Linear Regression

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Data

Given a table of numbers, what can you do?

Living area (feet^2)	#bedrooms	Price (1000$s)	.....
2104	3	400	
1600	3	330	
2400	3	369	
1416	2	232	
3000	4	540	
⋮	⋮	⋮	

→

	x_1	x_2	x_3	x_4	.....
Apt. 1	$x_1^{(1)}$	$x_2^{(1)}$	$x_3^{(1)}$	$x_4^{(1)}$	
Apt. 2	$x_1^{(2)}$	$x_2^{(2)}$	$x_3^{(2)}$	$x_4^{(2)}$	⋮
Apt. 3	$x_1^{(3)}$	$x_2^{(3)}$	$x_3^{(3)}$	$x_4^{(3)}$	
Apt. 4	$x_1^{(4)}$	$x_2^{(4)}$	$x_3^{(4)}$	$x_4^{(4)}$	
	⋮	⋮	⋮	⋮	

- Visualization: Look at it!
- Find statistical features: Mean, median, outliers etc.
- Clean it: missing values, …

What are the inputs and outputs?

- **Inputs**: quantities that are typically **given**
- **Outputs**: quantities we want to **predict**

Living area (feet^2)	#bedrooms	Price (1000$s)
2104	3	400
1600	3	330
2400	3	369
1416	2	232
3000	4	540
⋮	⋮	⋮

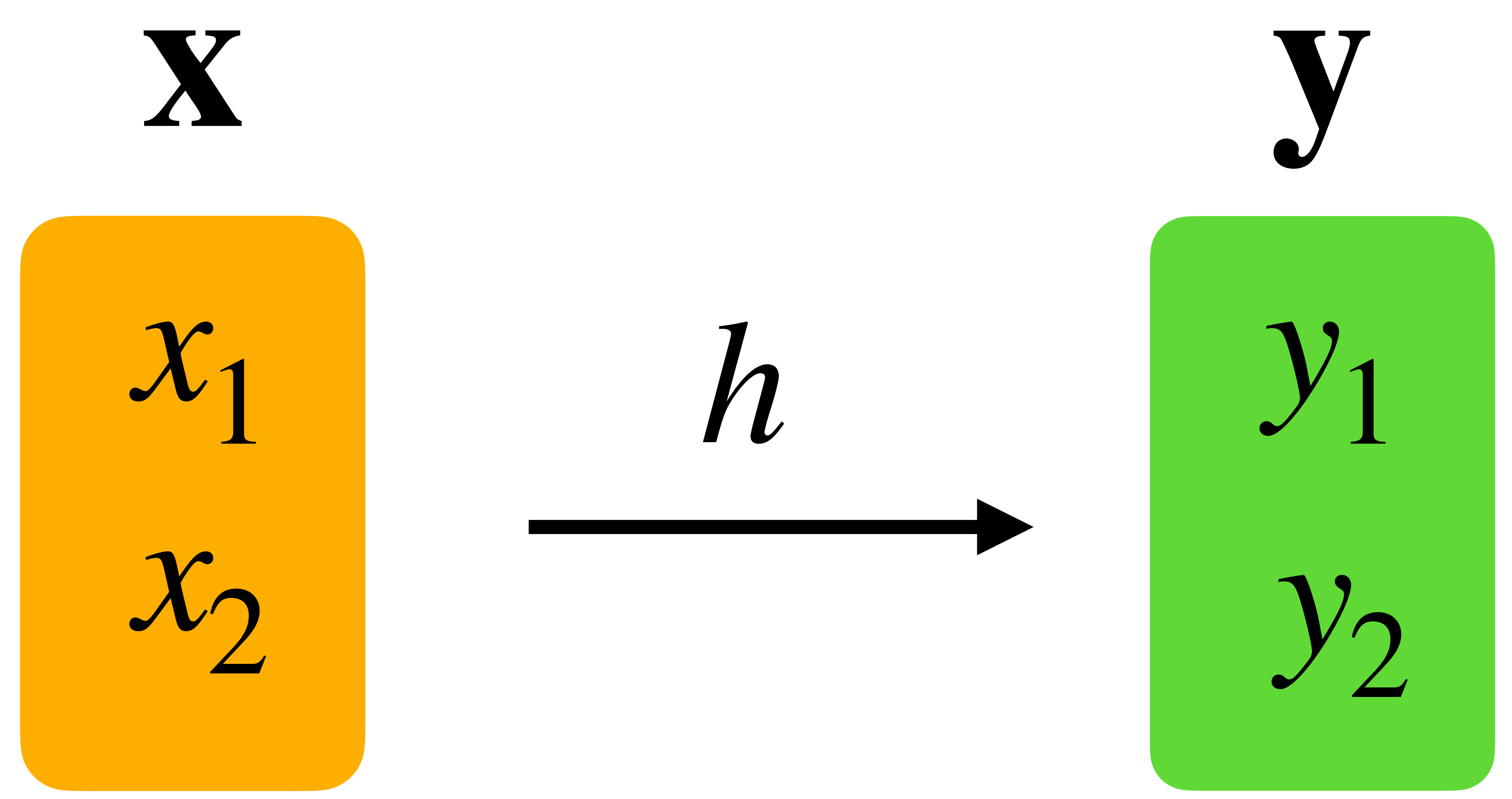
→

	Inputs		Outputs		
	x_1	x_2	x_3	x_4	.....
Apt. 1	$x_1^{(1)}$	$x_2^{(1)}$	$x_3^{(1)}$	$x_4^{(1)}$	
Apt. 2	$x_1^{(2)}$	$x_2^{(2)}$	$x_3^{(2)}$	$x_4^{(2)}$	⋮
Apt. 3	$x_1^{(3)}$	$x_2^{(3)}$	$x_3^{(3)}$	$x_4^{(3)}$	
Apt. 4	$x_1^{(4)}$	$x_2^{(4)}$	$x_3^{(4)}$	$x_4^{(4)}$	
	⋮	⋮	⋮	⋮	

Given inputs, predict outputs

	Inputs		Outputs	
	x_1	x_2	y_1	y_2
Apt. 1	$x_1^{(1)}$	$x_2^{(1)}$	$y_1^{(1)}$	$y_2^{(1)}$
Apt. 2	$x_1^{(2)}$	$x_2^{(2)}$	$y_1^{(2)}$	$y_2^{(2)}$
Apt. 3	$x_1^{(3)}$	$x_2^{(3)}$	$y_1^{(3)}$	$y_2^{(3)}$
Apt. 4	$x_1^{(4)}$	$x_2^{(4)}$	$y_1^{(4)}$	$y_2^{(4)}$
	$\vdots$	$\vdots$	$\vdots$	$\vdots$
Given Input	$x_1^{(n)}$	$x_2^{(n)}$	??	**Unknown output**

