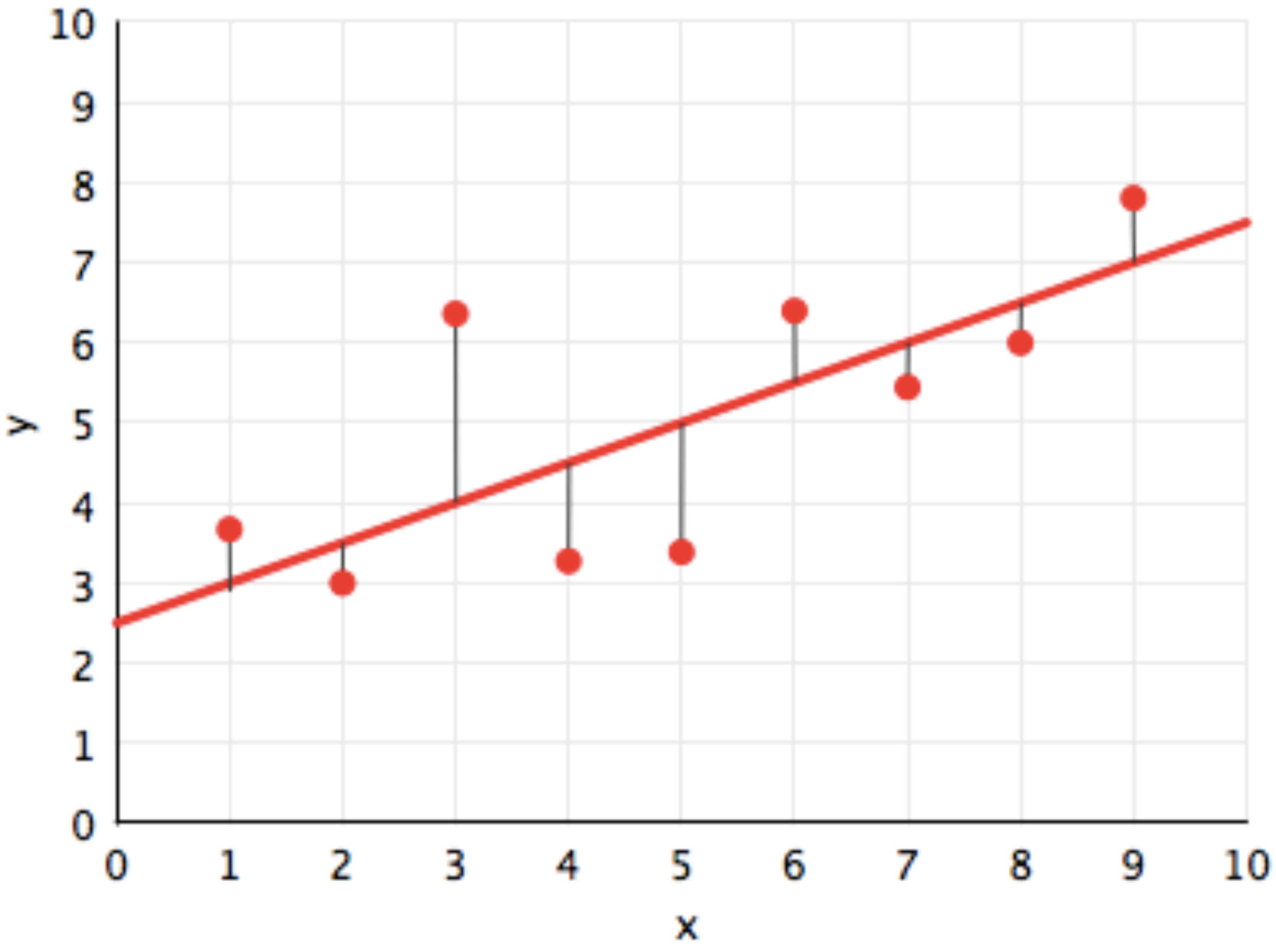
# Day 1 Session 1

## Linear Regression with Gradient Descent

# REGRESSION

- how many dollars will you spend?
- what is your creditworthiness
- how many people will vote for Bernie t days before election
- use to predict probabilities for classification
- causal modeling in econometrics



# HYPOTHESIS SPACES

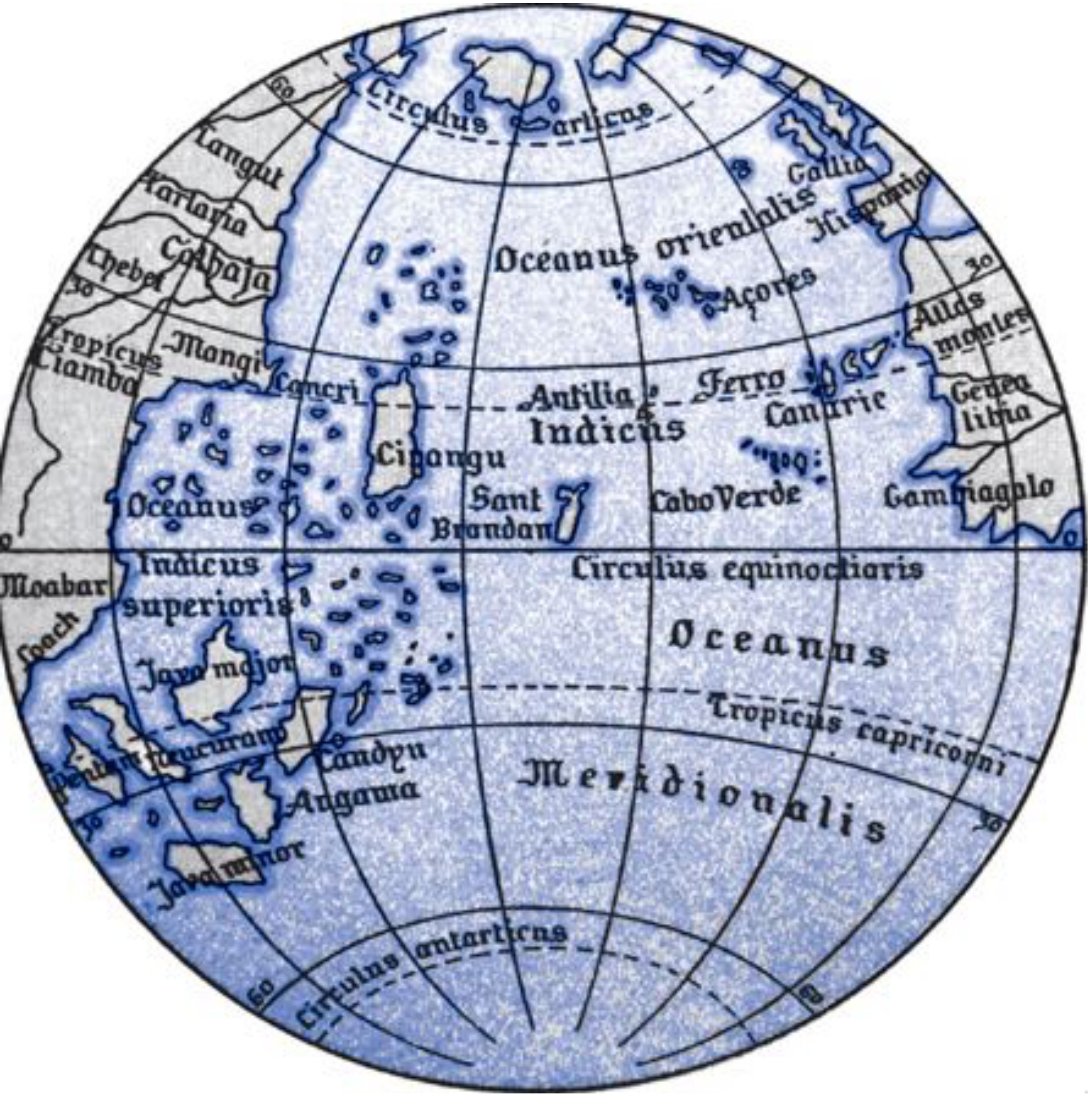
A polynomial looks so:

$$h(x) = \theta_0 + \theta_1 x^1 + \theta_2 x^2 + \ldots + \theta_n x^n = \sum_{i=0}^{n} \theta_i x^i$$

All polynomials of a degree or complexity $d$ constitute a hypothesis space.

$$\mathcal{H}_1 : h_1(x) = \theta_0 + \theta_1 x$$

$$\mathcal{H}_{20} : h_{20}(x) = \sum_{i=0}^{20} \theta_i x^i$$




# SMALL World vs BIG World

- *Small World* answers the question: given a model class (i.e. a Hypothesis space, whats the best model in it). It involves parameters. Its model checking.
- *BIG World* compares model spaces. Its model comparison with or without "hyperparameters".

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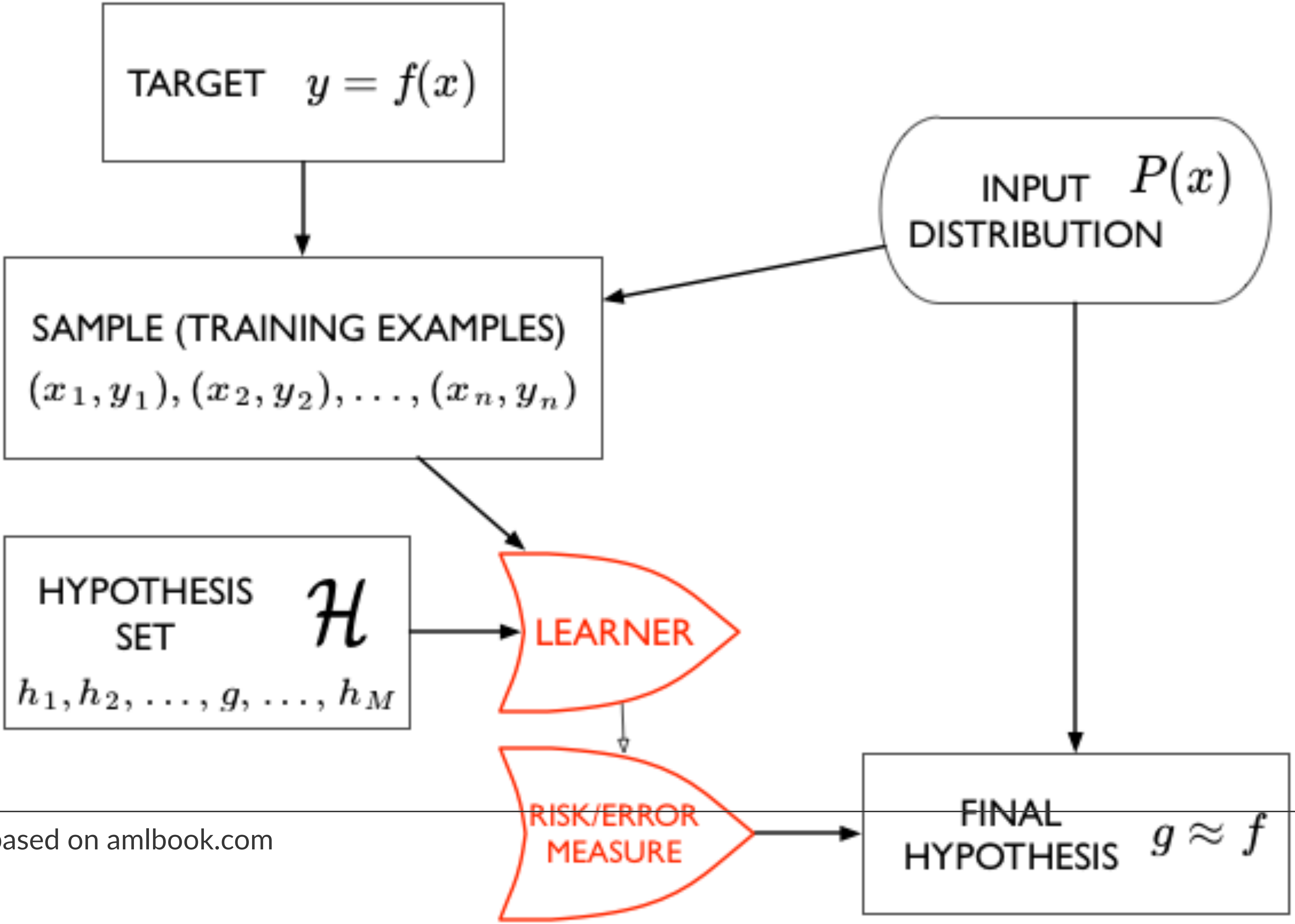



