Maximum Likelihood Estimation

Frequentist Statistics

Answers the question: **What is Data?** with

"data is a **sample** from an existing **population**"

- data is stochastic, variable
- model the sample. The model may have parameters
- find parameters for our sample. The parameters are considered **FIXED**.

Our coin flip example

- in our coins example, the true proportion, called p^* comes from all possible (infinite) coin flips. We never get to see this
- This of course depends on if our model describes the true generating process for the data, otherwise we can find a p^* given a population, but still have model mis-specification error
- if we are only given one (finite sample sized) replication, which is the situation in real life, we can only estimate a probability $\hat{p}$
- In our idealized, simulated case we have many M replications, and thus samples, and we can now find the **distribution** of estimated probab ilities $\hat{p}$

Lets start by focussing on how to find one $\hat{p}$

Likelihood

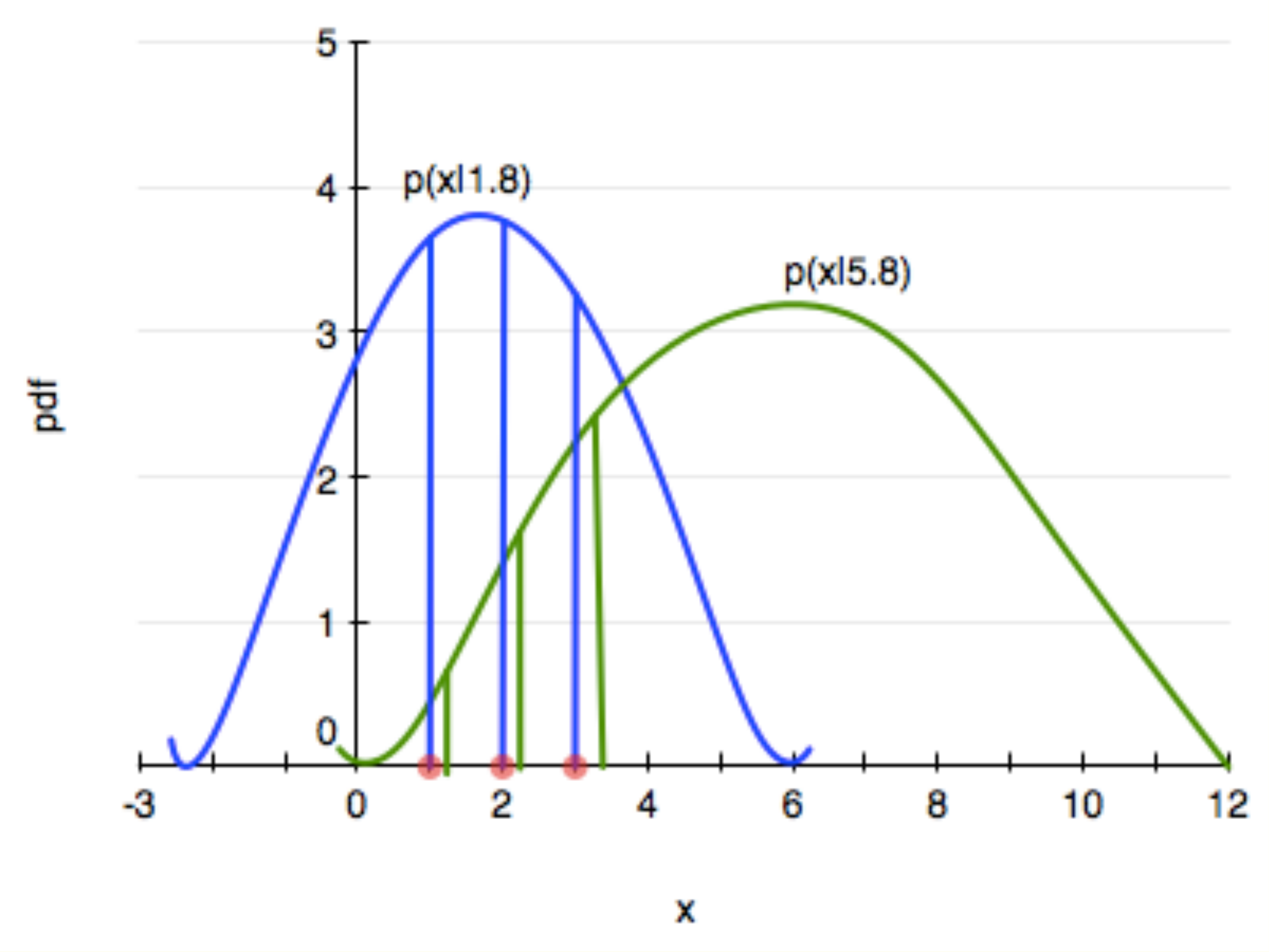
How likely it is to observe values $x_1, \ldots, x_n$ given the parameters θ?

$$L(\lambda) = P(\{x_i\}|\theta) = \prod_{i=1}^{n} P(x_i|\theta)$$

How likely are the observations if the model is true?

Remember, if your model describes the true generating process for the data, then there is some true θ^*. We dont know this. The best we can do is to estimate $\hat{\theta}$.

Maximum Likelihood estimation

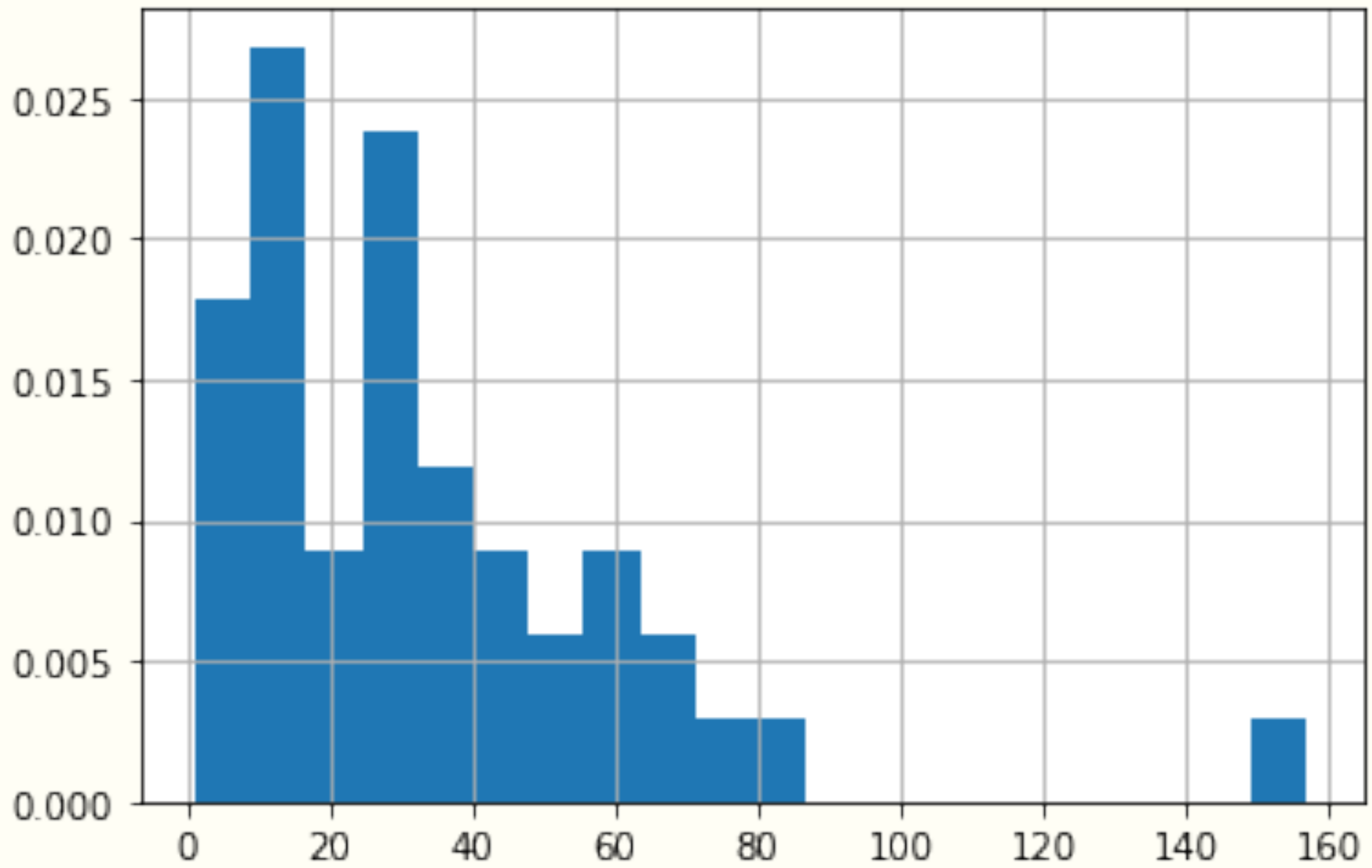


Example: Exponential Distribution Model

$$f(x;\lambda) = \begin{cases} \lambda e^{-\lambda x} & x \geq 0, \\ 0 & x < 0. \end{cases}$$

Describes the time between events in a homogeneous Poisson process (events occur at a constant average rate). Eg time buses arriving, radioactive decay, telephone calls and requests for a particular document on a web server

Consider the arrival times of the babies in a hospital. There is no reason to expect any specific clustering in time, so one could think of modelling the arrival of the babies via a poisson process.