Supervised Learning



Given the data,
find a **function** h, a.k.a **hypothesis**,
that predicts outputs, given inputs

$$\mathbf{y} = h(\mathbf{x})$$

Assume multiple inputs, 1 output

x_1	x_2	y	
Living area (feet^2)	#bedrooms	Price (1000\$s)	.....
2104	3	400	
1600	3	330	
2400	3	369	
1416	2	232	
3000	4	540	
⋮	⋮	⋮	

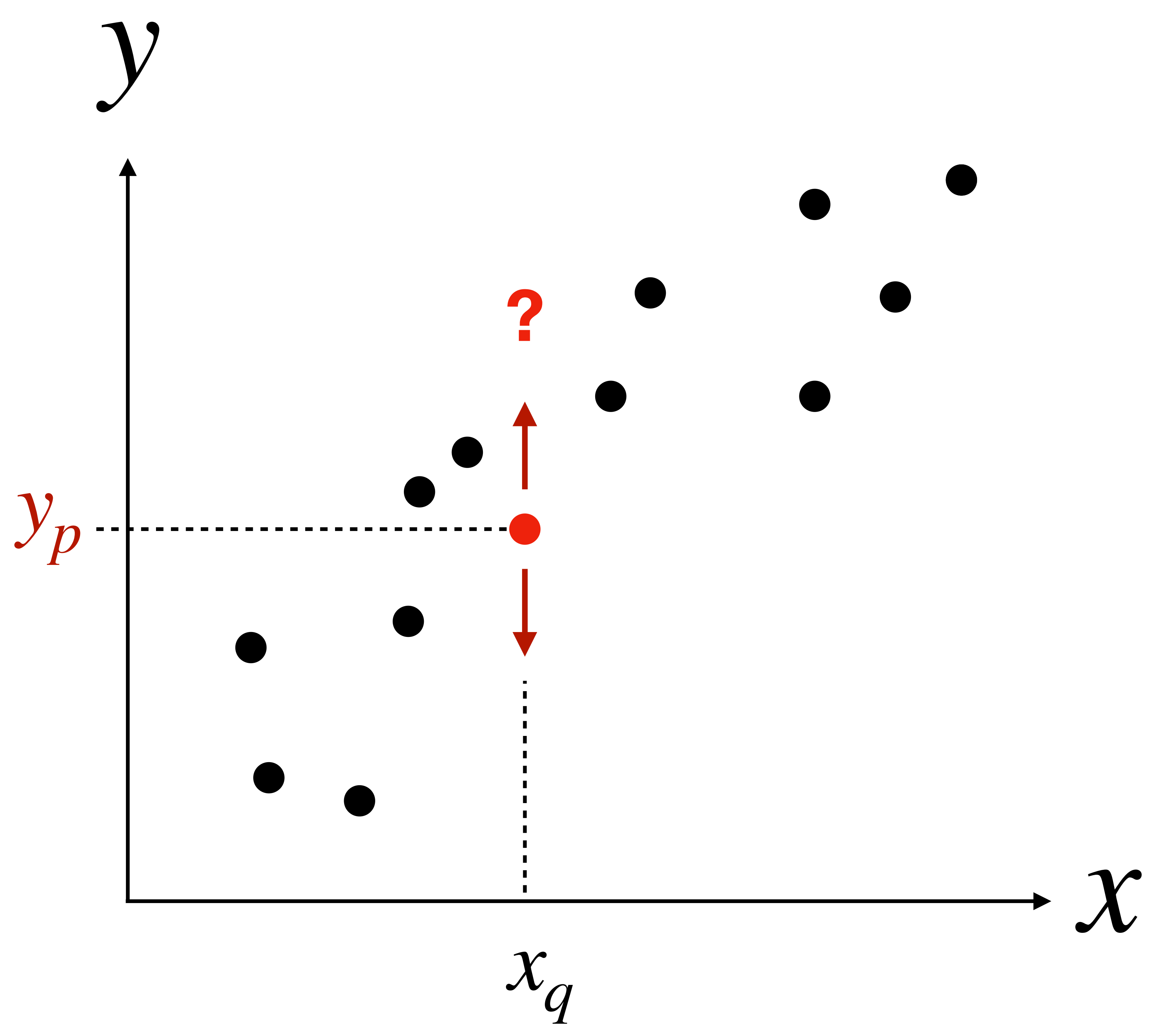
→

Inputs		Output
x_1	x_2	y
$x_1^{(1)}$	$x_2^{(1)}$	$y^{(1)}$
$x_1^{(2)}$	$x_2^{(2)}$	$y^{(2)}$
$x_1^{(3)}$	$x_2^{(3)}$	$y^{(3)}$
$x_1^{(4)}$	$x_2^{(4)}$	$y^{(4)}$
⋮	⋮	⋮