[*] image based on amlbook.com

Linear Regression

$$\hat{y} = f_\theta(x) = \theta^T x$$

Cost Function:

$$R(\theta) = \frac{1}{2}\sum_{i=1}^{m}(f_\theta(x^{(i)} - y^{(i)})^2$$

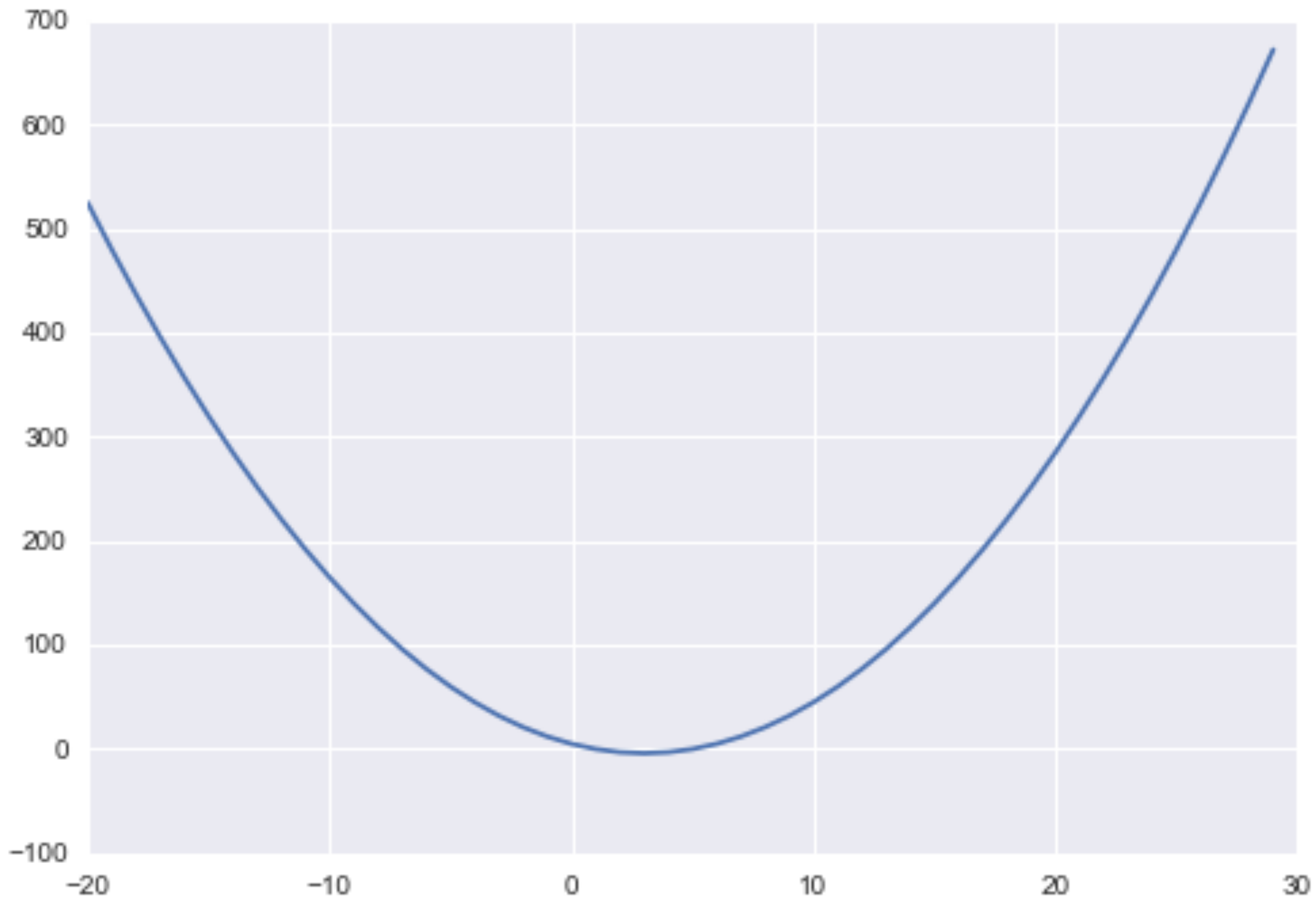
# MINIMIZE SQUARED ERROR

# Gradient ascent (descent)

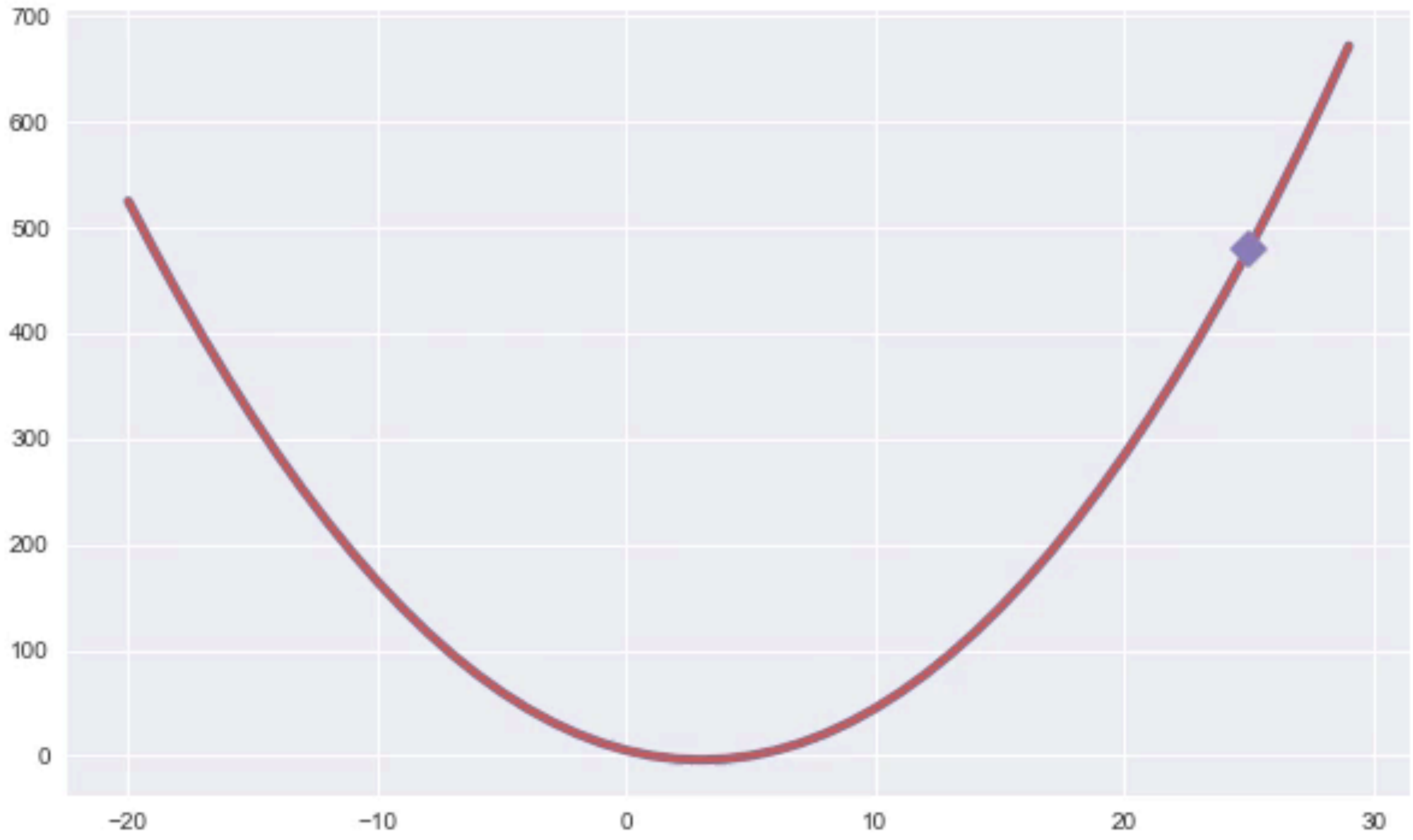
basically go opposite the direction of the derivative.

Consider the objective function:
$J(x) = x^2 - 6x + 5$

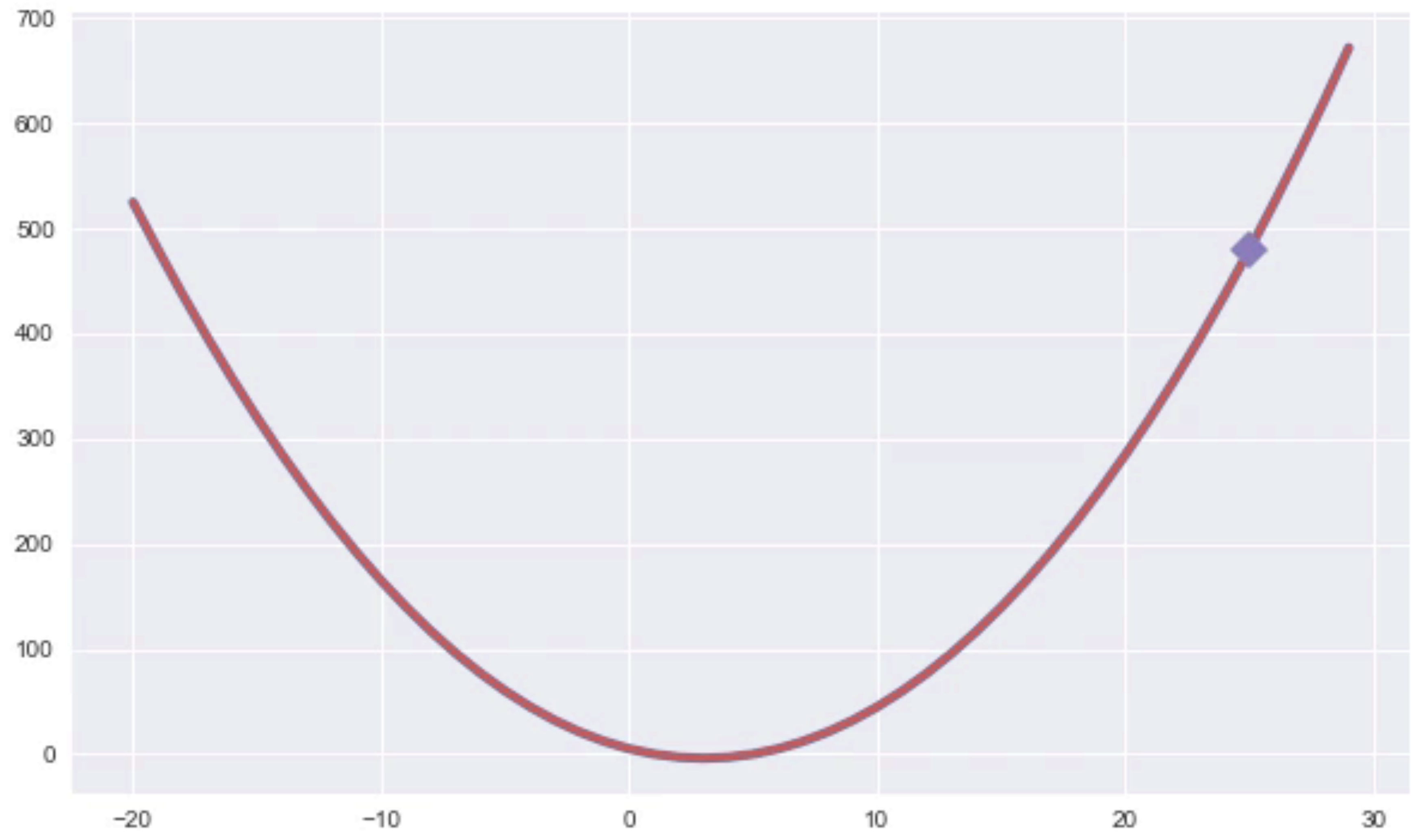
```
gradient = fprime(old_x)
move = gradient * step
current_x = old_x - move
```



