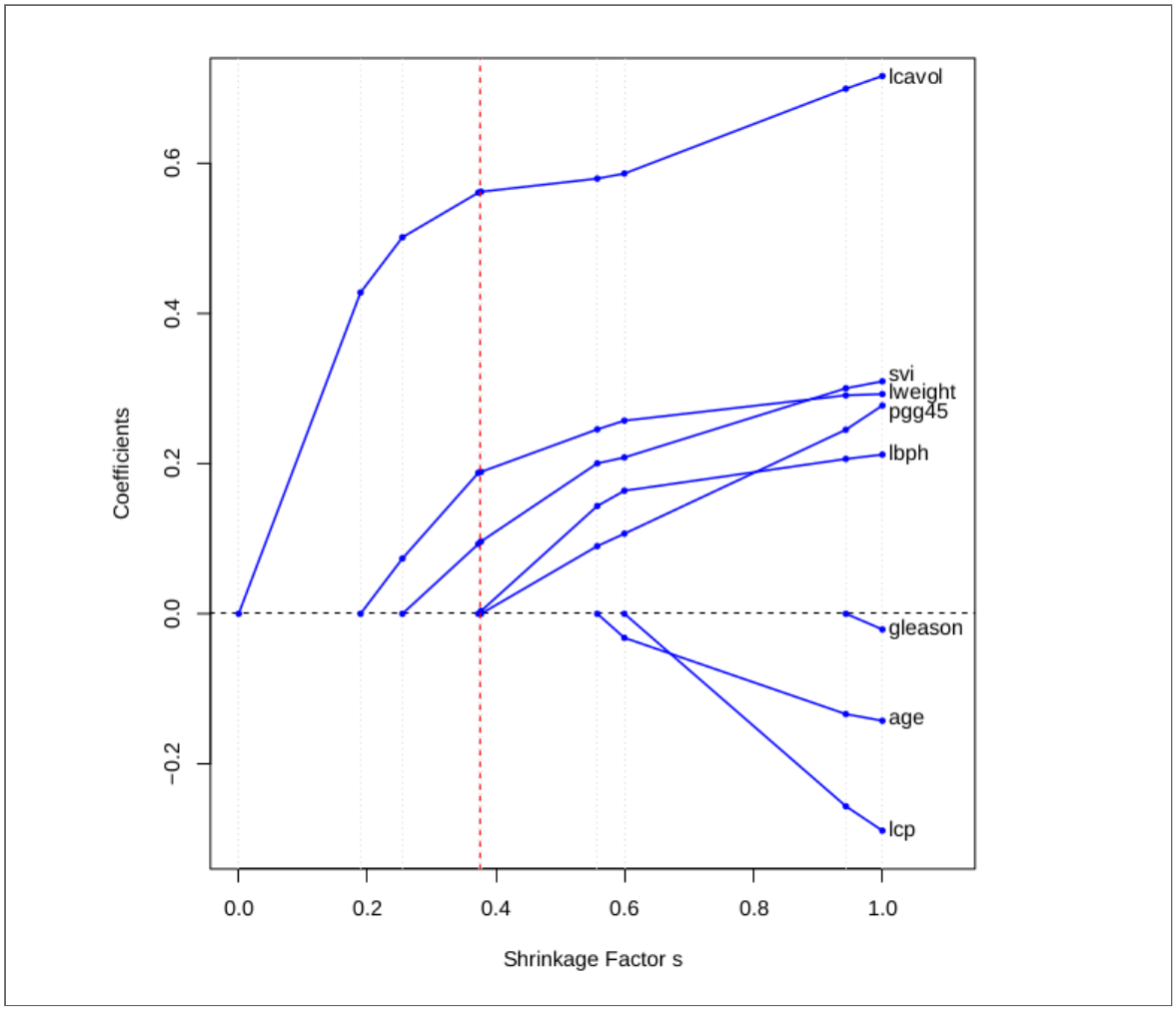
with the constraint that $\sum_{j=1}^{M} |\beta_j| < \lambda$

What area of the parameter space is allowed?

L1 Visual Aid



Controlling Regularization with λ



Building our own Logistic Regression