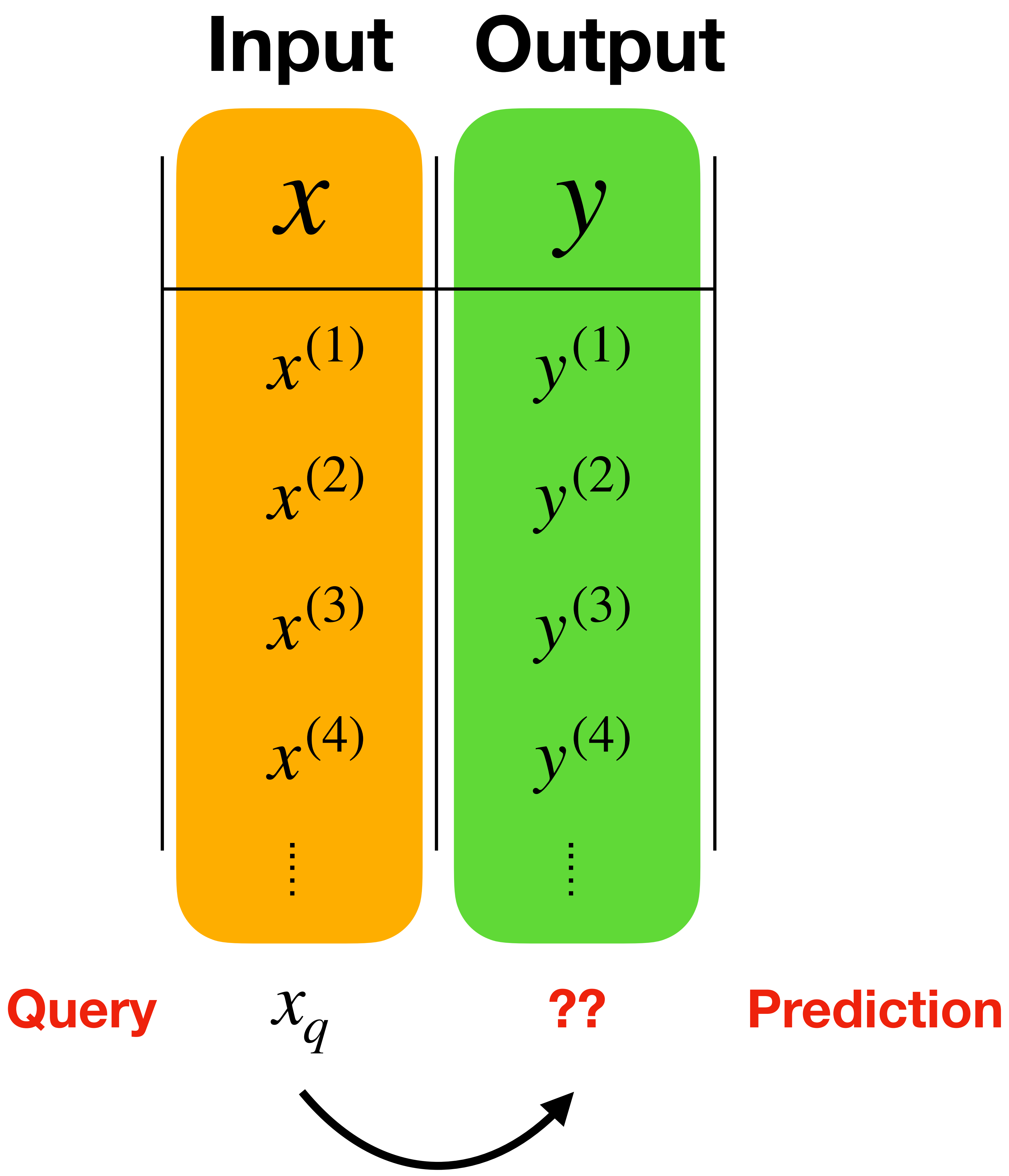
Given new input, what's the output?

(size) Input	(price) Output
x	y
$x^{(1)}$	$y^{(1)}$
$x^{(2)}$	$y^{(2)}$
$x^{(3)}$	$y^{(3)}$
$x^{(4)}$	$y^{(4)}$
⋮	⋮

Query x_q → y_p **??** **Prediction**

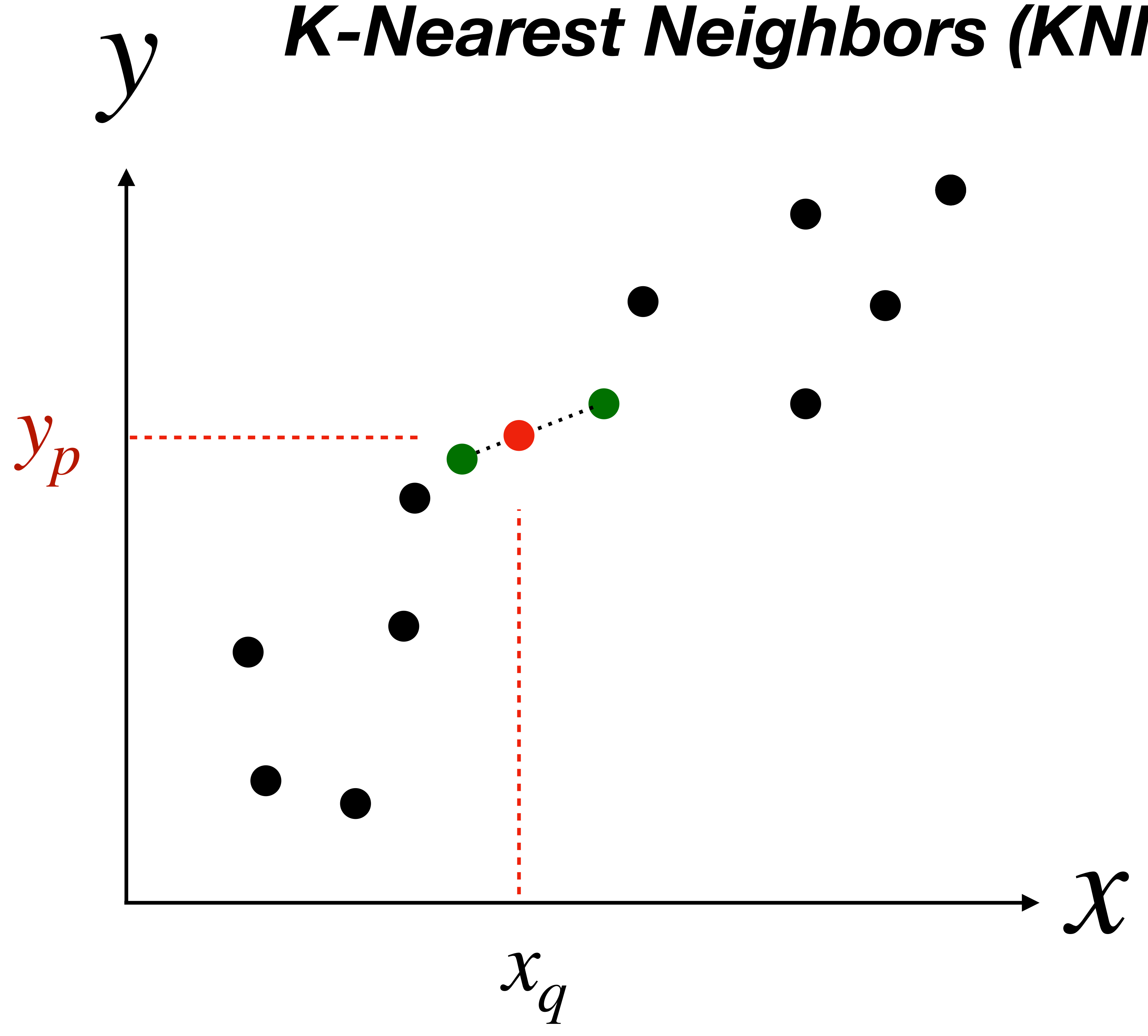


Given new input, what's the output?