log-likelihood

Maximize the likelihood, or more often (easier and more numerically stable), the log-likelihood

$$\ell(\lambda) = \sum_{i=1}^{n} ln(P(x_i \mid \lambda))$$

In the case of the exponential distribution we have:

$$\ell(lambda) = \sum_{i=1}^{n} ln(\lambda e^{-\lambda x_i}) = \sum_{i=1}^{n} (ln(\lambda) - \lambda x_i) \,.$$

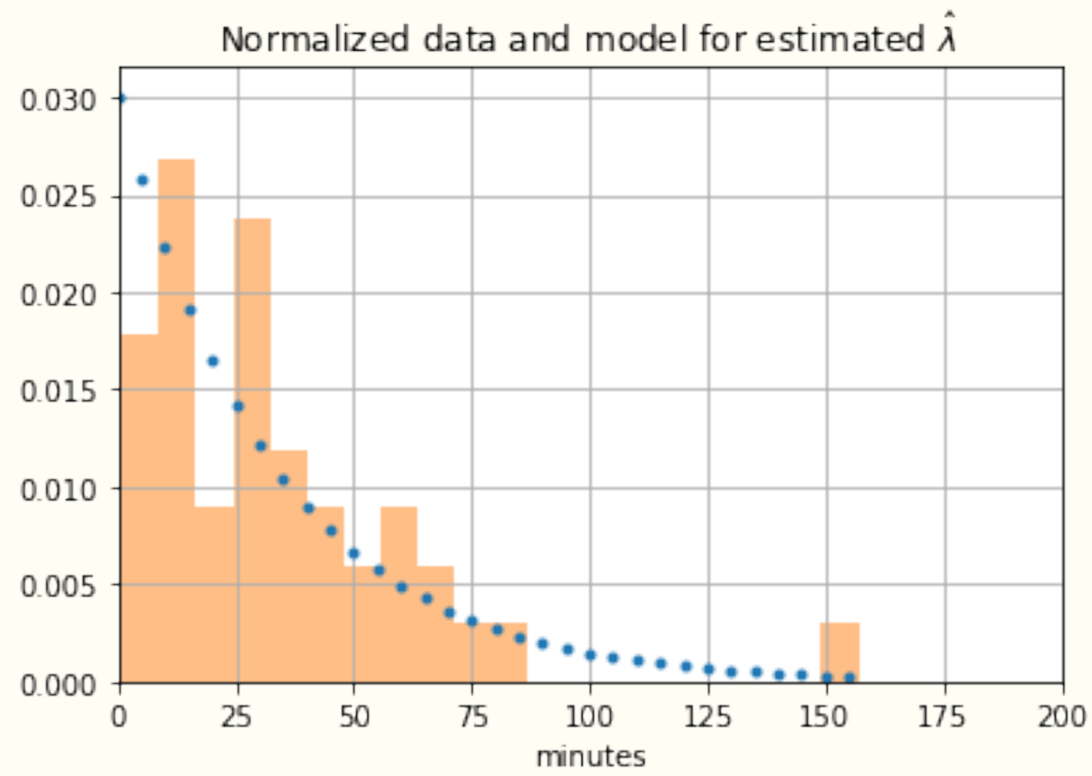
Maximizing this:

$$\frac{d\ell}{d\lambda} = \frac{n}{\lambda} - \sum_{i=1}^{n} x_i = 0$$

and thus:

$$\frac{1}{\hat{\lambda}_{MLE}} = \frac{1}{n}\sum_{i=1}^{n} x_i,$$

which is the sample mean of our sample.




```
lambda_from_mean = 1./timediffs.mean()
minutes=np.arange(0, 160, 5)
rv = expon(scale=1./lambda_from_mean)
plt.plot(minutes,rv.pdf(minutes),'.')
timediffs.hist(density=True, alpha=0.5, bins=20);
```

INFERENCE: True vs estimated

If your model describes the true generating process for the data, then there is some true θ^*.

We dont know this. The best we can do is to estimate $\hat{\theta}$.

Now, imagine that God gives you some M data sets **drawn** from the population, and you can now find θ on each such dataset.

So, we'd have M estimates.

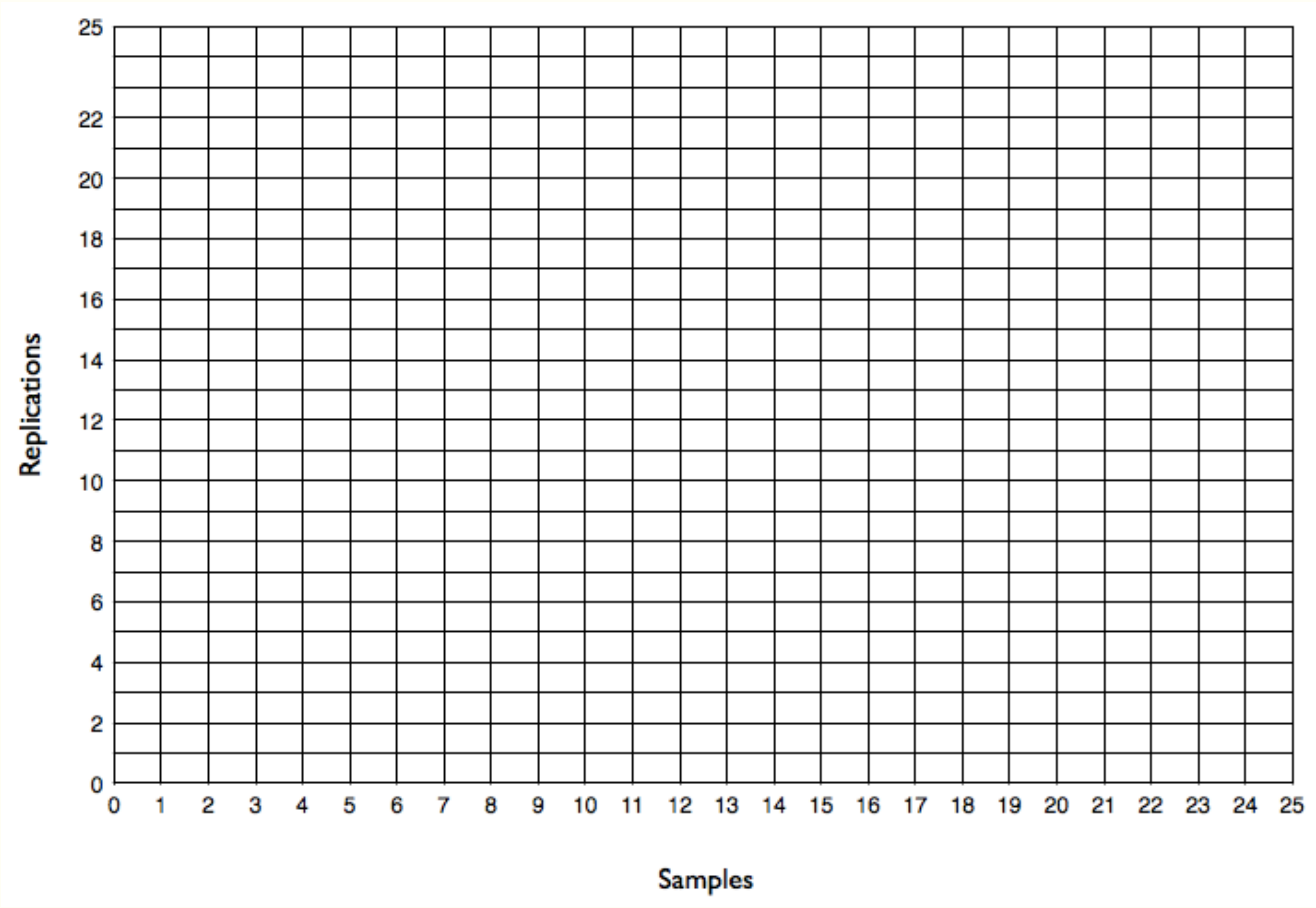
Sampling distribution

As we let $M \to \infty$, the distribution induced on $\hat{\theta}$ is the empirical **sampling distribution of the estimator**.

We could use the sampling distribution to get confidence intervals on θ.

But we dont have M samples. What to do?