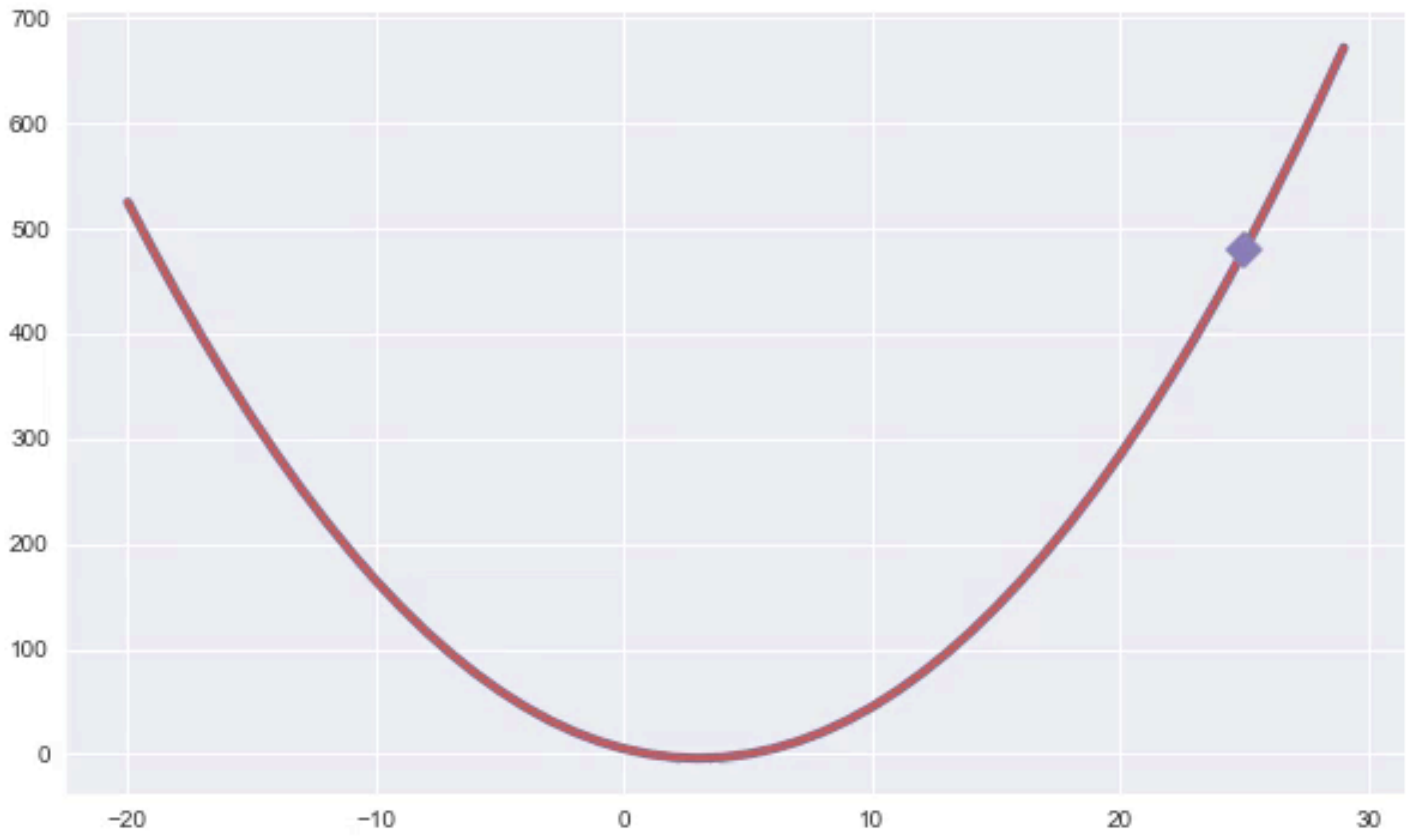
# good step size



# too big step size



# too small step size



# Gradient Descent.

We want:

$$\nabla_h R_{out}(h) = \nabla_h \int dx p(x,y) R_{out}(h(x), y)$$

For a particular sample, use the Law of Large numbers:

$$\nabla_h \hat{R_{out}}(h) \sim \nabla_h \frac{1}{N} \sum_{i \in \mathcal{D}} R_{in}(h(\hat{x_i}), y_i)$$

# Gradient Descent

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

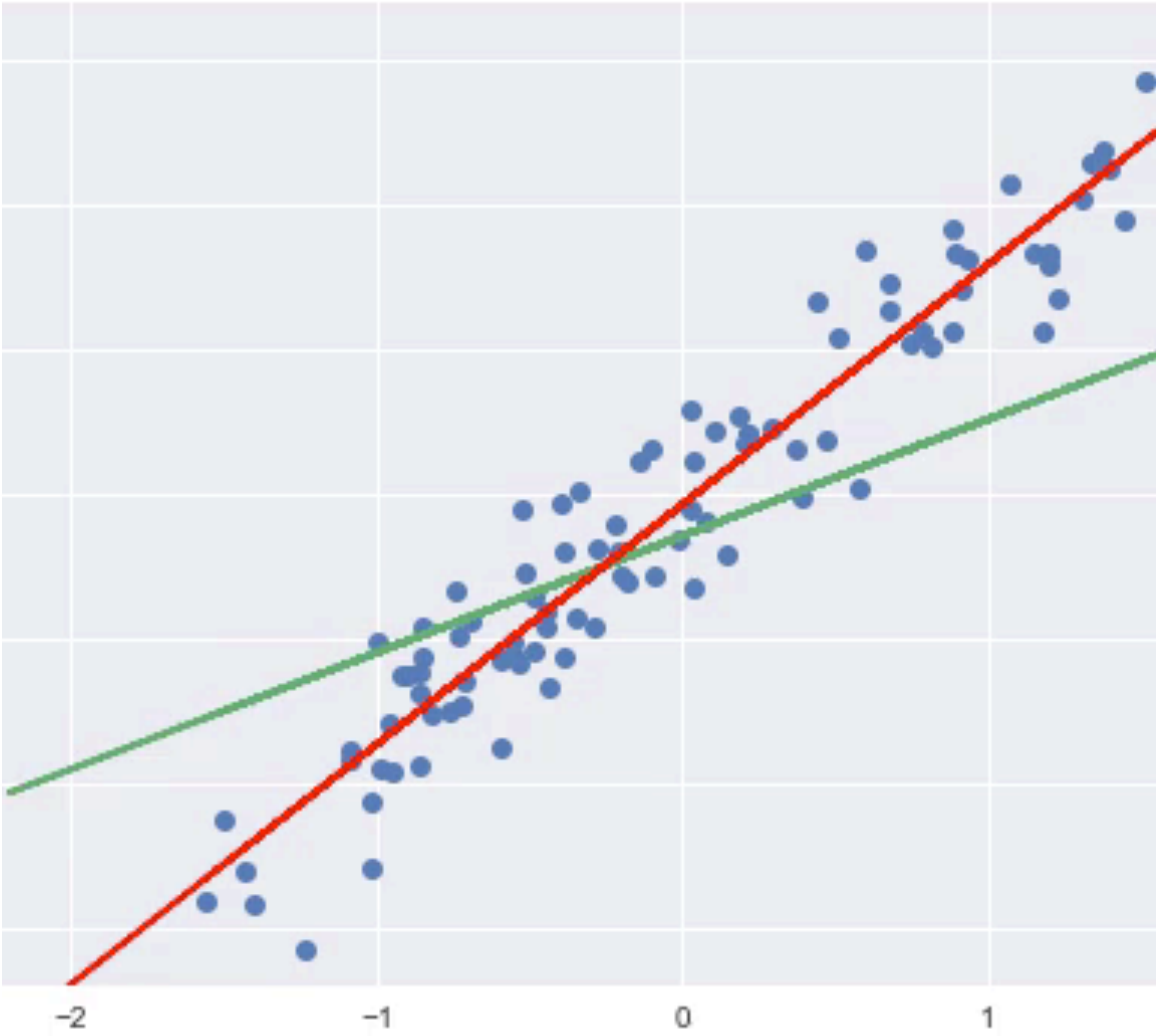
where $\eta$ is the learning rate.

ENTIRE DATASET NEEDED

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

# Linear Regression: Gradient Descent

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m} (y^{(i)} - f_\theta(x^{(i)}))x_j^{(i)}$$



# Stochastic Gradient Descent

$$\theta := \theta - \alpha \nabla_\theta R_i(\theta)$$

ONE POINT AT A TIME

For Linear Regression:

$$\theta_j := \theta_j + \alpha (y^{(i)} - f_\theta(x^{(i)})) x_j^{(i)}$$

```
for i in range(nb_epochs):
  np.random.shuffle(data)
  for example in data:
    params_grad = evaluate_gradient(loss_function, example, params)
    params = params - learning_rate * params_grad
```