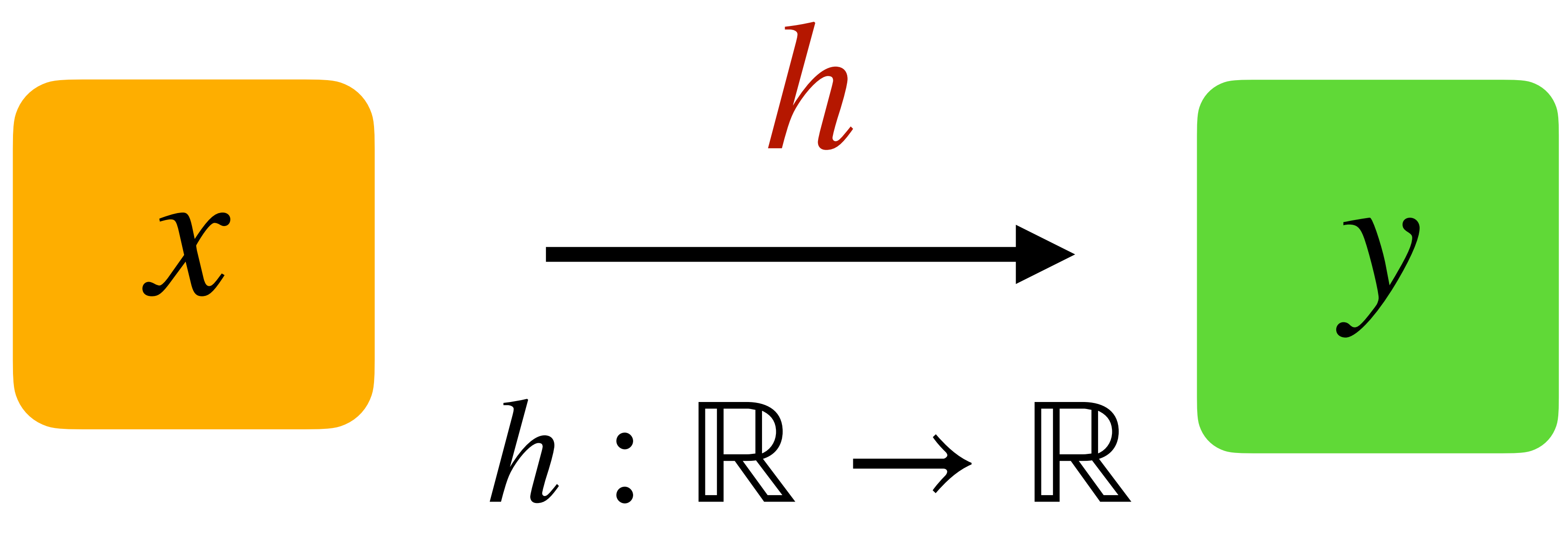


Weighted average of surrounding points

K-Nearest Neighbors (KNN)

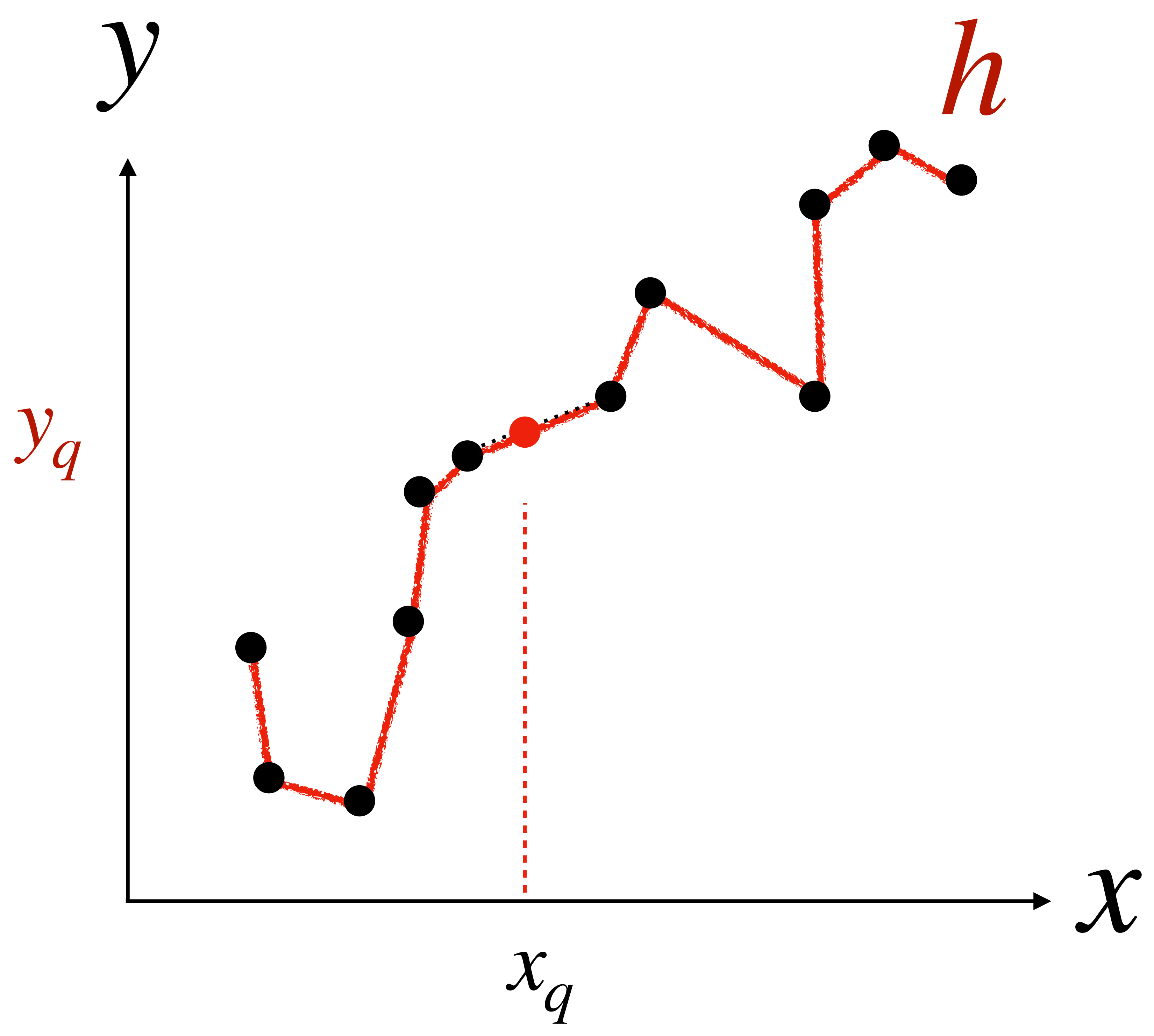


Given new input, what's the output?