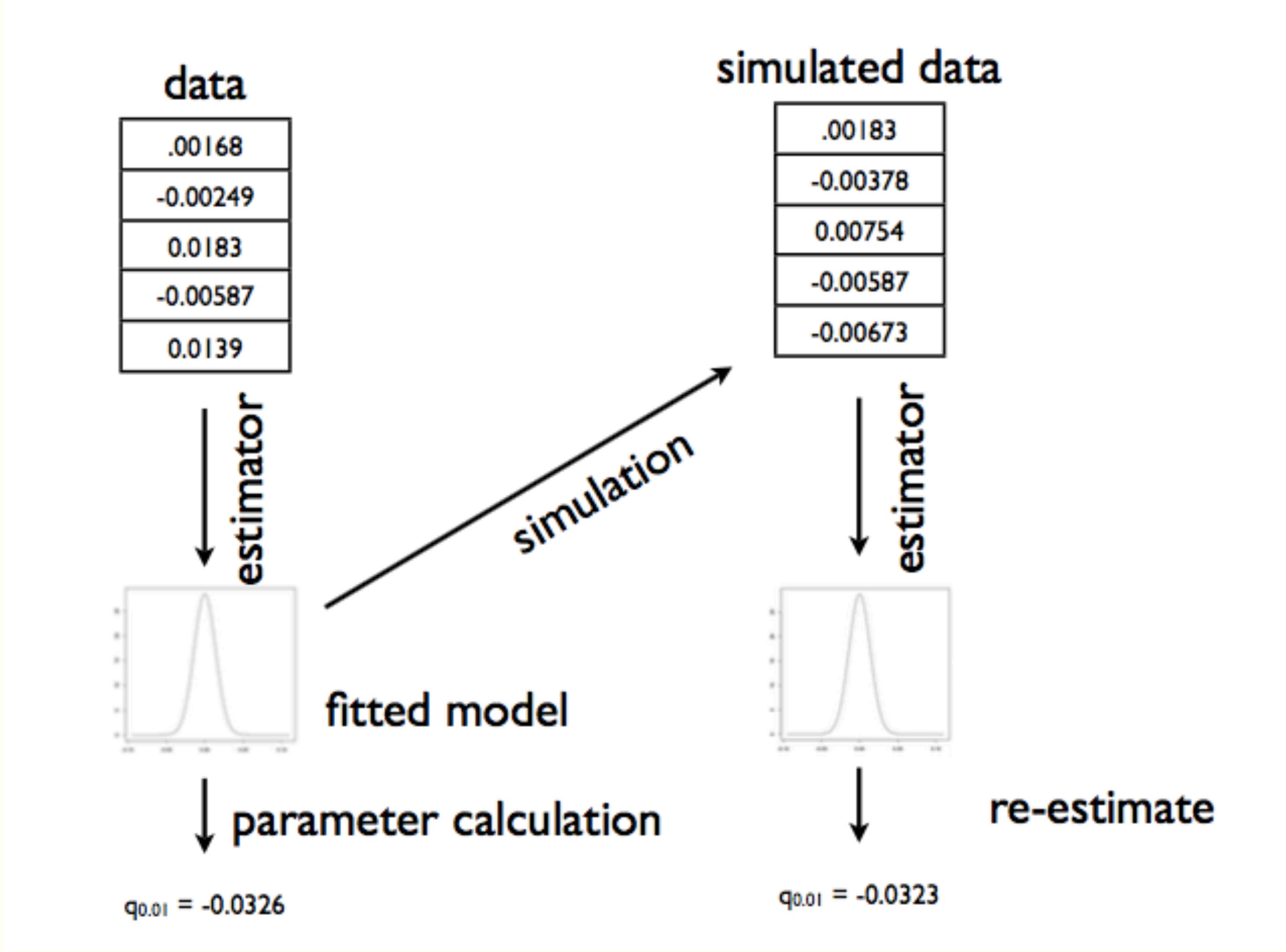
M samples of N data points



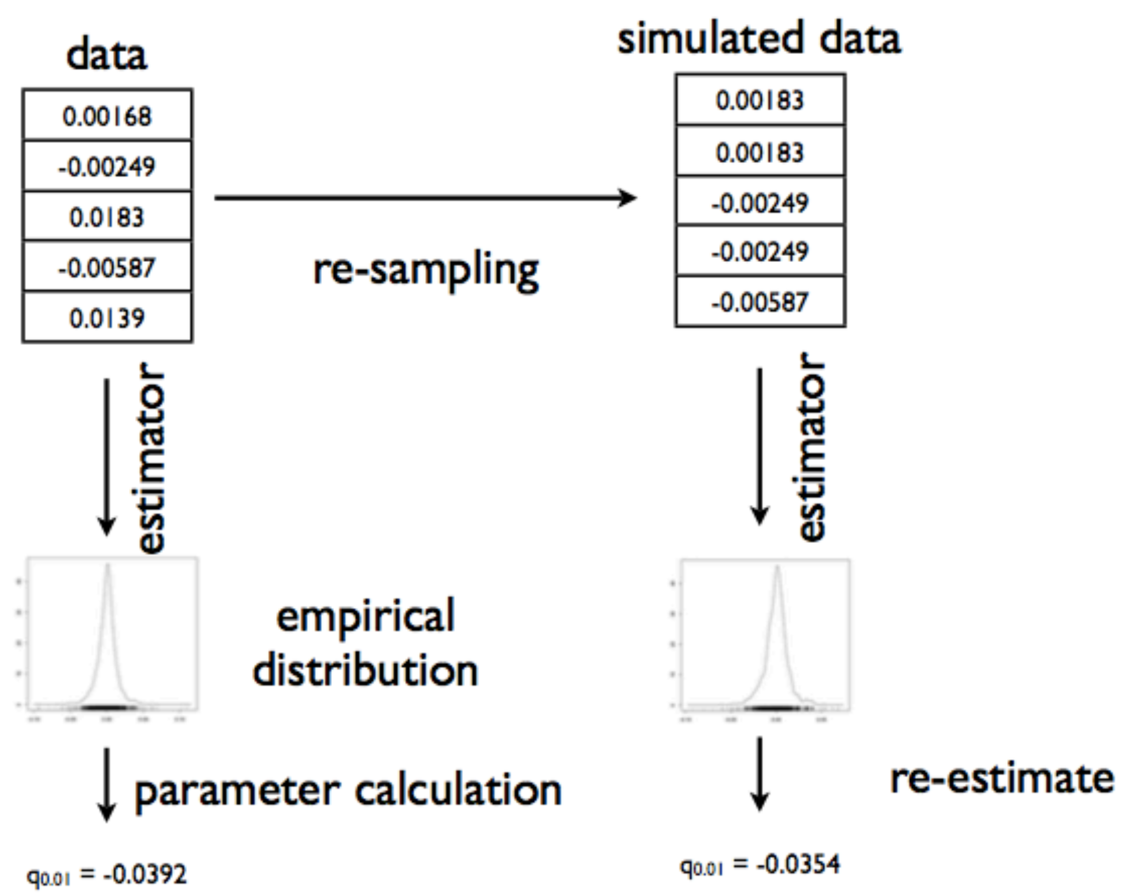
Bootstrap

- If we knew the true parameters of the population, we could generate M fake datasets.
- we dont, so we use our estimate $\hat{\theta}$ to generate the datasets
- this is called the Parametric Bootstrap
- usually best for statistics that are variations around truth

(diagram from Shalizi)



Non Parametric Bootstrap[1]



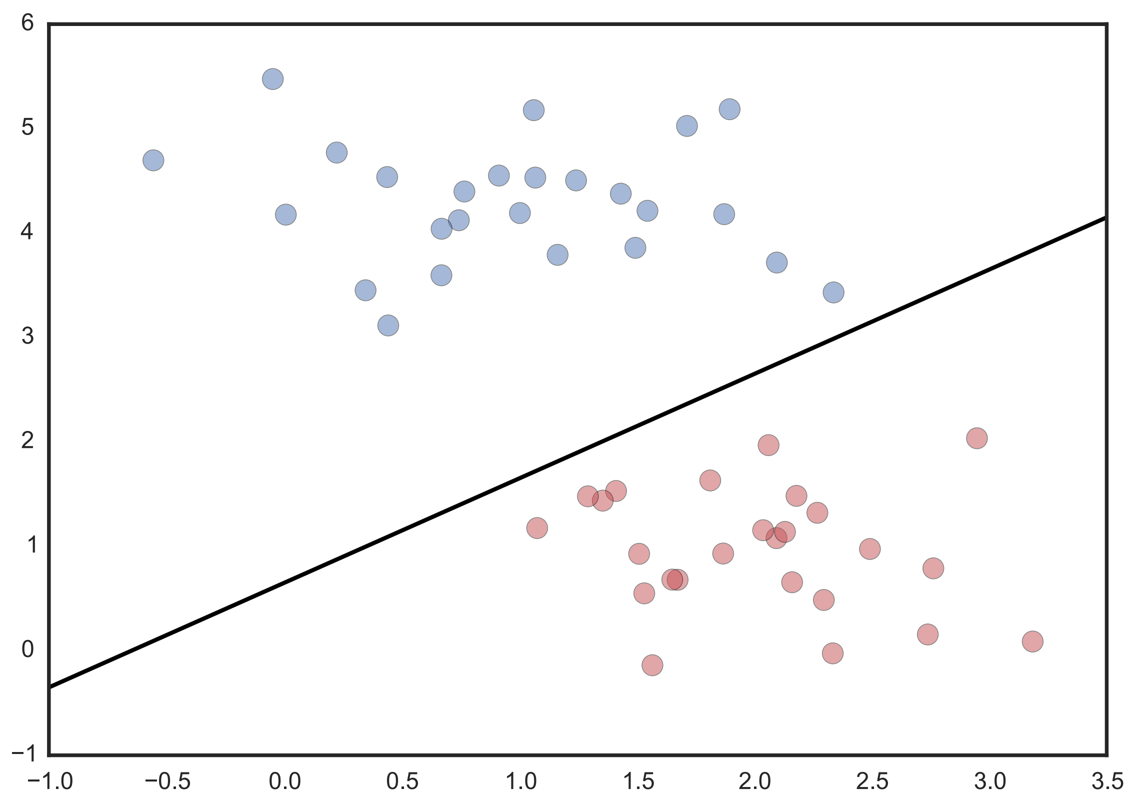
Specification error: what if the model isnt quite good?

Then Sample with replacement the X from our original sample D, generating many fake datasets.

Use the empirical distribution!