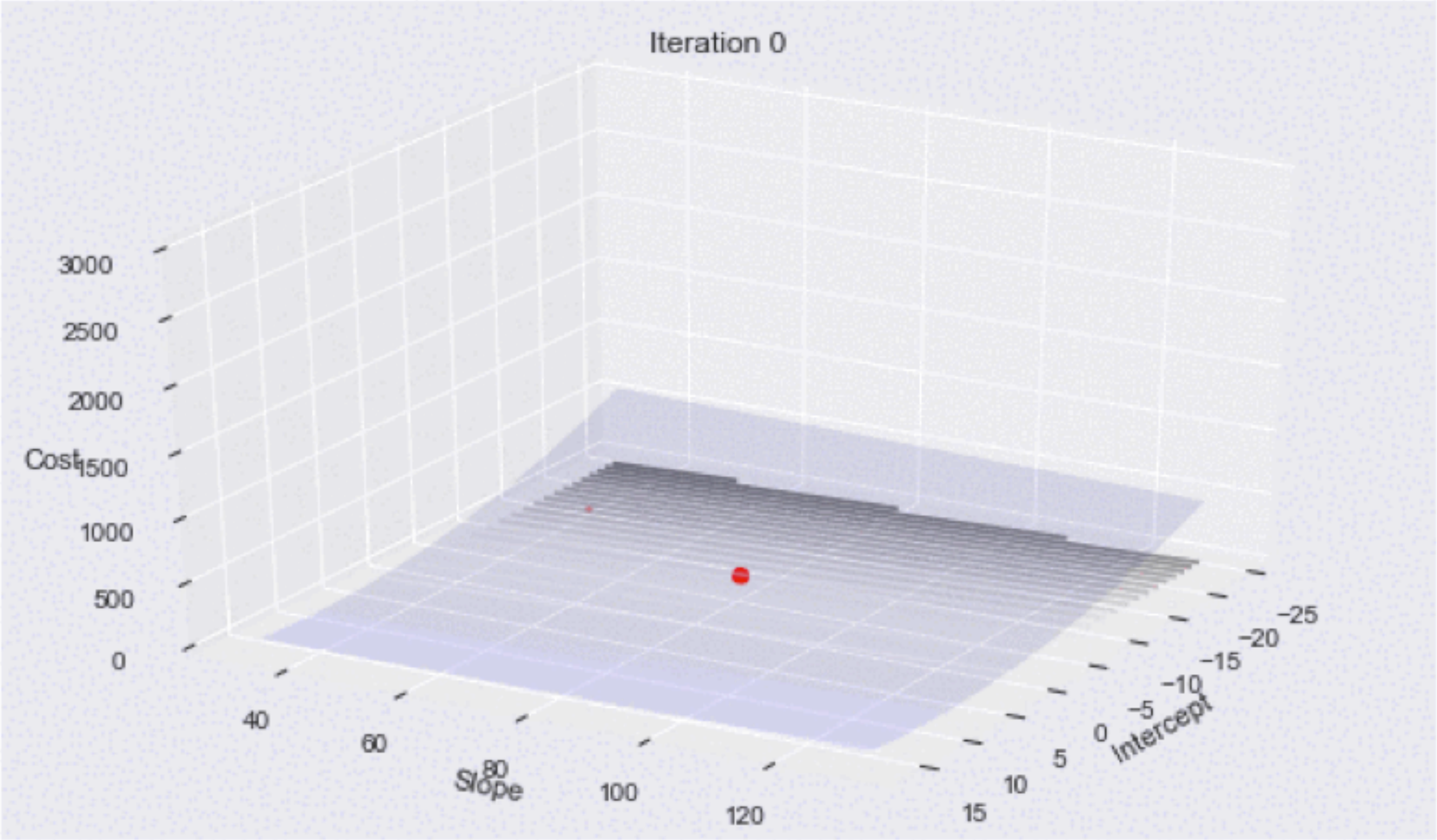
# Mini-Batch SGD (the most used)

$$\theta := \theta - \eta \nabla_\theta J(\theta; x^{(i:i+n)}; y^{(i:i+n)})$$

```
for i in range(mb_epochs):
  np.random.shuffle(data)
  for batch in get_batches(data, batch_size=50):
    params_grad = evaluate_gradient(loss_function, batch, params)
    params = params - learning_rate * params_grad
```

# Mini-Batch: do some at a time

- the risk surface changes at each gradient calculation
- thus things are noisy
- cumulated risk is smoother, can be used to compare to SGD
- epochs are now the number of times you revisit the full dataset
- shuffle in-between to provide even more stochasticity


Iteration 0
Cost
3000
2500
2000
1500
1000
500
0
Slope
40
60
80
100
120
Intercept
−25
−20
−15
−10
−5
0
5
10
15

# 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**.

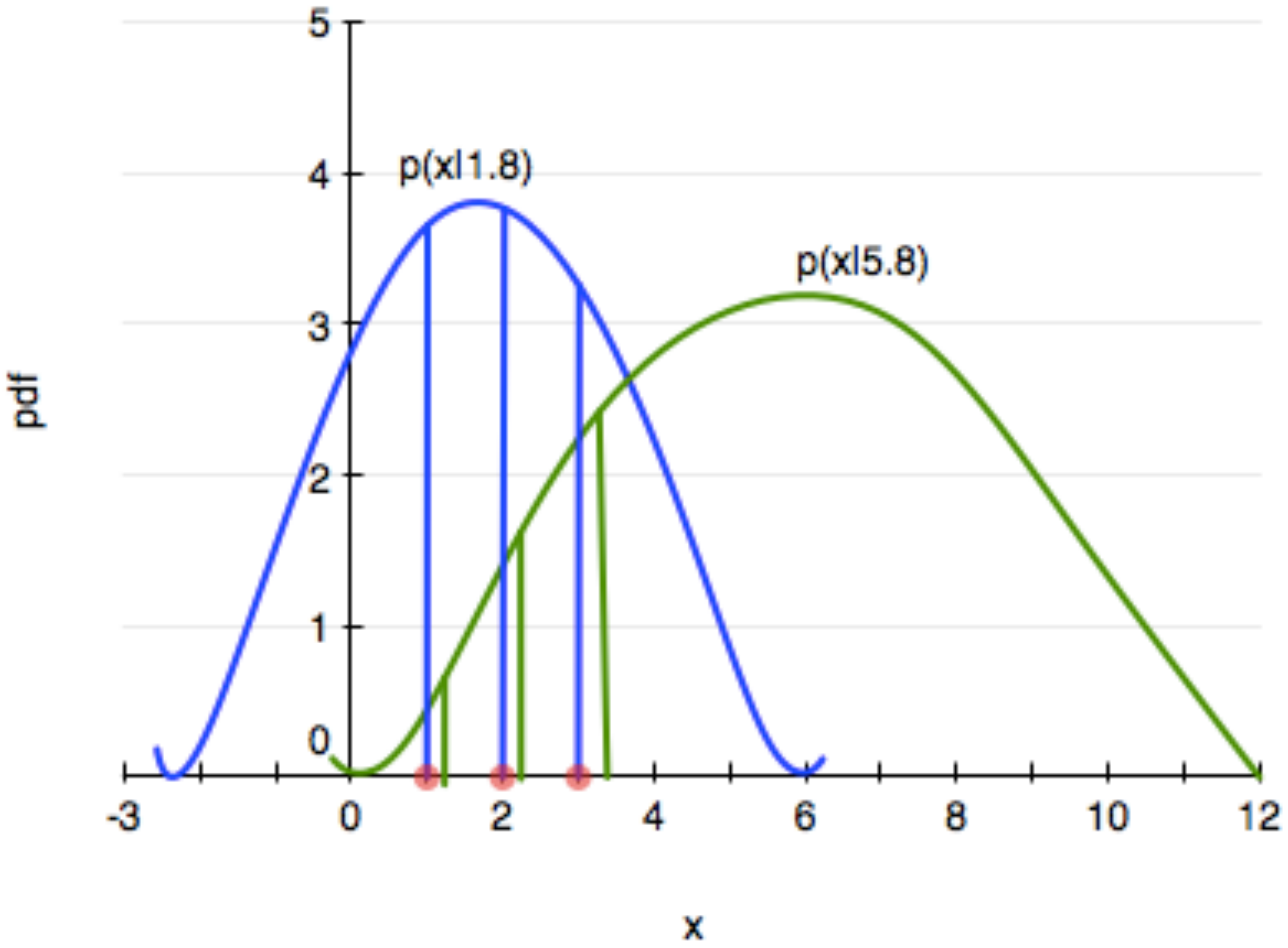
# Likelihood

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

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

How likely are the observations if the model is true?

# Maximum Likelihood estimation



We have data on the wing length in millimeters of a nine members of a particular species of moth. We wish to make inferences from those measurements on the population quantities $\mu$ and $\sigma$.

Y = [16.4, 17.0, 17.2, 17.4, 18.2, 18.2, 18.2, 19.9, 20.8]

Let us assume a gaussian pdf:

$$p(y|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\left(\frac{y-\mu}{2\sigma}\right)^2}$$

# Gaussian Distribution

# MLE Estimators

LIKELIHOOD: $p(y_1, \ldots, y_n | \mu, \sigma^2) = \prod_{i=1}^{n} p(y_i | \mu, \sigma^2)$

$$= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\left(\frac{(y_i-\mu)^2}{2\sigma^2}\right)} = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{1}{2}\sum_i \frac{(y_i - \mu)^2}{\sigma^2}\right\}$$

Take partials for $\hat{\mu}_{MLE}$ and $\hat{\sigma}^2_{MLE}$

# MLE for Moth Wing

$$\hat{\mu}_{MLE} = \frac{1}{N}\sum_i y_i = \bar{Y};\ \hat{\sigma}^2_{MLE} = \frac{1}{N}\sum_i (Y_i - \bar{Y}^2)$$

$\hat{\sigma}^2_{MLE}$ is a biased estimator of the population variance, while $\hat{\mu}_{MLE}$ is an unbiased estimator.

That is, $E_D[\hat{\mu}_{MLE}] = \mu$, where the $D$ subscripts means the expectation with respect to the predictive, or data-sampling, or data generating distribution.

VALUES: `sigma 1.33 mu 18.14`

# 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 between buses arriving.

# 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.

# True vs estimated

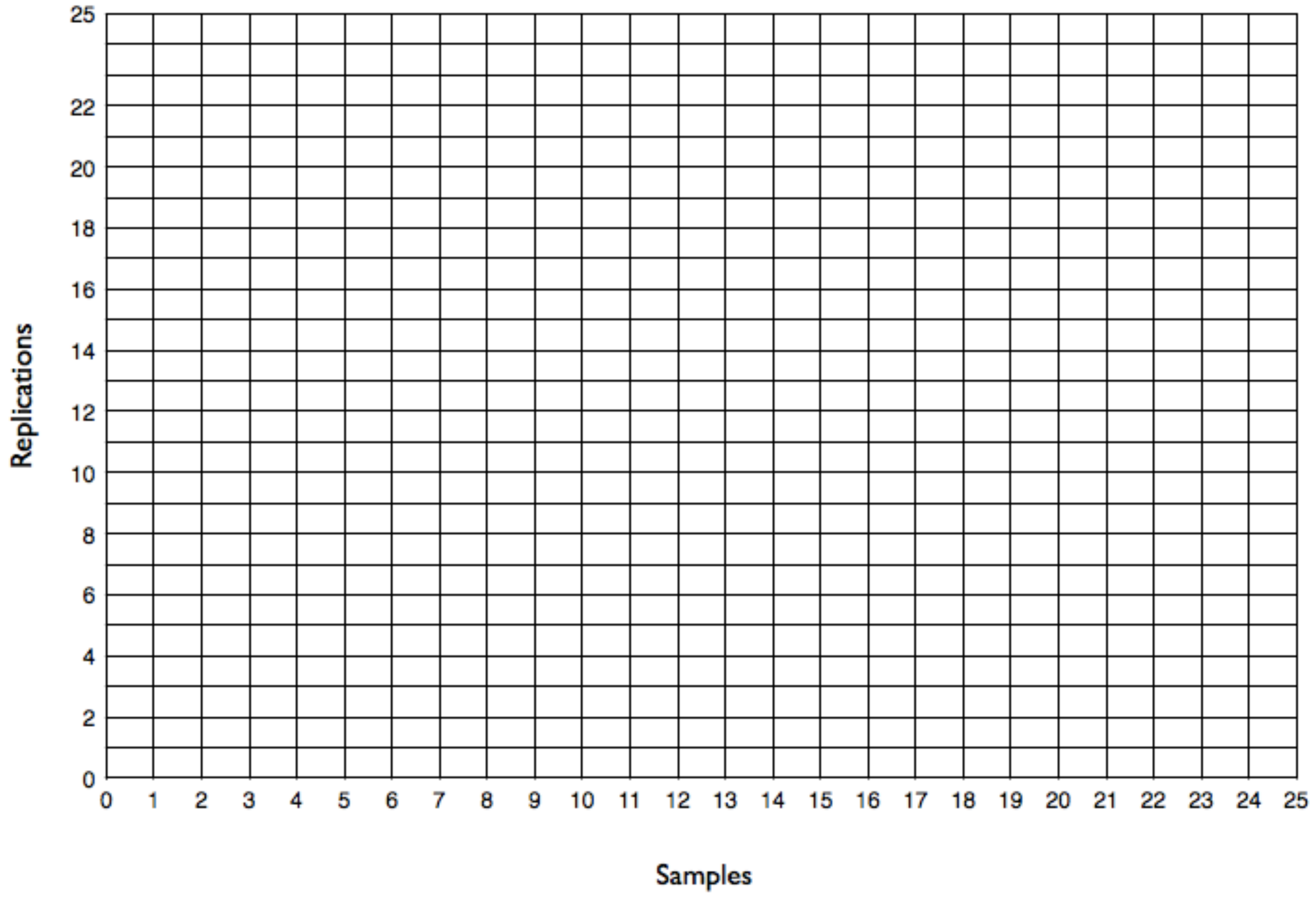
If your model describes the true generating process for the data, then there is some true $\mu^*$.