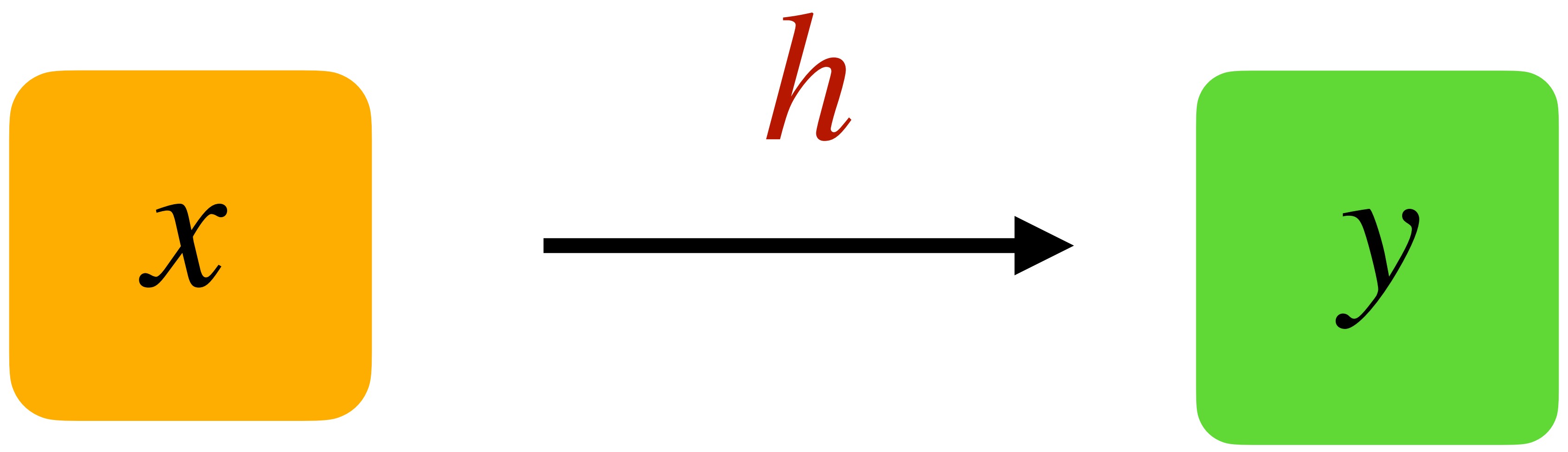


Given the data,
find a **function** h, a.k.a **hypothesis,**
that predicts an output, given an input

Linear Interpolation

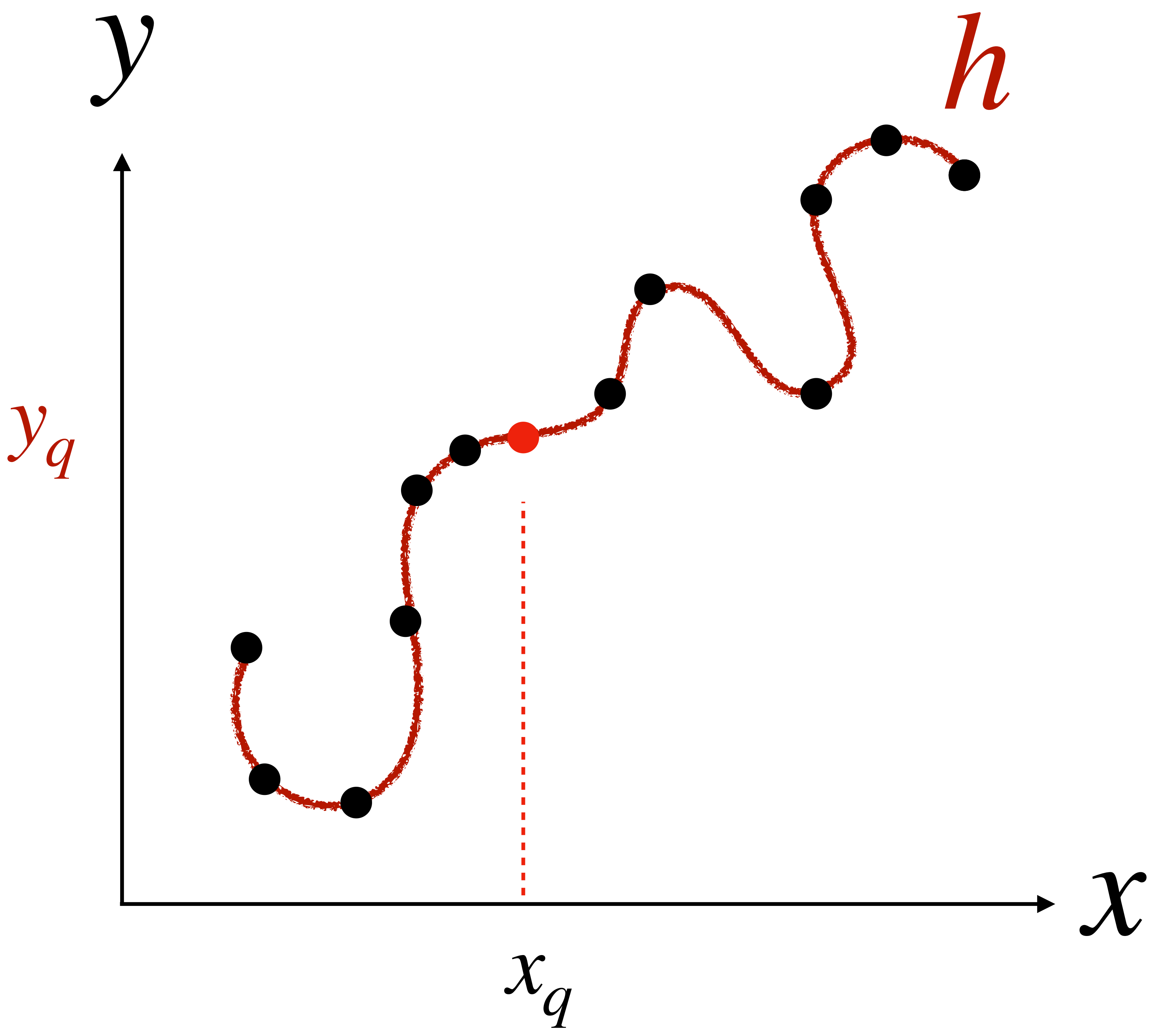


Given new input, what's the output?