[1] (from Shalizi)

CLASSIFICATION



- will a customer churn?
- is this a check? For how much?
- a man or a woman?
- will this customer buy?
- do you have cancer?
- is this spam?
- whose picture is this?
- what is this text about?[j]

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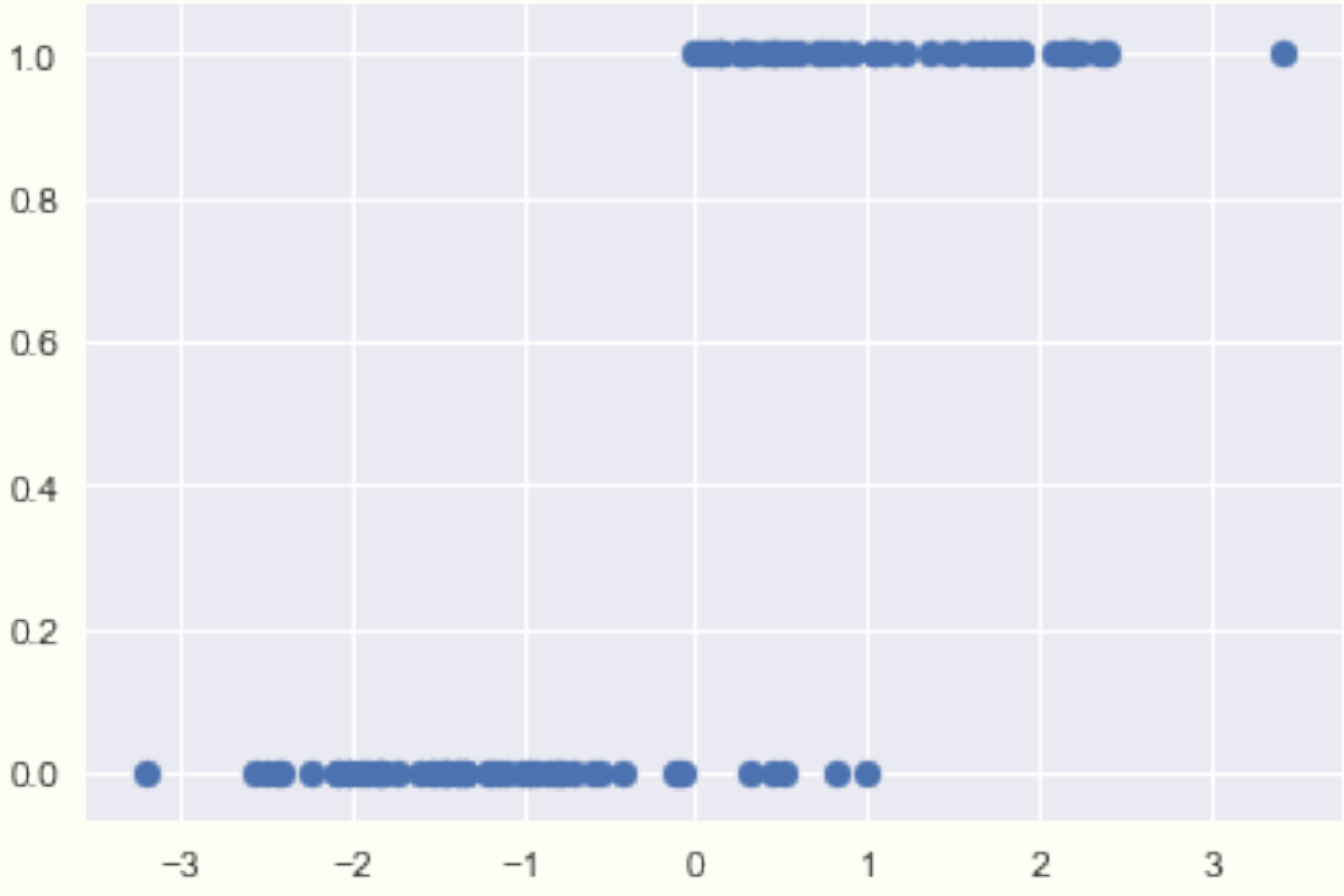
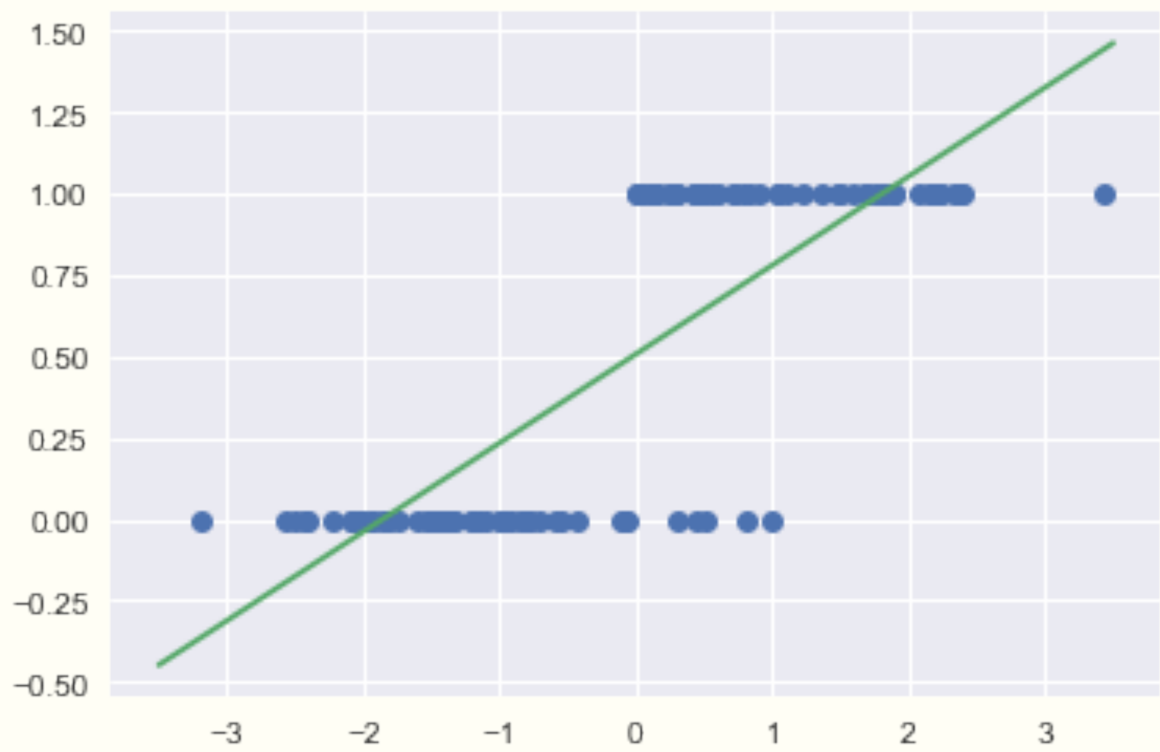
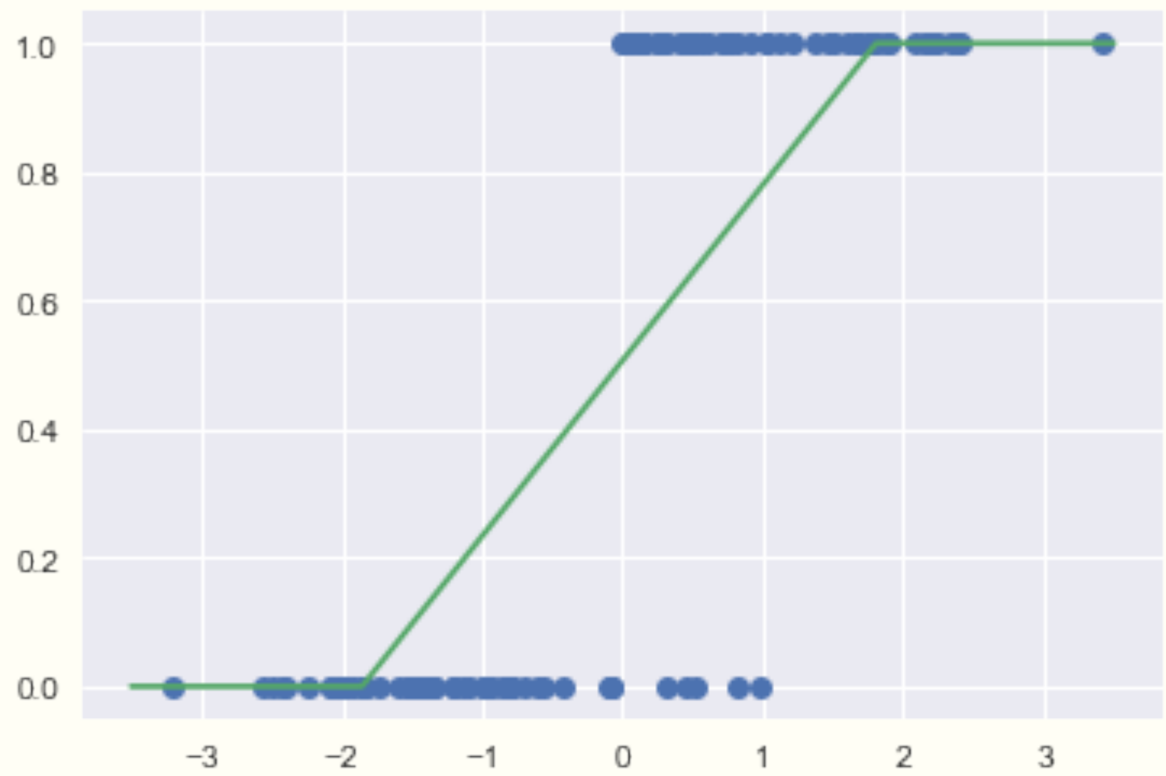
[j] image from code in http://bit.ly/1Azg29G