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

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

So, we'd have M estimates.

# M samples of N data points



# Sampling distribution

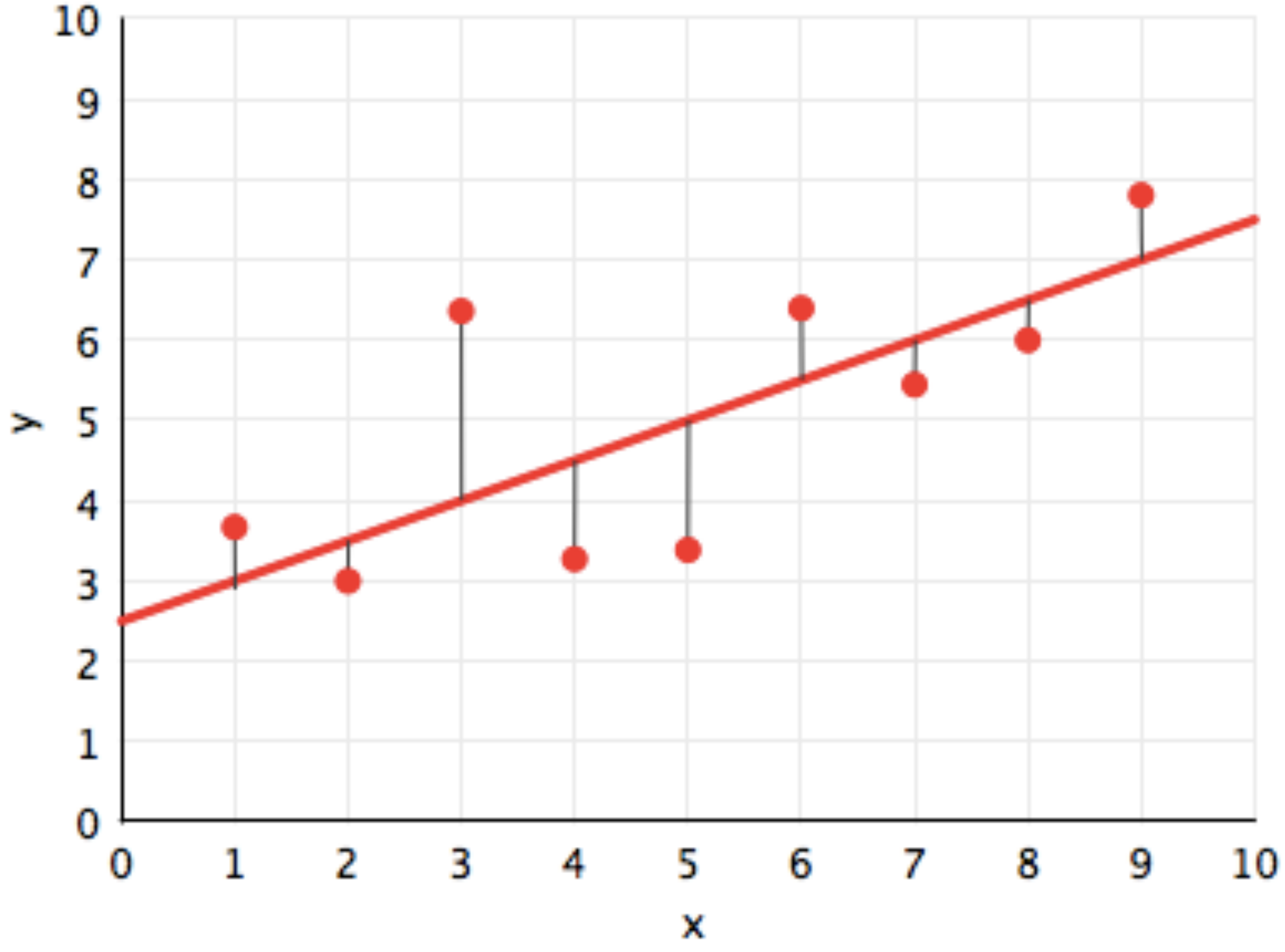
As we let $M \to \infty$, the distribution induced on $\hat{\mu}$ is the empirical **sampling distribution of the estimator**.

$\mu$ could be $\lambda$, our parameter, or a mean, a variance, etc

We could use the sampling distribution to get confidence intervals on $\lambda$.

But we dont have M samples. What to do?

# REGRESSION

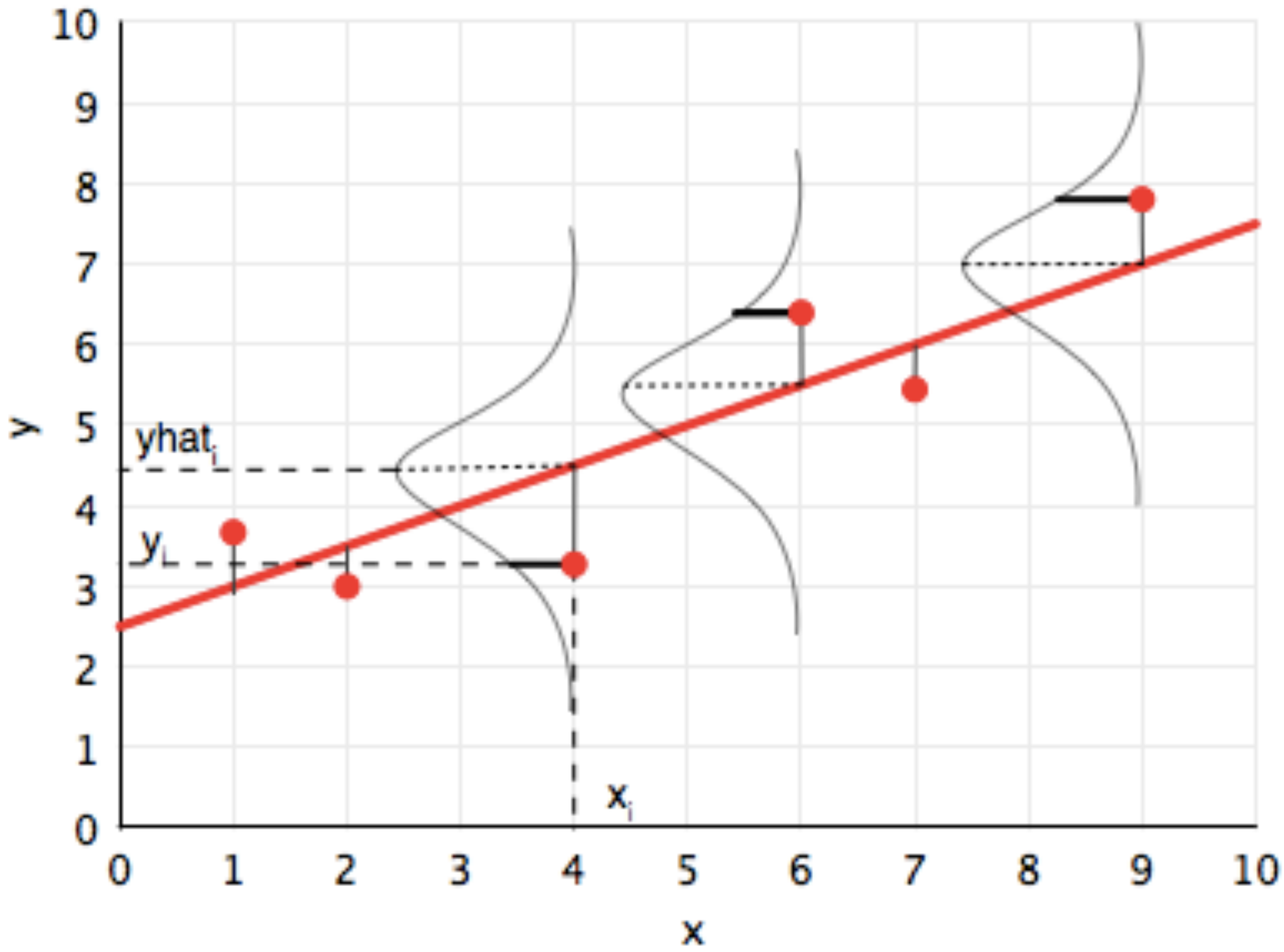


# Regression Noise Sources

- lack of knowledge of the true generating process
- sampling
- measurement error
- lack of knowledge of $x$

No more $y = f(x)$. Need $y = f(x) + \epsilon$.

or a $P(y \mid x)$



10
9
8
7
6
5
4
3
2
1
0
y
yhat$_i$
$y_i$
$x_i$
0
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2
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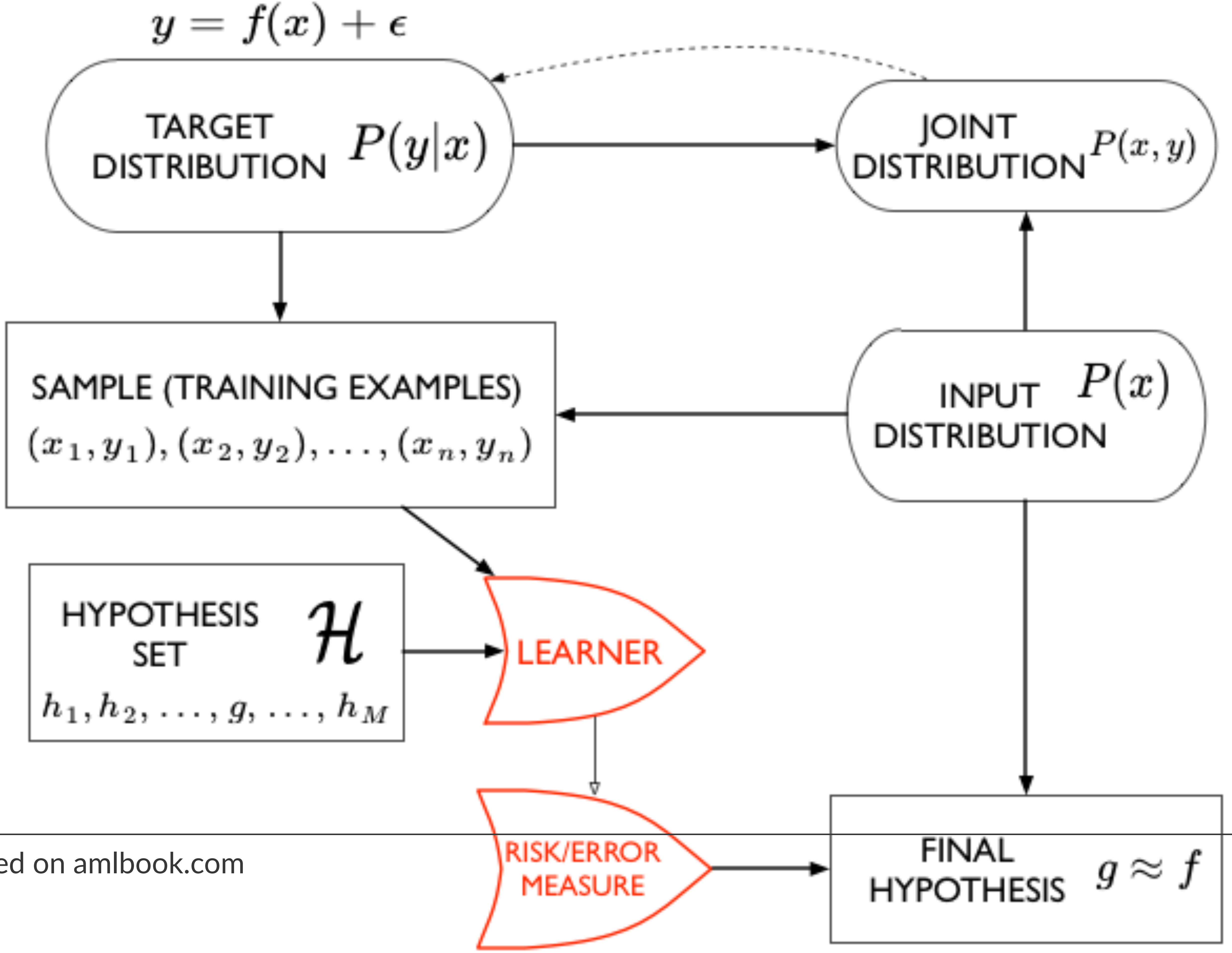
6
7
8
9
10
x