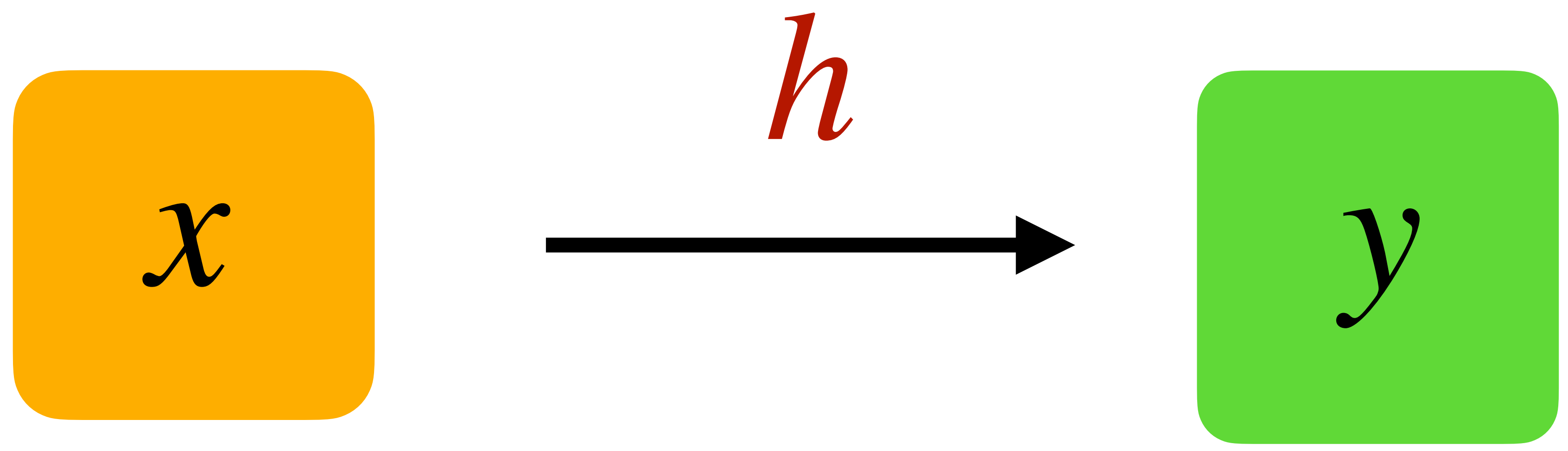


Given the data,
find a **function** h, a.k.a **hypothesis,**
that predicts an output, given an input

Polynomial Interpolation

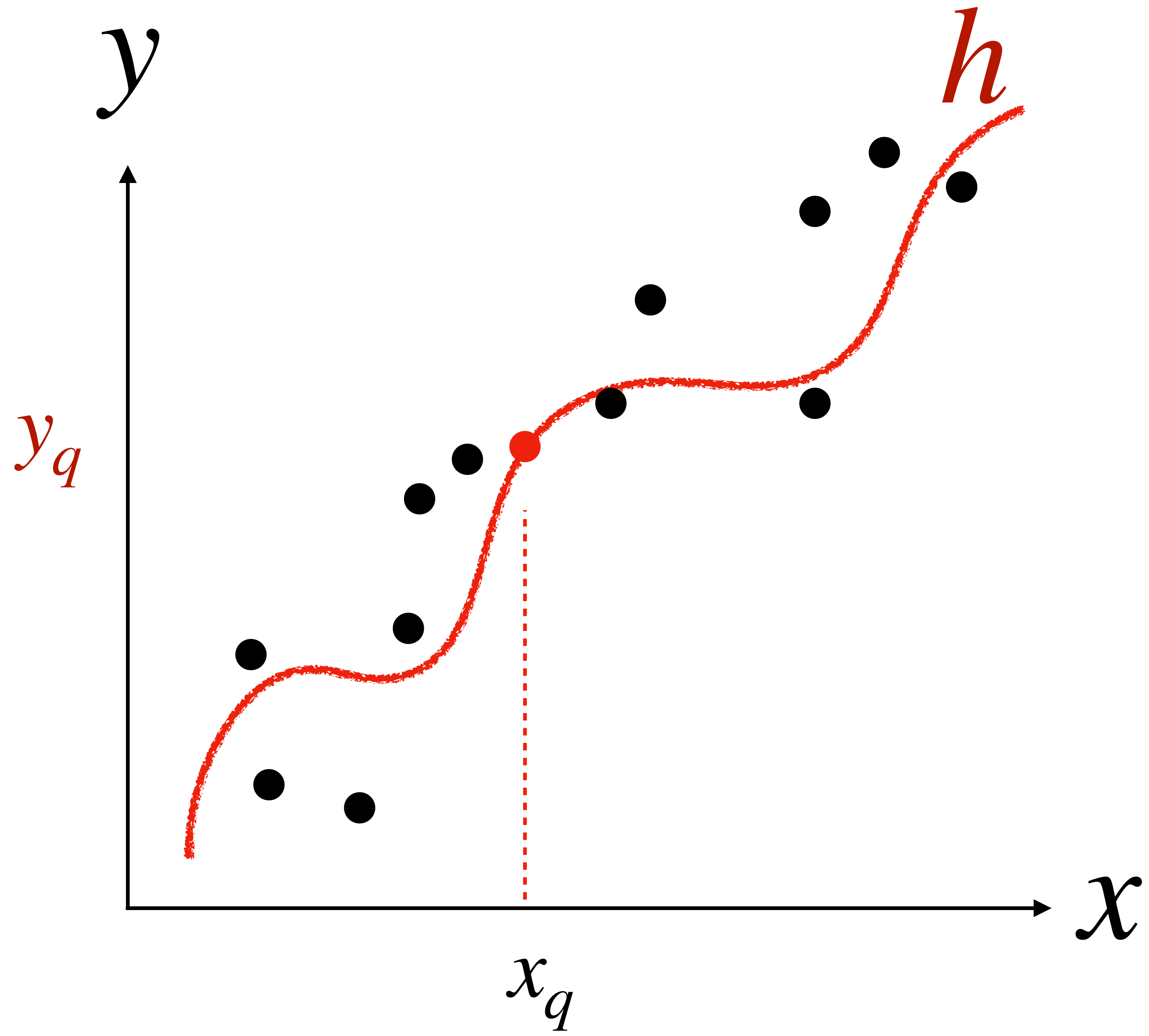


Given new input, what's the output?