1-D classification problem

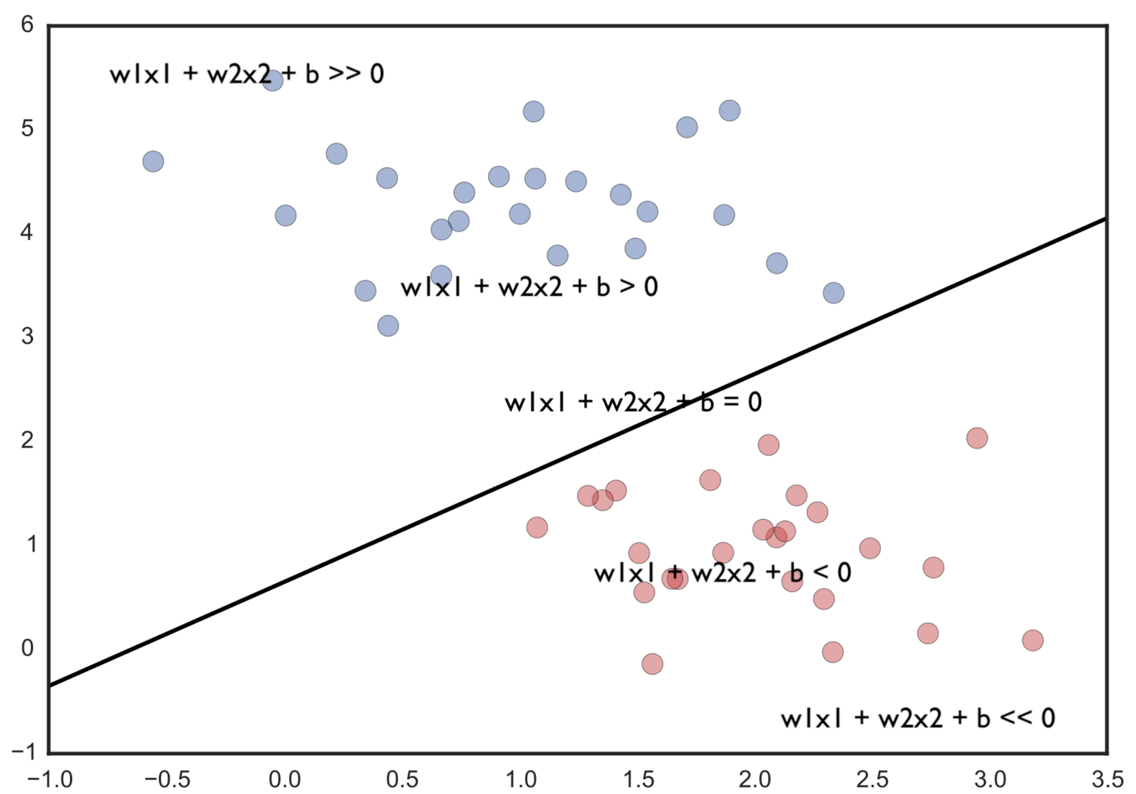


1-D Using Linear regression





Logistic regression..split via line



Draw a line in feature space that divides the '1' (blue) samples from the '0' (red)samples.

Now, a line has the form $w_1x_1 + w_2x_2 + b = 0$ in 2-dimensions.

Our classification rule then becomes:

$$y = 1, \;\; \mathbf{w}\cdot\mathbf{x} + b \geq 0$$
$$y = 0, \;\; \mathbf{w}\cdot\mathbf{x} + b < 0$$

Highly positive and negative values go far from this line!

Sigmoid Function

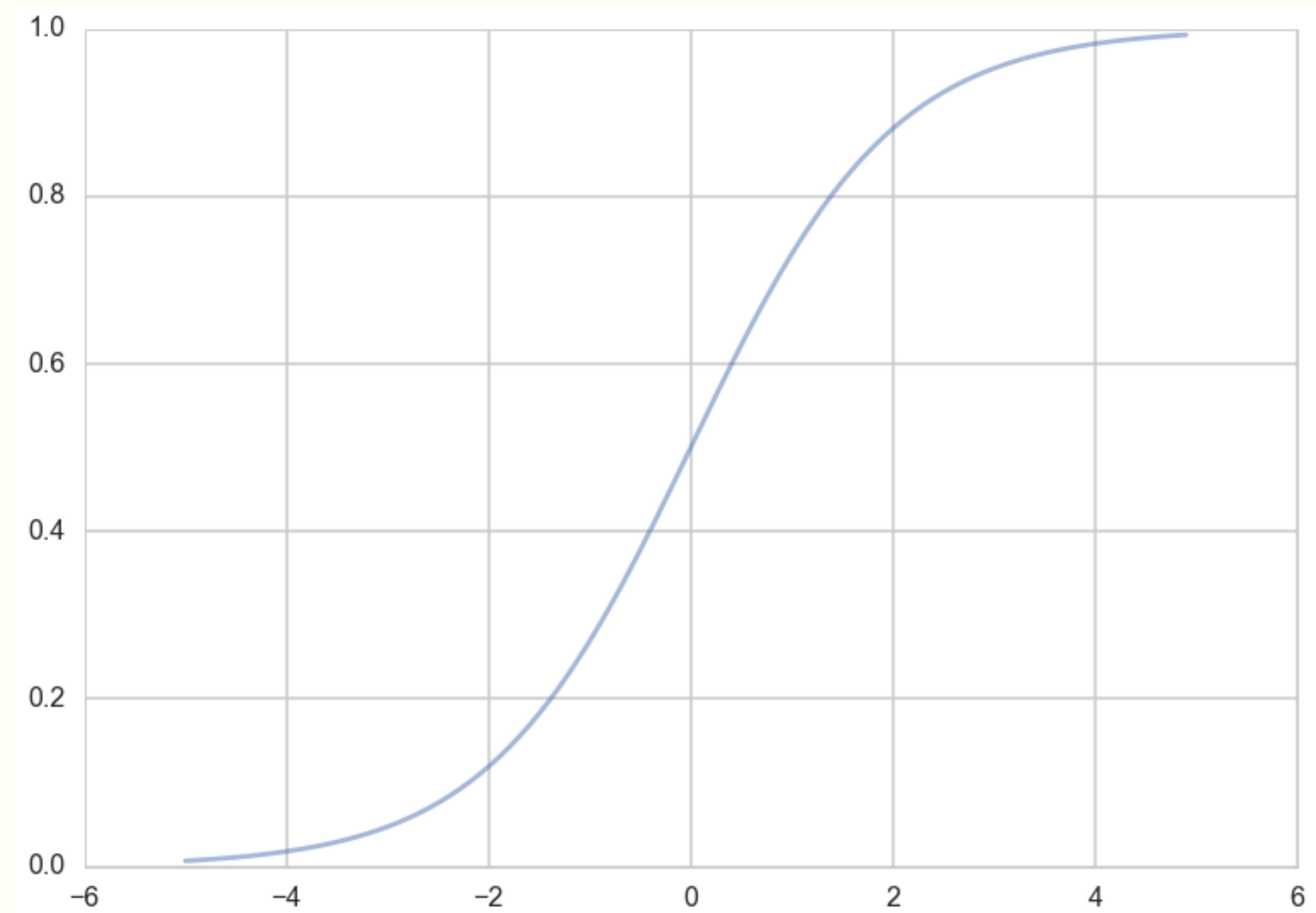
Consider the **sigmoid** function:

$$h(z) = \frac{1}{1+e^{-z}}$$ with the identification

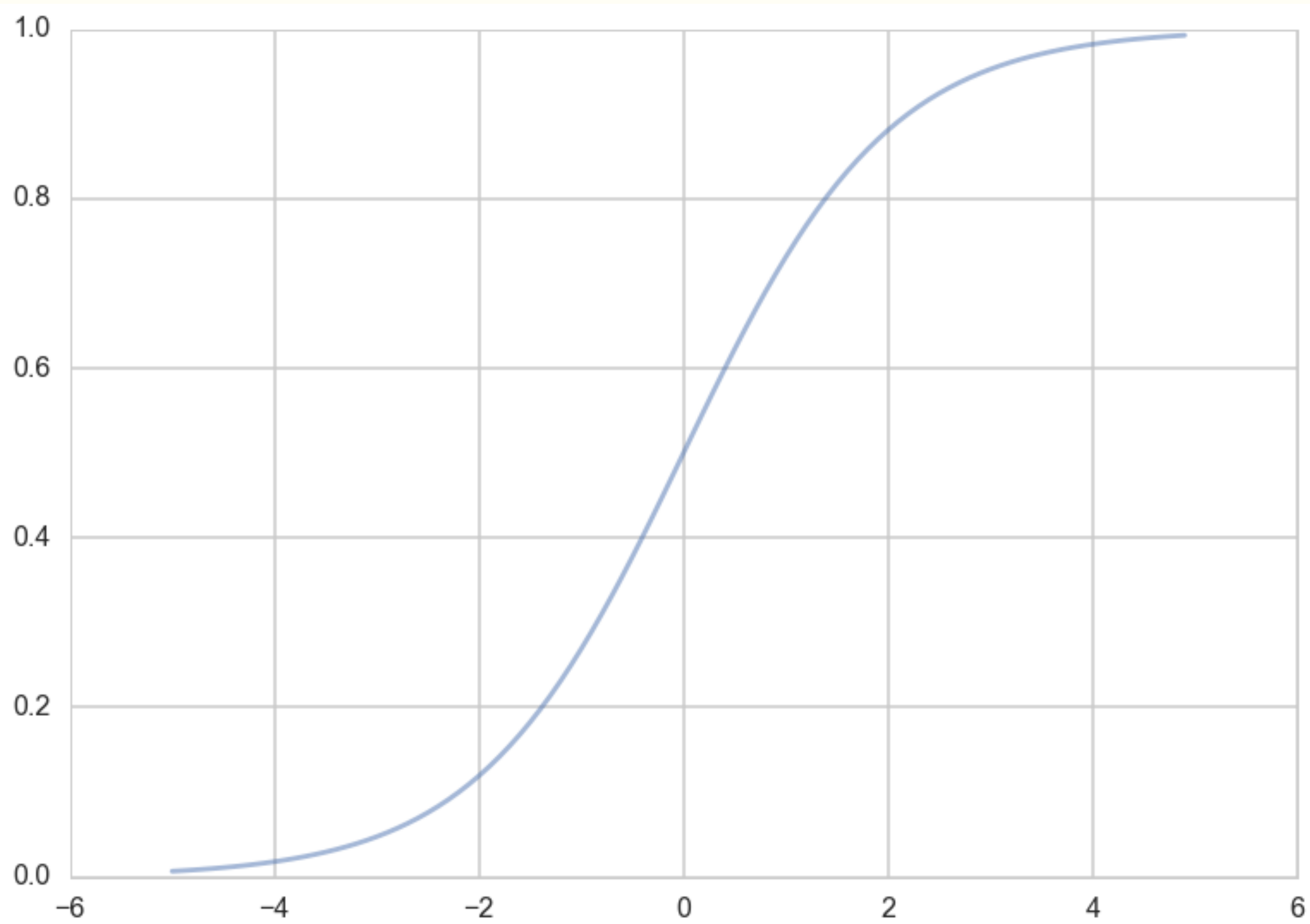
$$z = \mathbf{w} \cdot \mathbf{x} + b$$

- At $z = 0$ this function has the value 0.5.
- If $z > 0, h > 0.5$ and as $z \to \infty, h \to 1$.
- If $z < 0, h < 0.5$ and as $z \to -\infty$, $h \to 0$.

As long as we identify any value of $h > 0.5$ as classified to '1', and any $h < 0.5$ as 0, we can achieve what we wished above.



Sigmoid Probability



The further away we are from the dividing line, the better our classification.
As $z \to \infty, h \to 1$. As $z \to -\infty, h \to 0$.

Pure certainty of a '1' and of not being a '1', respectively.

Identify: $h(z) = \dfrac{1}{1+e^{-z}}$ as the **probability that the data point is a '1'**.

Since $z = \mathbf{w} \cdot \mathbf{x} + b$, this is a affine function FOLLOWED by a **non-linearity**. This is called a Generalized Linear Model (GLM).

Bernoulli

Then, the conditional probabilities of $y = 1$ or $y = 0$ given a particular data point's features $\mathbf{x}$ are:

$$P(y = 1|\mathbf{x}) = h(\mathbf{w} \cdot \mathbf{x} + b)$$
$$P(y = 0|\mathbf{x}) = 1 - h(\mathbf{w} \cdot \mathbf{x} + b).$$

These two can be written together as

$$P(y|\mathbf{x}, \mathbf{w}) = h(\mathbf{w} \cdot \mathbf{x} + b)^y \left(1 - h(\mathbf{w} \cdot \mathbf{x} + b)\right)^{1-y}$$

MLE for Logistic Regression

- "Squeeze" linear regression through a **Sigmoid** function
- this bounds the output to be a probability
- now multiply probabilities to get the "maximum likelihood" of the data, given the parameters.

Multiplying over the samples we get:

$$P(y|\mathbf{x},\mathbf{w}) = P(\{y_i\}|\{\mathbf{x}_i\},\mathbf{w}) =$$

$$\prod_{y_i \in \mathcal{D}} P(y_i|\mathbf{x}_i,\mathbf{w}) = \prod_{y_i \in \mathcal{D}} h(\mathbf{w}\cdot\mathbf{x}_i + b)^{y_i}(1 - h(\mathbf{w}\cdot\mathbf{x}_i + b))^{(1-y_i)}$$

maximum likelihood estimation maximises the **likelihood of the sample y**, or alternately the log-likelihood,

$$\mathcal{L} = P(y \mid \mathbf{x},\mathbf{w}).\ \text{OR}\ \ell = log(P(y \mid \mathbf{x},\mathbf{w}))$$

Thus

$$\ell = log\left(\prod_{y_i \in \mathcal{D}} h(\mathbf{w}\cdot\mathbf{x}_i + b)^{y_i}(1 - h(\mathbf{w}\cdot\mathbf{x}_i + b))^{(1-y_i)}\right)$$

$$= \sum_{y_i \in \mathcal{D}} log\left(h(\mathbf{w}\cdot\mathbf{x}_i + b)^{y_i}(1 - h(\mathbf{w}\cdot\mathbf{x}_i + b))^{(1-y_i)}\right)$$

$$= \sum_{y_i \in \mathcal{D}} log\, h(\mathbf{w}\cdot\mathbf{x}_i + b)^{y_i} + log\,(1 - h(\mathbf{w}\cdot\mathbf{x}_i + b))^{(1-y_i)}$$

$$= \sum_{y_i \in \mathcal{D}} (y_i log(h(\mathbf{w}\cdot\mathbf{x} + b)) + (1 - y_i) log(1 - h(\mathbf{w}\cdot\mathbf{x} + b)))$$

Logistic Regression: NLL

The negative of this log likelihood (NLL), also called *cross-entropy*.

$$NLL = -\sum_{y_i \in \mathcal{D}} (y_i log(h(\mathbf{w} \cdot \mathbf{x} + b)) + (1 - y_i) log(1 - h(\mathbf{w} \cdot \mathbf{x}) + b))$$

Gradient: $\nabla_{\mathbf{w}} NLL = \sum_i \mathbf{x}_i^T (p_i - y_i) = \mathbf{X}^T \cdot (\mathbf{p} - \mathbf{w})$

Hessian: $H = \mathbf{X}^T diag(p_i(1 - p_i))\mathbf{X}$ positive definite $\implies$ convex

How to calculate?

Use Layers.

```
class Layer:
    def __init__(self, name):
        self.name = name
        self.params = {}
        self.grads = {}
    def forward(self, inputs):
        raise NotImplementedError
    def backward(self, grad):
        raise NotImplementedError
```

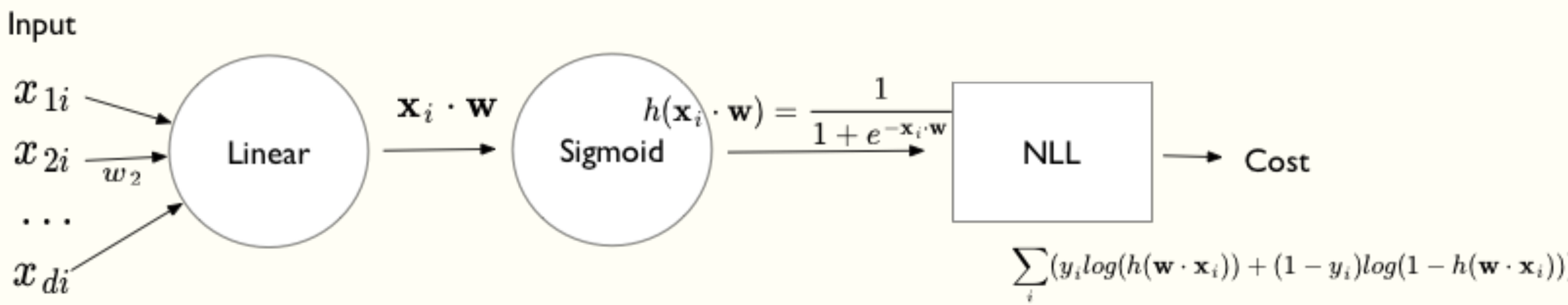
Layers replace functions.

You can think of 3 layers in Logistic Regression.

1. Affine Function
2. Sigmoid
3. Loss.

We will feed the gradients backward from loss to affine.

Layer based diagram



$$z_{0i} = x_i,\ z_{1i} = wx_i + b,\ z_{2i} = h(z_{1i}),\ Loss = -\sum_i y_i log(z_{2i} + (1-y_i) log(1-z_{2i})$$

Backpropagation

The *forward* mode, implemented with dunder `__call__` makes a **prediction**, thus:

$\mathbf{M}odel = (\mathbf{f}^3(\mathbf{f}^2(\mathbf{f}^1(\mathbf{x})))),\ \ Loss = f^4(\mathbf{M}odel)$. Loss is scalar.

Backpropagation: pass gradients **back** through layers:

$$\nabla_{\mathbf{x}} Loss = \frac{\partial f^4}{\partial \mathbf{f}^3}\frac{\partial \mathbf{f}^3}{\partial \mathbf{f}^2}\frac{\partial \mathbf{f}^2}{\partial \mathbf{f}^1}\frac{\partial \mathbf{f}^1}{\partial \mathbf{x}} = (((\frac{\partial f^4}{\partial \mathbf{f}^3}\frac{\partial \mathbf{f}^3}{\partial \mathbf{f}^2})\frac{\partial \mathbf{f}^2}{\partial \mathbf{f}^1})\frac{\partial \mathbf{f}^1}{\partial \mathbf{x}})$$

You **pass in** vector, **always** multiply vector by matrix, get **vector**, pass it **back**. Huge Memory Savings!