*




[*] image based on amlbook.com

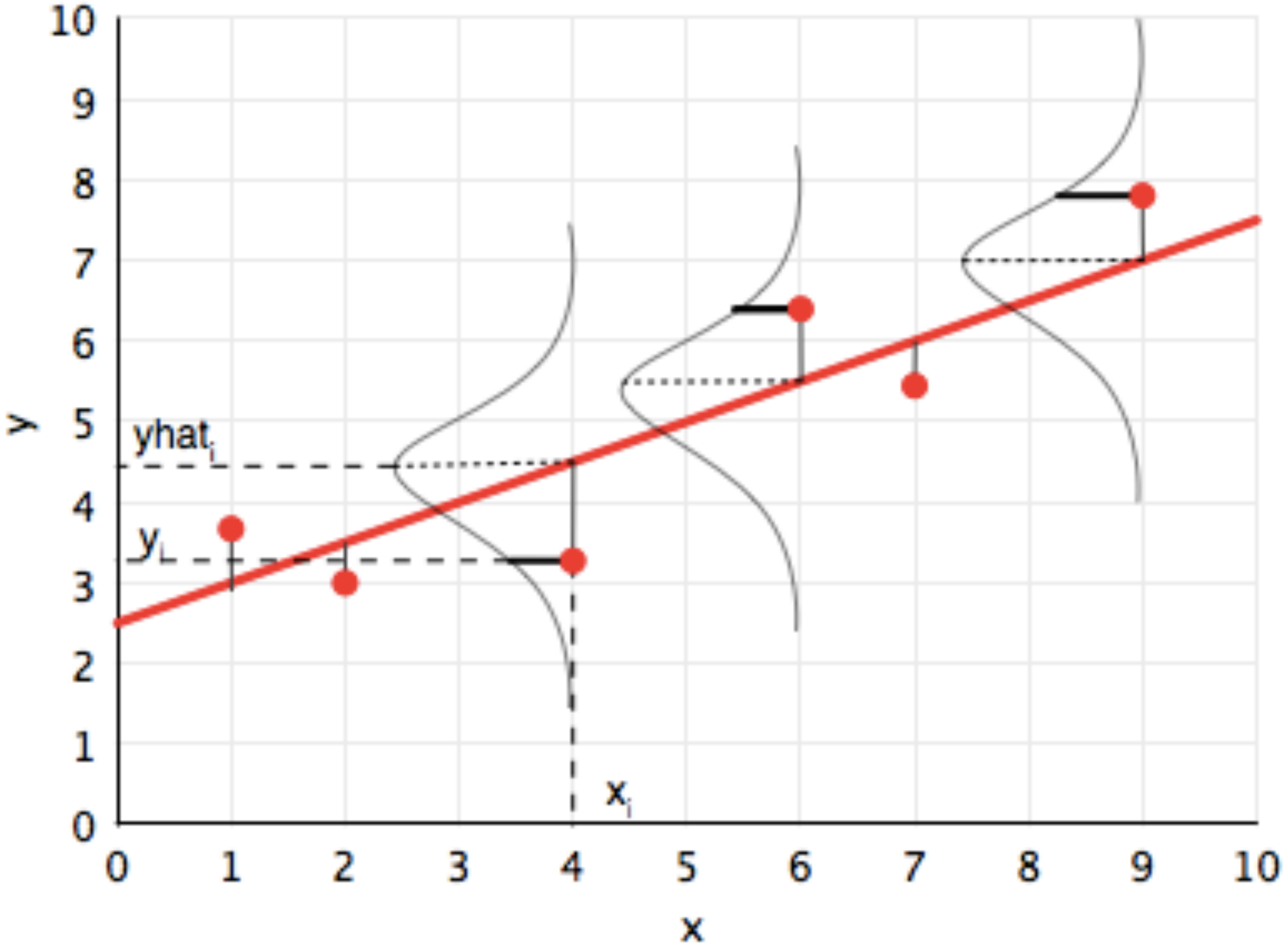
# Gaussian Distribution assumption

Each $y_i$ is gaussian distributed with mean $\mathbf{w} \cdot \mathbf{x}_i$ (the y predicted by the regression line) and variance $\sigma^2$:

$$y_i \sim N(\mathbf{w} \cdot \mathbf{x}_i, \sigma^2).$$

$$N(\mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(y-\mu)^2/2\sigma^2},$$

# Linear Regression MLE



We can then write the likelihood:

$$\mathcal{L} = p(\mathbf{y}|\mathbf{x}, \mathbf{w}, \sigma) = \prod_i p(\mathbf{y}_i|\mathbf{x}_i, \mathbf{w}, \sigma)$$

$$\mathcal{L} = (2\pi\sigma^2)^{(-n/2)} e^{\frac{-1}{2\sigma^2}\sum_i (y_i - \mathbf{w}\cdot\mathbf{x}_i)^2}.$$

The log likelihood $\ell$ then is given by:

$$\ell = \frac{-n}{2} log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_i (y_i - \mathbf{w}\cdot\mathbf{x}_i)^2.$$

# Maximizing gives:

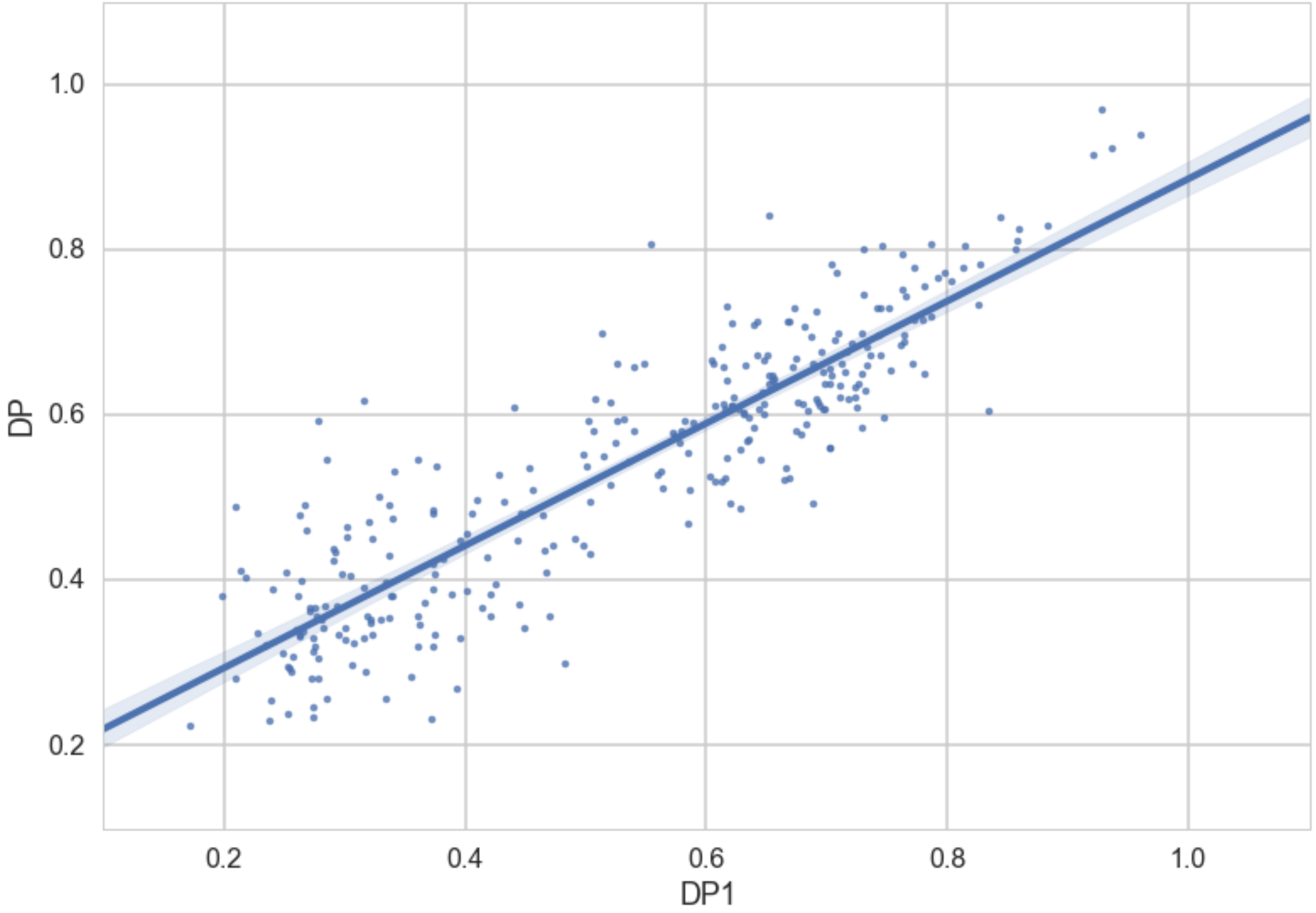
$$\mathbf{w}_{MLE} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y},$$

where we stack rows to get:

$$\mathbf{X} = stack(\{\mathbf{x}_i\})$$

$$\sigma^2_{MLE} = \frac{1}{n}\sum_i (y_i - \mathbf{w}\cdot\mathbf{x}_i)^2.$$

# Example: House Elections



# From Likelihood to Predictive Distribution

- the band on the previous graph is the sampling distribution of the regression line, or a representation of the sampling distribution of the $\mathbf{w}$.