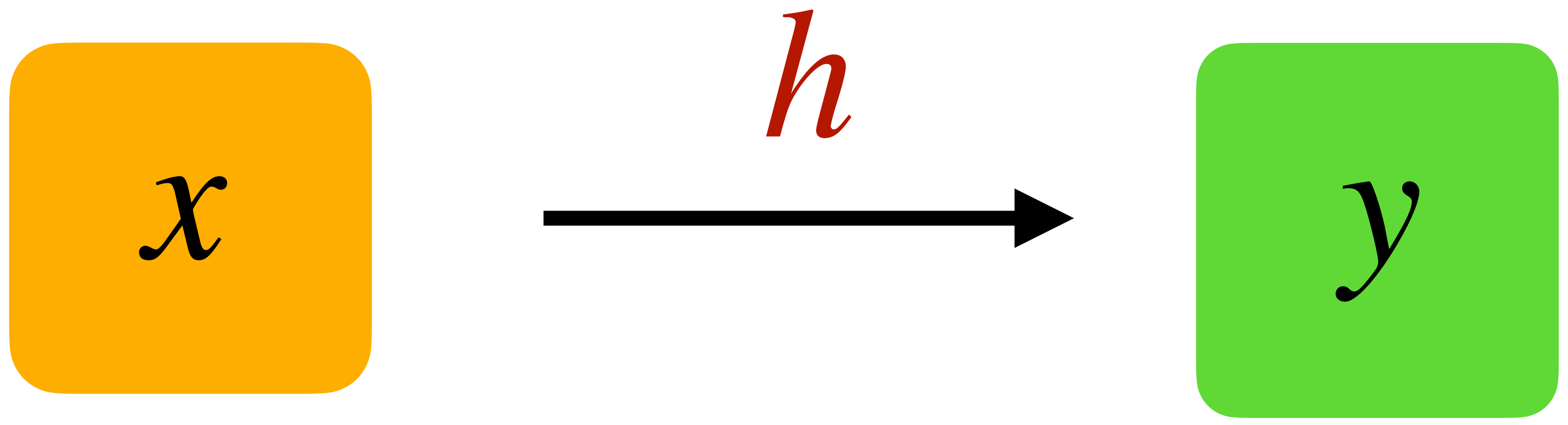
Given the data,
find a **function** h, a.k.a **hypothesis,**
that predicts an output, given an input

Some other function?



Given new input, what's the output?

Assume a linear hypothesis

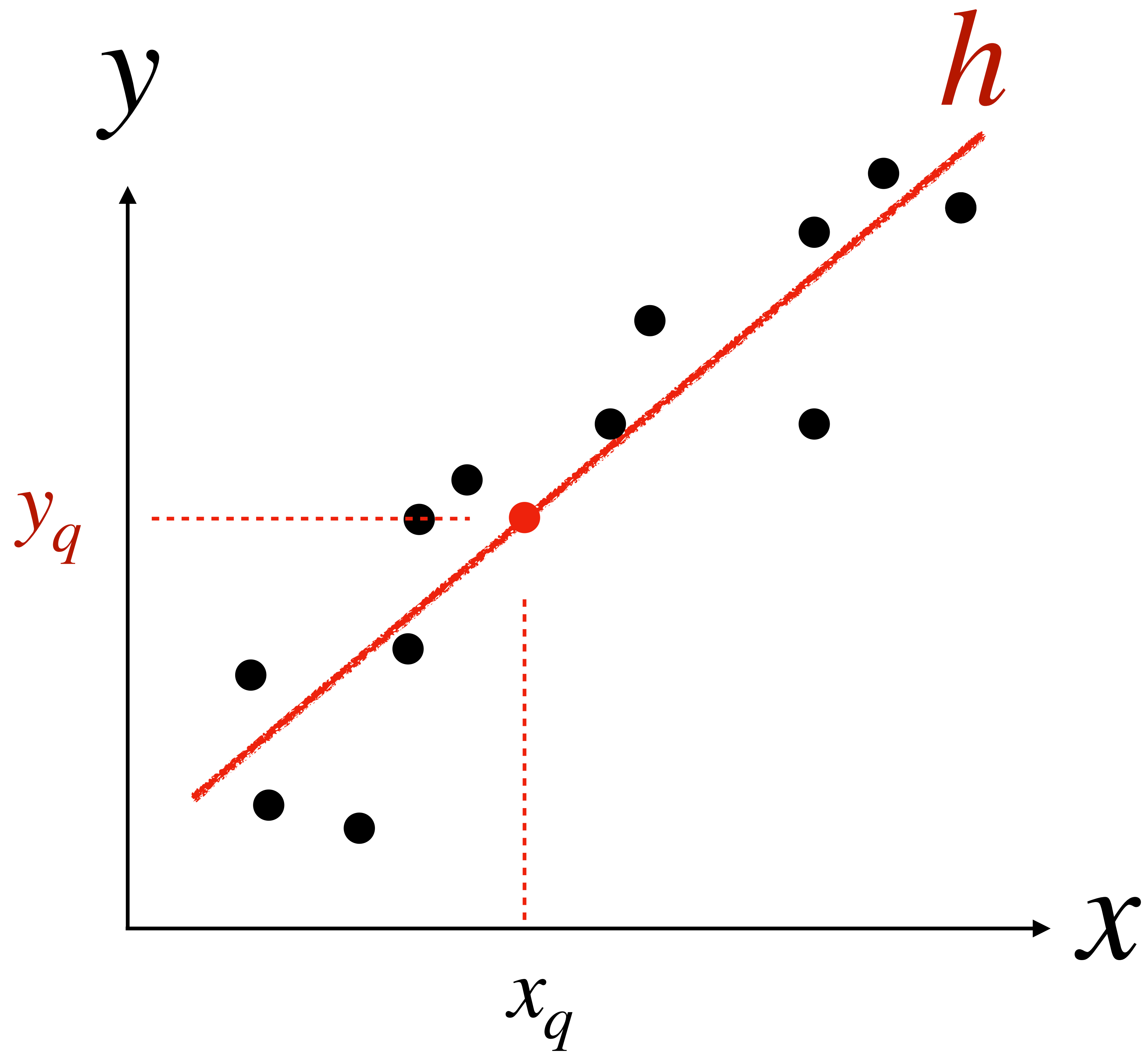


$$h(x) = ax + b$$

What are the best a and b that fit the data?