Affine Layer

```
class Affine(Layer):
    def __init__(self, name, input_dims):
        super().__init__(name)
        self.params['w'] = np.random.randn(input_dims, 1)
        self.params['b'] = np.random.randn(1,)
        self.grads['w'] = np.zeros((input_dims, 1))
        self.grads['b'] = np.array([0.])

    def forward(self, inputs):
        self.inputs = inputs
        return inputs@self.params['w'] + self.params['b']

    def backward(self, grad):
        # (m,n) @ (n,  1) = (m, 1)
        #print("gradshape", grad.shape)
        self.grads['w'] = self.inputs.T @ grad
        # (n, 1) @ (n, 1) = (1,)
        self.grads['b'] = np.sum(grad, axis=0)
        # return (n, 1) @ (1 , m) = (n, m)
        return grad@self.params['w'].T
```

Already done these!

$$\frac{\partial Loss}{\partial \theta^0} = \sum_u \delta_u^1 \frac{\partial z_{1,u}}{\partial \theta^0}$$

$$\frac{\partial Loss}{\partial w} = \sum_u \delta_u^1 \frac{\partial z_{1,u}}{\partial w} =$$

`self.inputs.T @ grad`

$$\frac{\partial Loss}{\partial z_{0u}} = \sum_v \delta_v^1 \frac{\partial z_{1,v}}{\partial z_{0u}} =$$

`grad@self.params['w'].T`

$$\frac{\partial Loss}{\partial b} = \sum_u \delta_u^1 \frac{\partial z_{1,u}}{\partial b} =$$

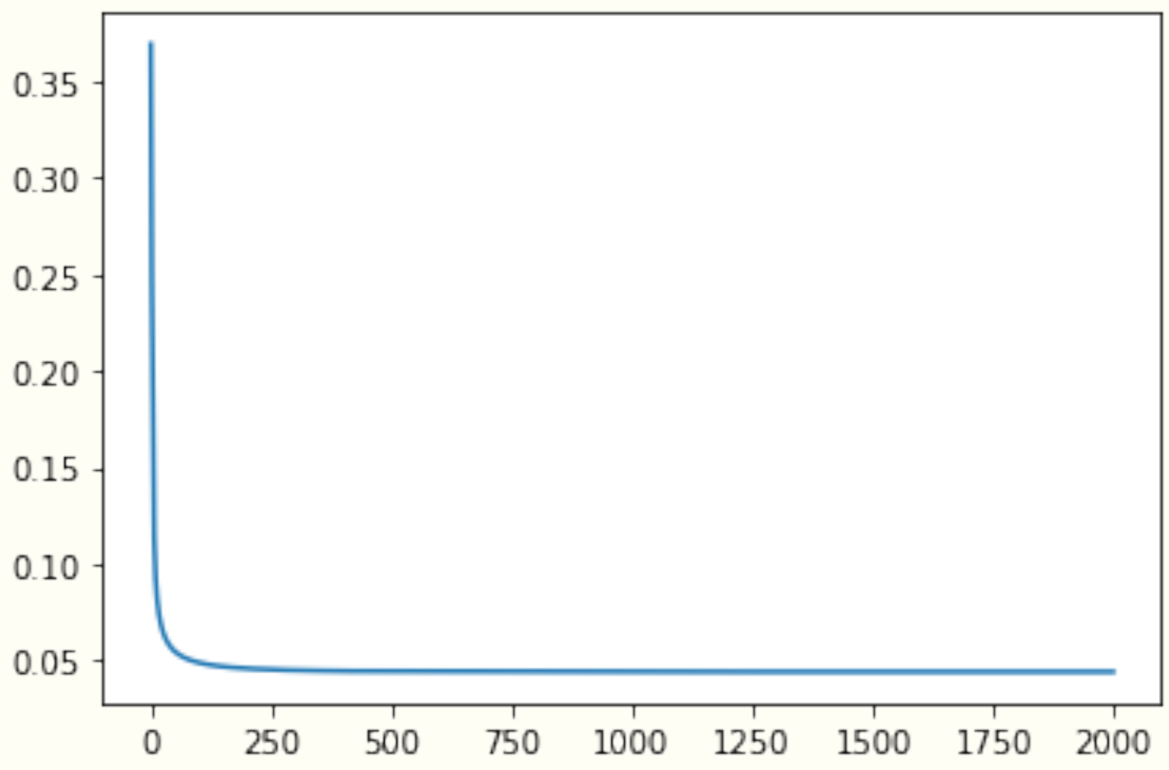
`np.sum(grad, axis=0)`

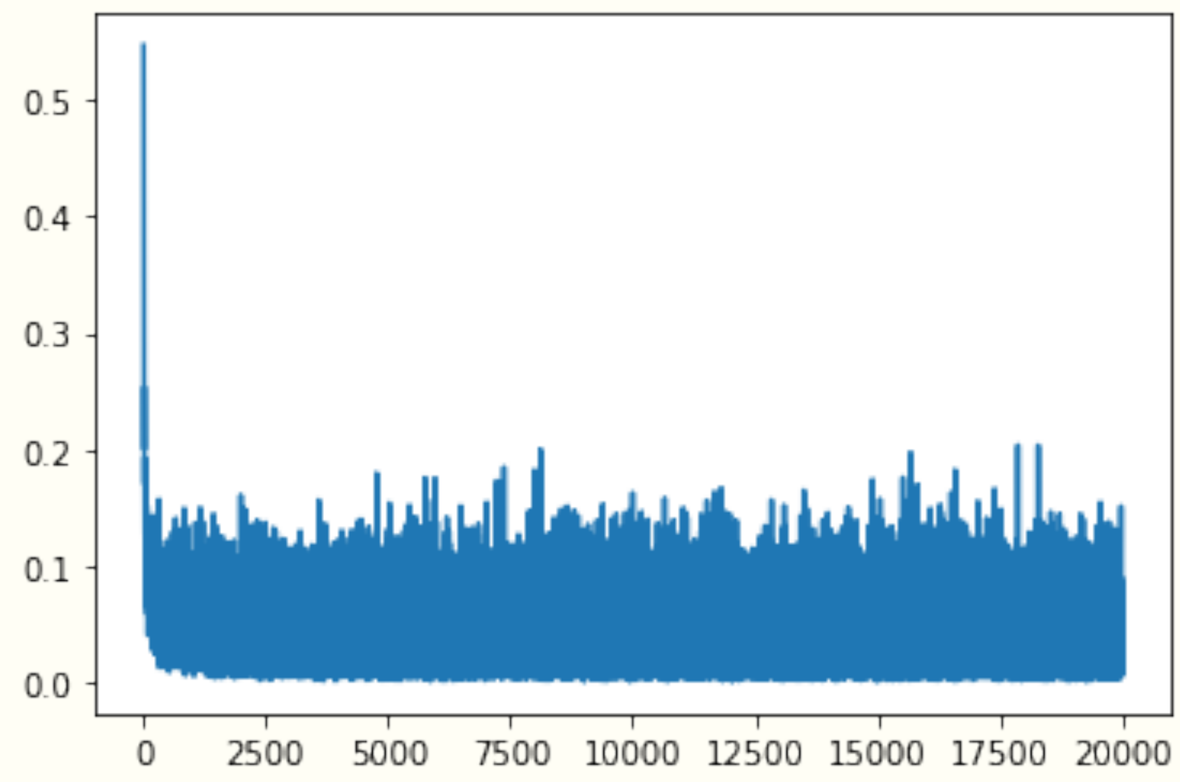
`Model` holds everything together

```
class Model:
    def __init__(self, layers):
        self.layers = layers

    def forward(self, inputs):
        for layer in self.layers:
            inputs = layer.forward(inputs)
        return inputs

    def backward(self, grad):
        for layer in reversed(self.layers):
            grad = layer.backward(grad)
        return grad

    def params_and_grads(self):
        for layer in self.layers:
            for name, param in layer.params.items():
                grad = layer.grads[name]
                yield layer, name, param, grad
```

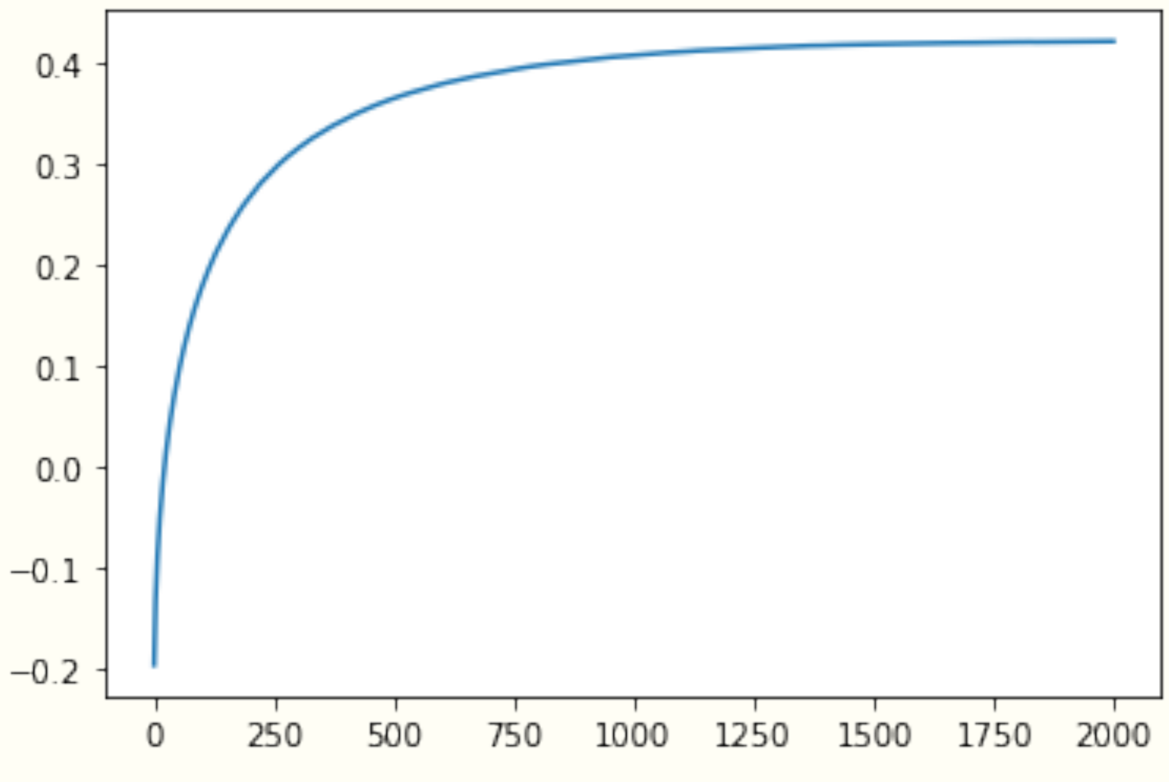
- Dunder `forward` runs through the layers forward, making a prediction.
- `backward` runs through them in reversed order, passing the returned gradient with respect to a layer's inputs backwards through the model.
- in python software, `backward` is implemented automatically!!