- $p(y|\mathbf{x}, \mu_{MLE}, \sigma^2_{MLE})$ is a probability distribution

- thought of as $p(y^*|\mathbf{x}^*, \{\mathbf{x}_i, y_i\}, \mu_{MLE}, \sigma^2_{MLE})$, it is a predictive distribution for as yet unseen data $y^*$ at $\mathbf{x}^*$, or the sampling distribution for data, or the data-generating distribution, at the new covariates $\mathbf{x}^*$. This is a wider band.

| | | | |
|---|---|---|---|
| **Dep. Variable:** | DP | **R-squared:** | 0.806 |
| **Model:** | OLS | **Adj. R-squared:** | 0.804 |
| **Method:** | Least Squares | **F-statistic:** | 612.0 |
| **Date:** | Tue, 13 Oct 2015 | **Prob (F-statistic):** | 1.04e-105 |
| **Time:** | 16:33:01 | **Log-Likelihood:** | 368.81 |
| **No. Observations:** | 298 | **AIC:** | -731.6 |
| **Df Residuals:** | 295 | **BIC:** | -720.5 |
| **Df Model:** | 2 | | |
| **Covariance Type:** | nonrobust | | |

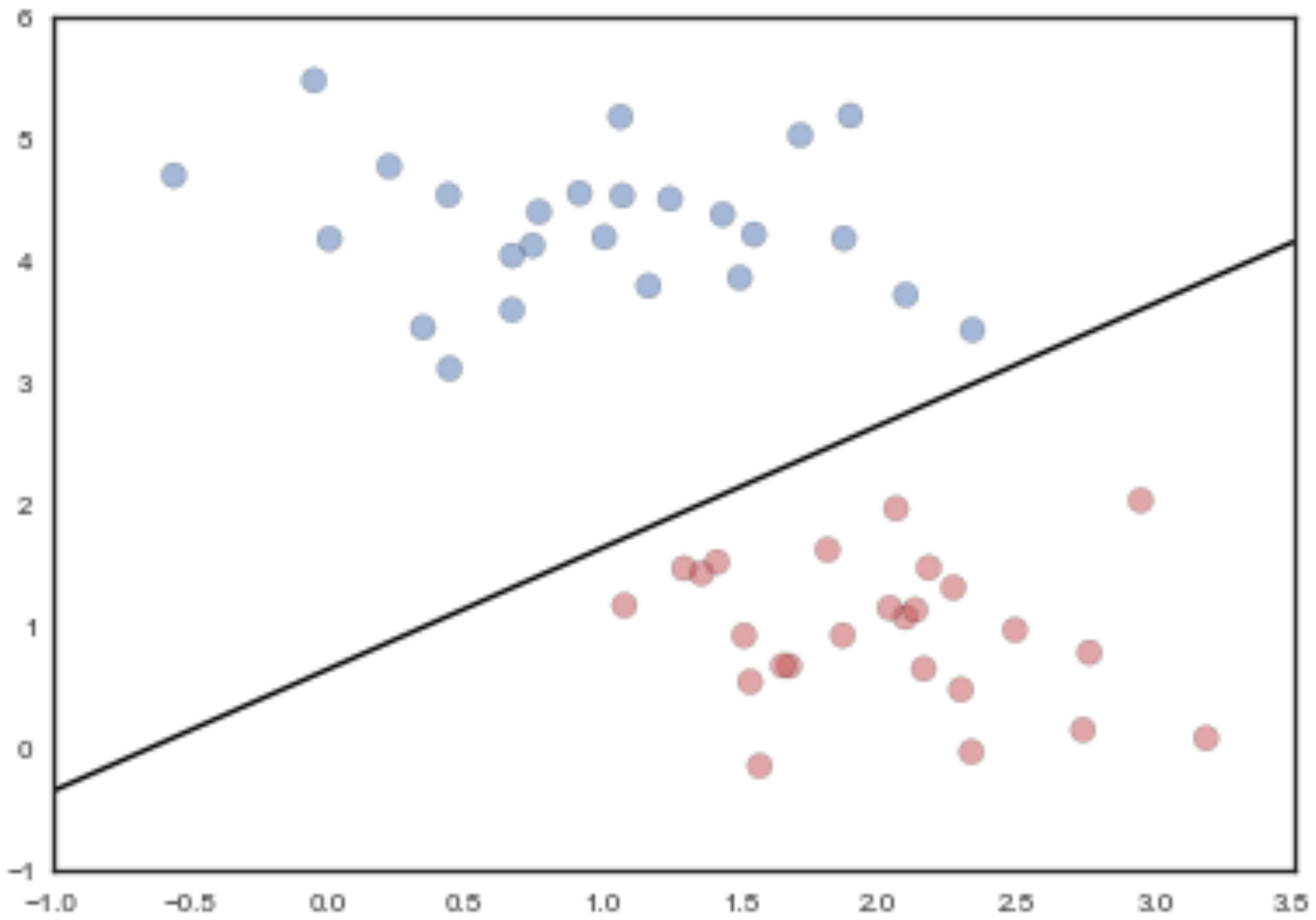
| | coef | std err | t | P>\|t\| | [95.0% Conf. Int.] |
|---|---|---|---|---|---|
| **Intercept** | 0.2326 | 0.020 | 11.503 | 0.000 | 0.193 0.272 |
| **DP1** | 0.5622 | 0.040 | 14.220 | 0.000 | 0.484 0.640 |
| **I** | 0.0429 | 0.008 | 5.333 | 0.000 | 0.027 0.059 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 7.465 | **Durbin-Watson:** | 1.728 |
| **Prob(Omnibus):** | 0.024 | **Jarque-Bera (JB):** | 7.316 |
| **Skew:** | 0.374 | **Prob(JB):** | 0.0258 |
| **Kurtosis:** | 3.174 | **Cond. No.** | 13.1 |

`Dem_Perc(t) ~ Dem_Perc(t-2) + I`

- done in statsmodels
- From Gelman and Hwang

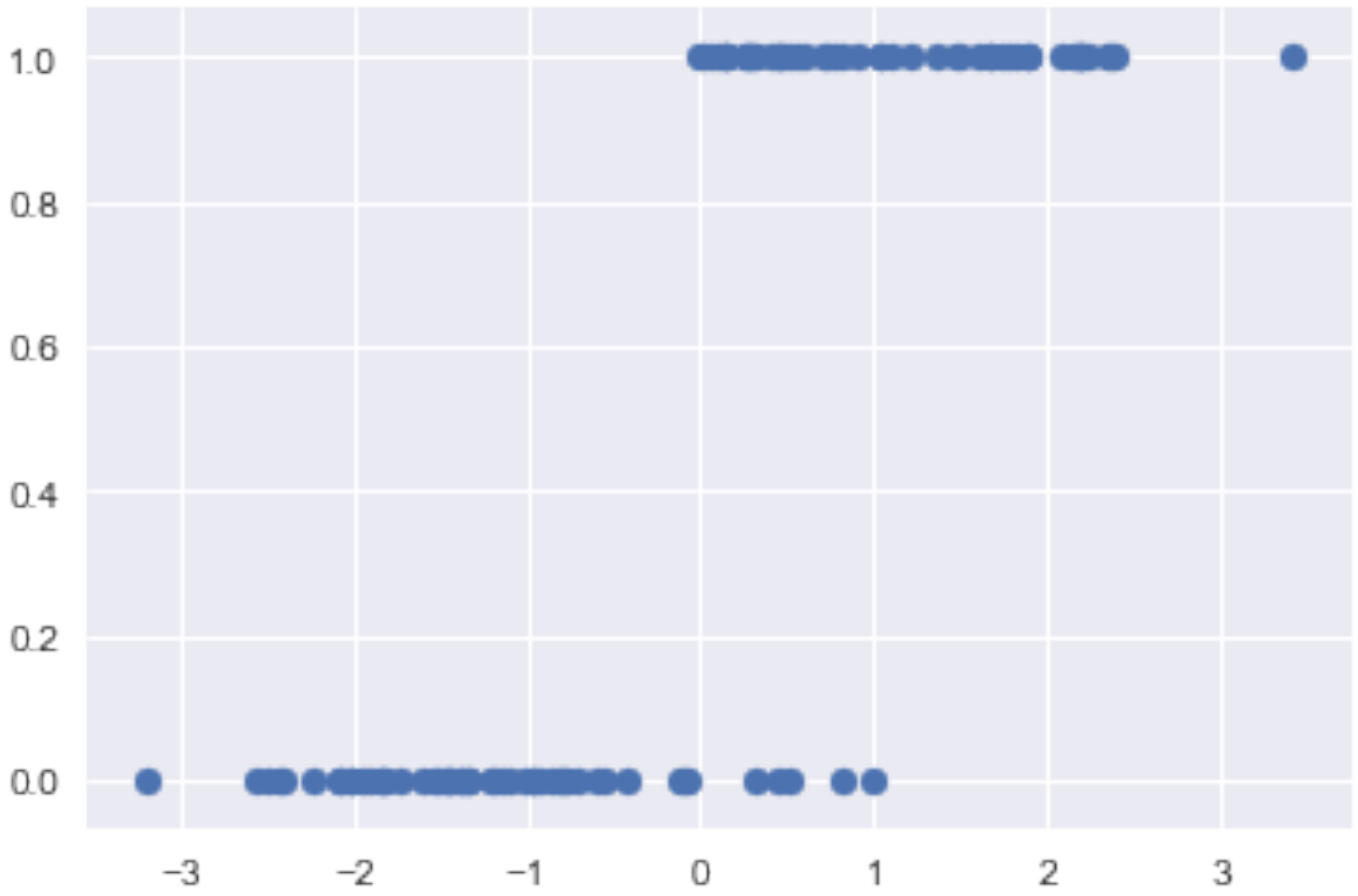
# CLASSIFICATION



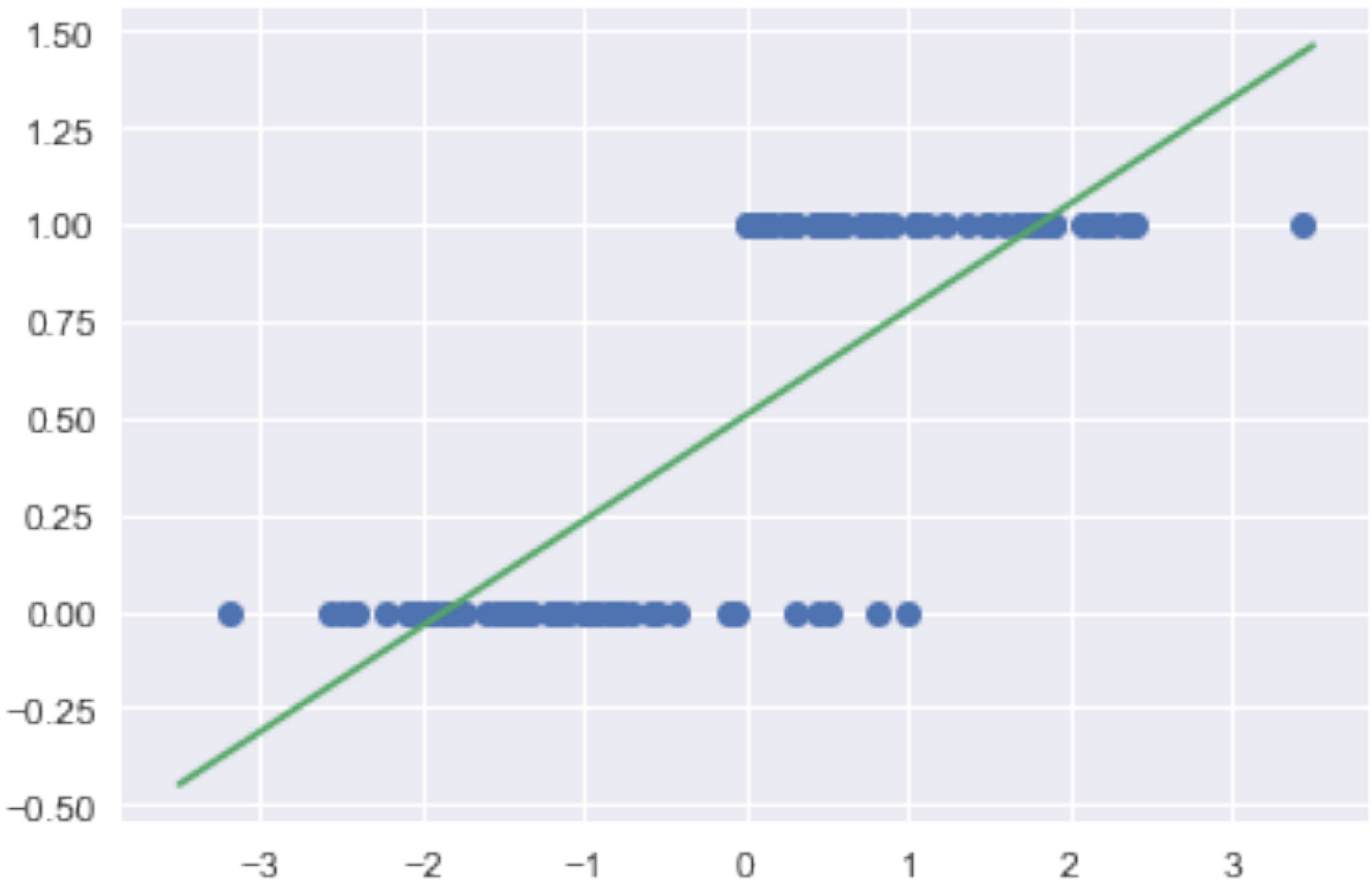

- will a customer churn?
- is this a check? For how much?
- a man or a woman?
- will this customer buy?
- do you have cancer?
- is this spam?
- whose picture is this?
- what is this text about?[j]

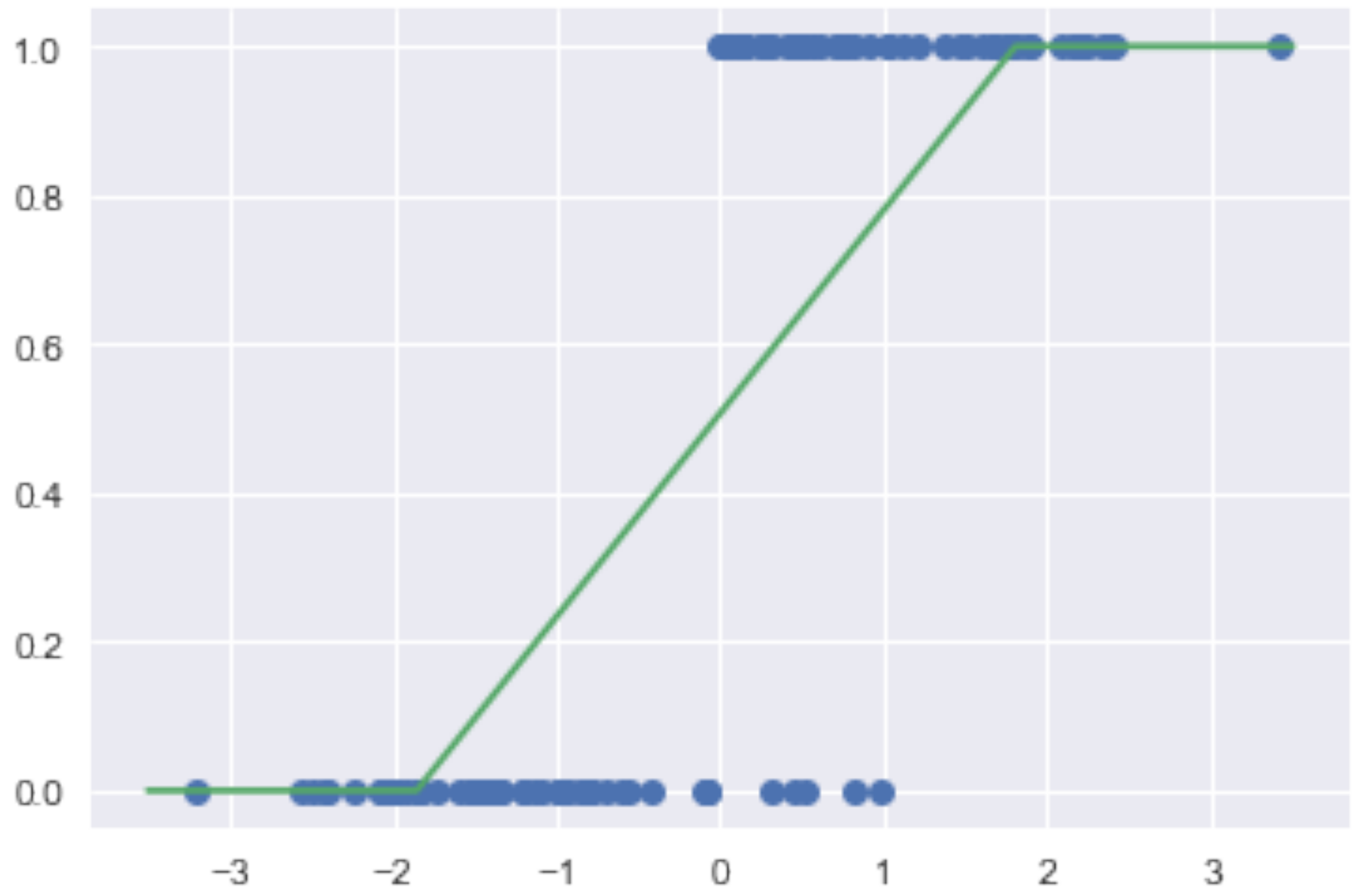
[j] image from code in http://bit.ly/1Azg29G

# 1-D classification problem



# 1-D Using Linear regression



# MLE for Logistic Regression

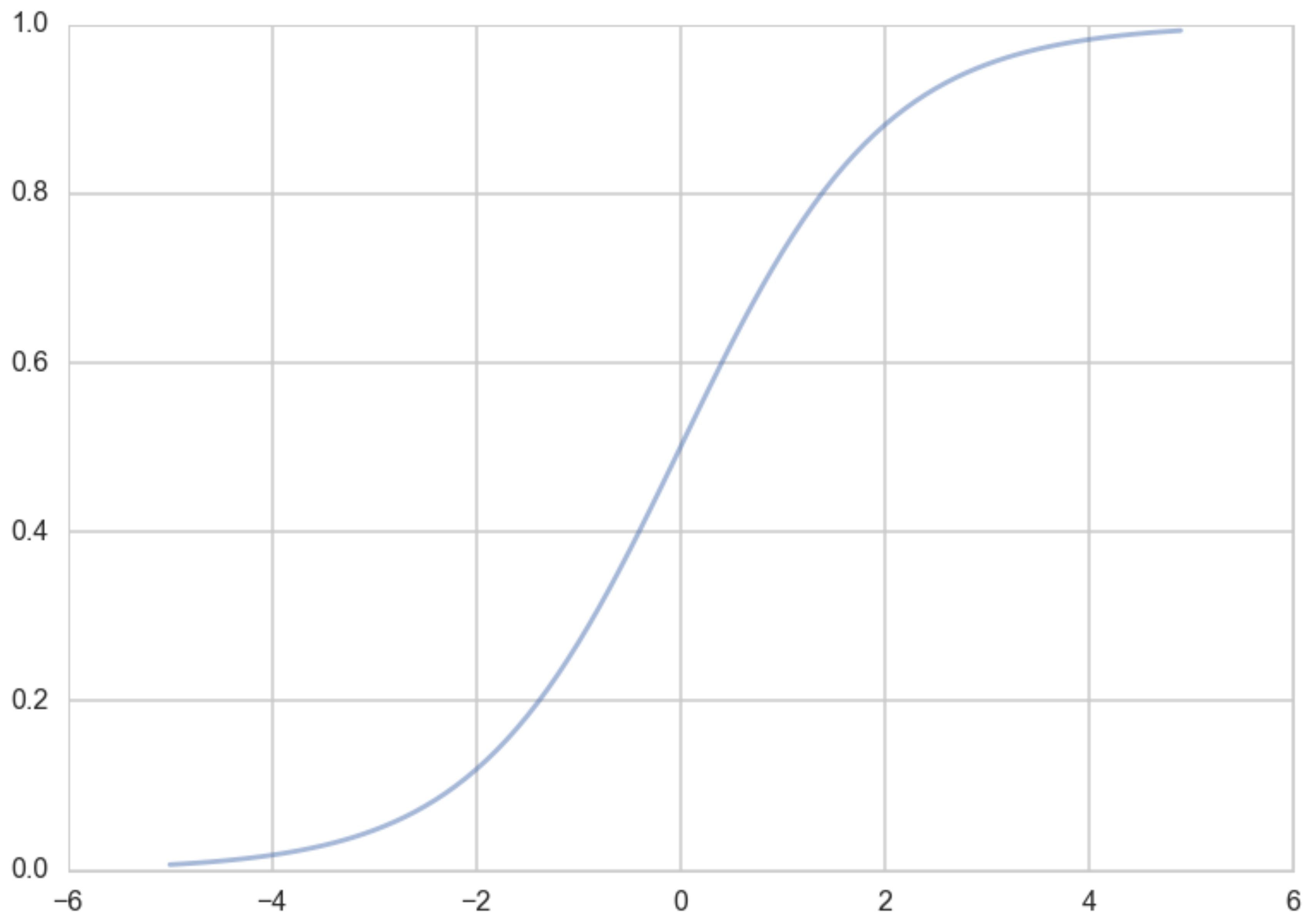
- example of a Generalized Linear Model (GLM)
- "Squeeze" linear regression through a **Sigmoid** function
- this bounds the output to be a probability
- What is the sampling Distribution?

# Sigmoid function

This function is plotted below:

```
h = lambda z: 1./(1+np.exp(-z))
zs=np.arange(-5,5,0.1)
plt.plot(zs, h(zs), alpha=0.5);
```

Identify: $z = \mathbf{w} \cdot \mathbf{x}$ and $h(\mathbf{w} \cdot \mathbf{x})$ with the probability that the sample is a '1' ($y = 1$).



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

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

These two can be written together as

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

BERNOULLI!!

# Bernoulli Distribution

Multiplying over the samples we get:

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

A noisy $y$ is to imagine that our data $\mathcal{D}$ was generated from a joint probability distribution $P(x, y)$. Thus we need to model $y$ at a given $x$, written as $P(y \mid x)$, and since $P(x)$ is also a probability distribution, we have:

$$P(x, y) = P(y \mid x)P(x),$$

Indeed its important to realize that a particular sample can be thought of as a draw from some "true" probability distribution.

**maximum likelihood** estimation maximises the **likelihood of the sample y**,

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

Again, we can equivalently maximize

$$\ell = log(P(y \mid \mathbf{x}, \mathbf{w}))$$

Thus

$$
\begin{aligned}
\ell &= log\left(\prod_{y_i\in\mathcal{D}} h(\mathbf{w}\cdot\mathbf{x}_i)^{y_i}(1-h(\mathbf{w}\cdot\mathbf{x}_i))^{(1-y_i)}\right)\\
&= \sum_{y_i\in\mathcal{D}} log\left(h(\mathbf{w}\cdot\mathbf{x}_i)^{y_i}(1-h(\mathbf{w}\cdot\mathbf{x}_i))^{(1-y_i)}\right)\\
&= \sum_{y_i\in\mathcal{D}} log\, h(\mathbf{w}\cdot\mathbf{x}_i)^{y_i} + log\,(1-h(\mathbf{w}\cdot\mathbf{x}_i))^{(1-y_i)}\\
&= \sum_{y_i\in\mathcal{D}} (y_i log(h(\mathbf{w}\cdot\mathbf{x})) + (1-y_i)log(1-h(\mathbf{w}\cdot\mathbf{x})))
\end{aligned}
$$

Use Convex optimization!

# 1-D Using Logistic regression