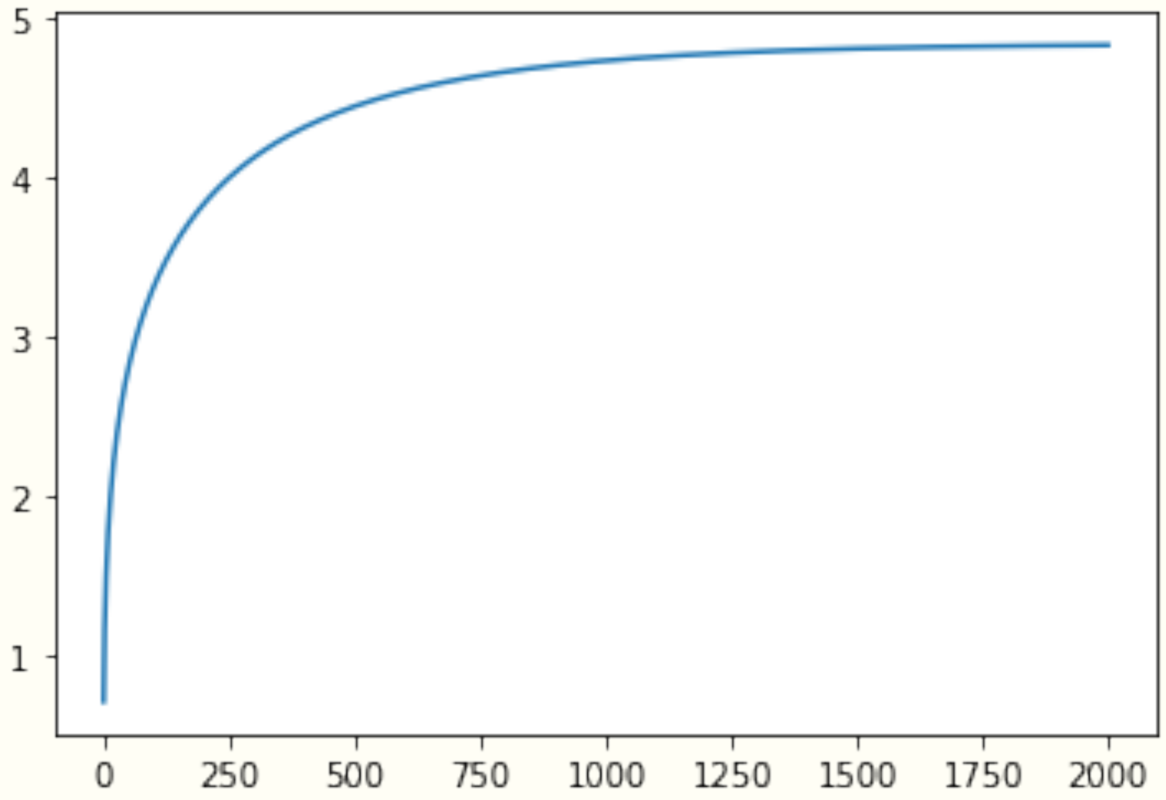
Losses


0.35
0.30
0.25
0.20
0.15
0.10
0.05
0
250
500
750
1000
1250
1500
1750
2000

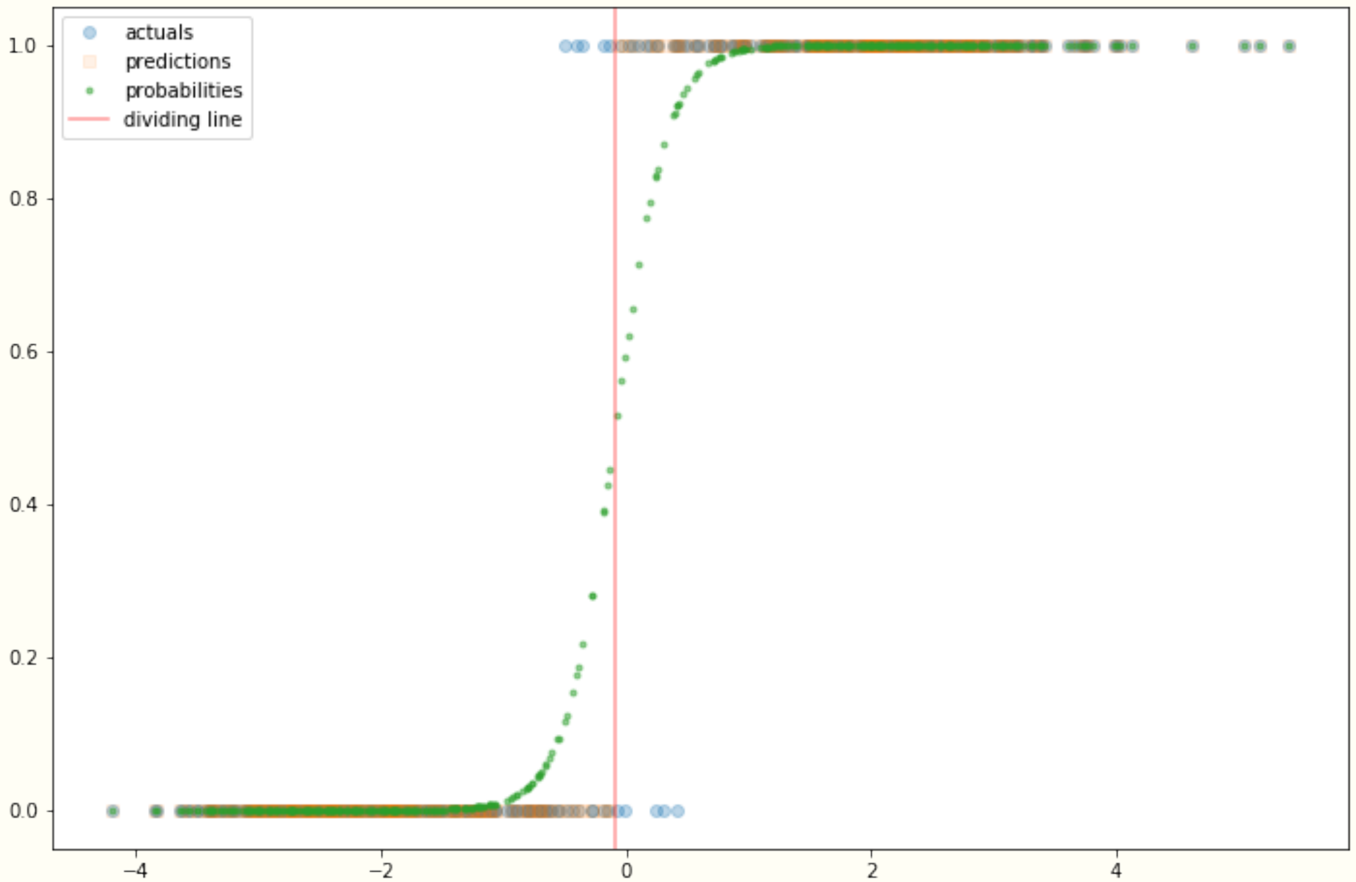

0.5
0.4
0.3
0.2
0.1
0.0
0
2500
5000
7500
10000
12500
15000
17500
20000

Parameters


0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
250
500
750
1000
1250
1500
1750
2000


5
4
3
2
1
0
250
500
750
1000
1250
1500
1750
2000

Classification Using Logistic regression



$$z = wx = b$$

$$p = h(z) = \frac{1}{1+e^{-z}} = \frac{1}{1+e^{-(wx+b)}}$$

if $p \geq 0.5$ classify as positive. We make some misclassifications:

```
Pred    0     1
     [[245,   5],   0
      [  5, 245]]   1
                    Obsv
```

Sampling Distribution

We have focussed on prediction here.

But its important to realize that a particular sample of 1's and 0s can be thought of as a draw from some "true" probability distribution.

The various "datasets" that can be generated given our probabilities are the samples, and you can get sampling distributions on w and b.

Gradient Descent

$$\theta := \theta - \eta \nabla_\theta J(\theta) = \theta - \eta \sum_{i=1}^{m} \nabla J_i(\theta)$$

where η is the learning rate.

ENTIRE DATASET NEEDED

```
for i in range(n_epochs):
  params_grad = evaluate_gradient(loss_function, data, params)
  params = params - learning_rate * params_grad`
```