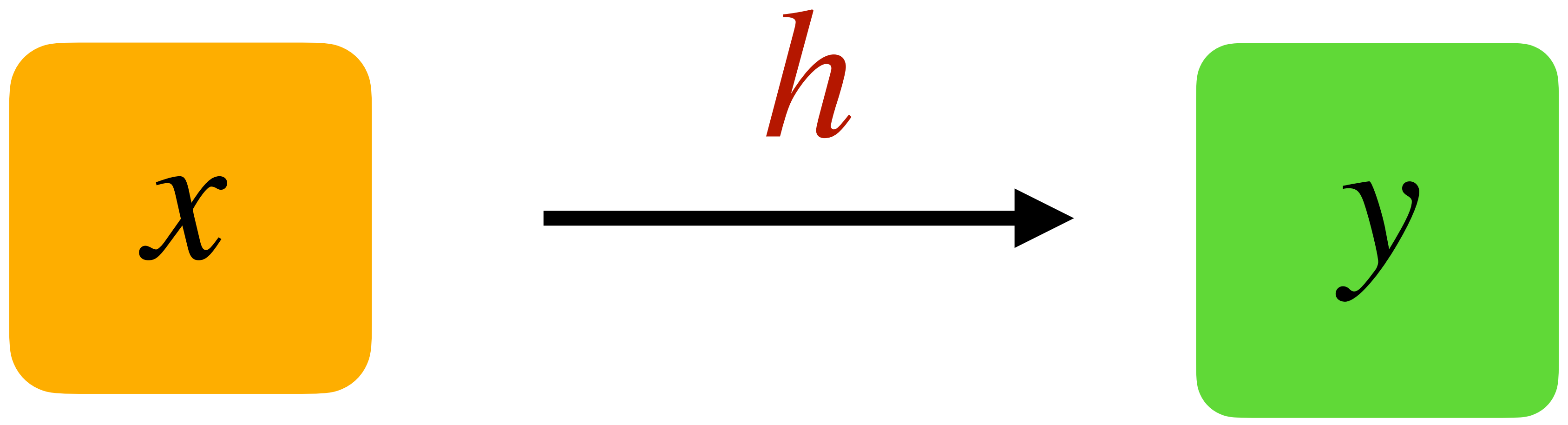
a, b **are fitting parameters**

Linear function



Assume a linear hypothesis

Assume a linear hypothesis



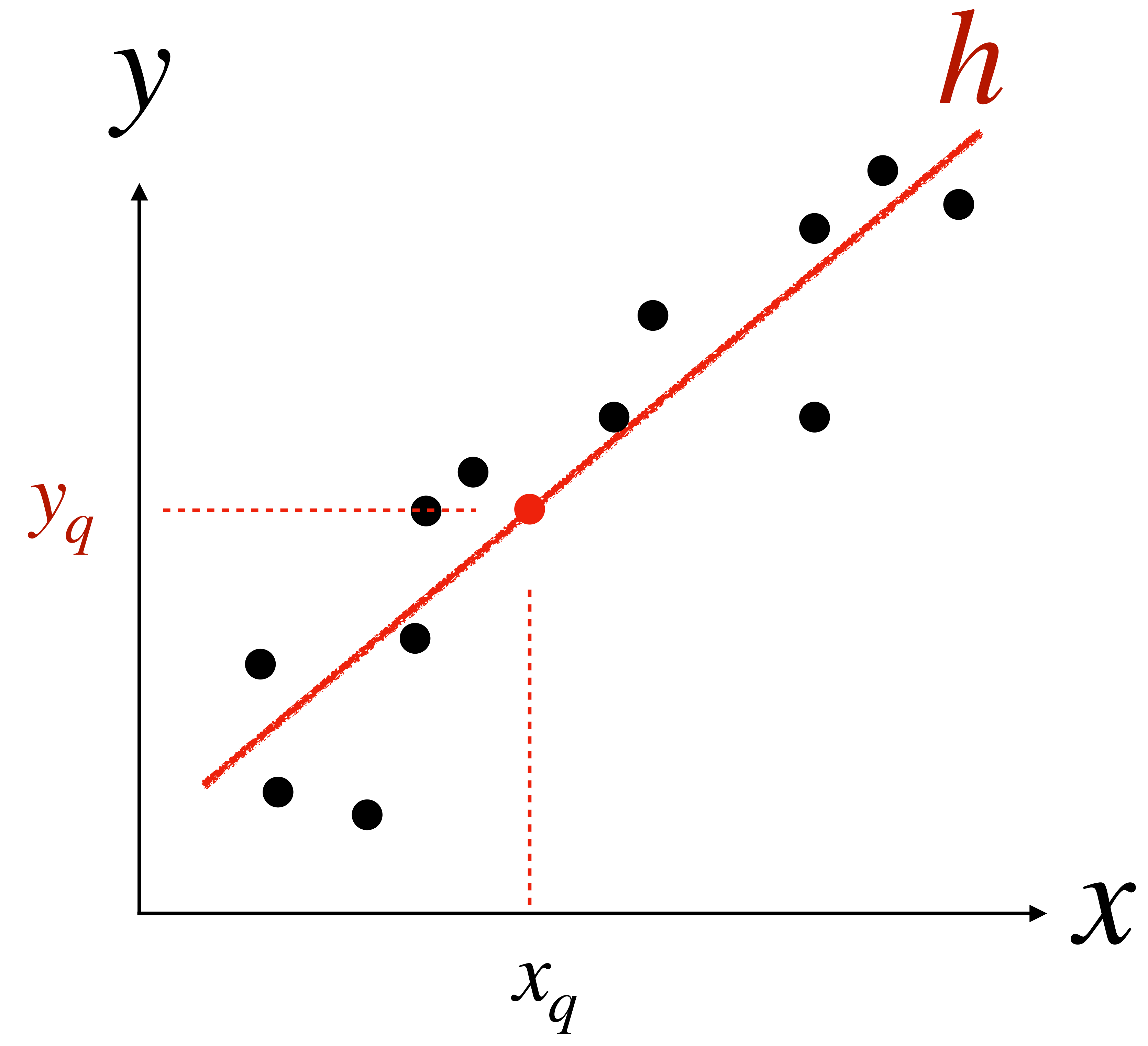
$$h_\theta(x) = \theta_0 + \theta_1 x$$

$$h_\theta(x) = [\theta_0, \theta_1] \cdot [1, x]$$

Unknown parameters | Input features

$$\theta \cdot \mathbf{x}$$

Linear function



What's the best $\theta = [\theta_0, \theta_1]$, given the data ?

What happens if we have **more inputs**?

Assume a linear hypothesis

$\mathbf{x} \xrightarrow{h} y$

$h : \mathbb{R}^n \to \mathbb{R}$

$$h_\theta(\mathbf{x}) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \ldots$$

$$h_\theta(\mathbf{x}) = \underbrace{[\theta_0, \theta_1, \theta_2, \theta_3, \ldots]^\top}_{\theta} \cdot \underbrace{[1, x_1, x_2, x_3, \ldots]^\top}_{\mathbf{x}}$$

weights — θ

inputs — $\mathbf{x}$

$$h_\theta(\mathbf{x}) = \theta \cdot \mathbf{x} = \theta^\top \mathbf{x}$$

Inputs		Output
x_1	x_2	y
$x_1^{(1)}$	$x_2^{(1)}$	$y^{(1)}$
$x_1^{(2)}$	$x_2^{(2)}$	$y^{(2)}$
$x_1^{(3)}$	$x_2^{(3)}$	$y^{(3)}$
$x_1^{(4)}$	$x_2^{(4)}$	$y^{(4)}$
$\vdots$	$\vdots$	$\vdots$

How do we pick the best parameters θ ?

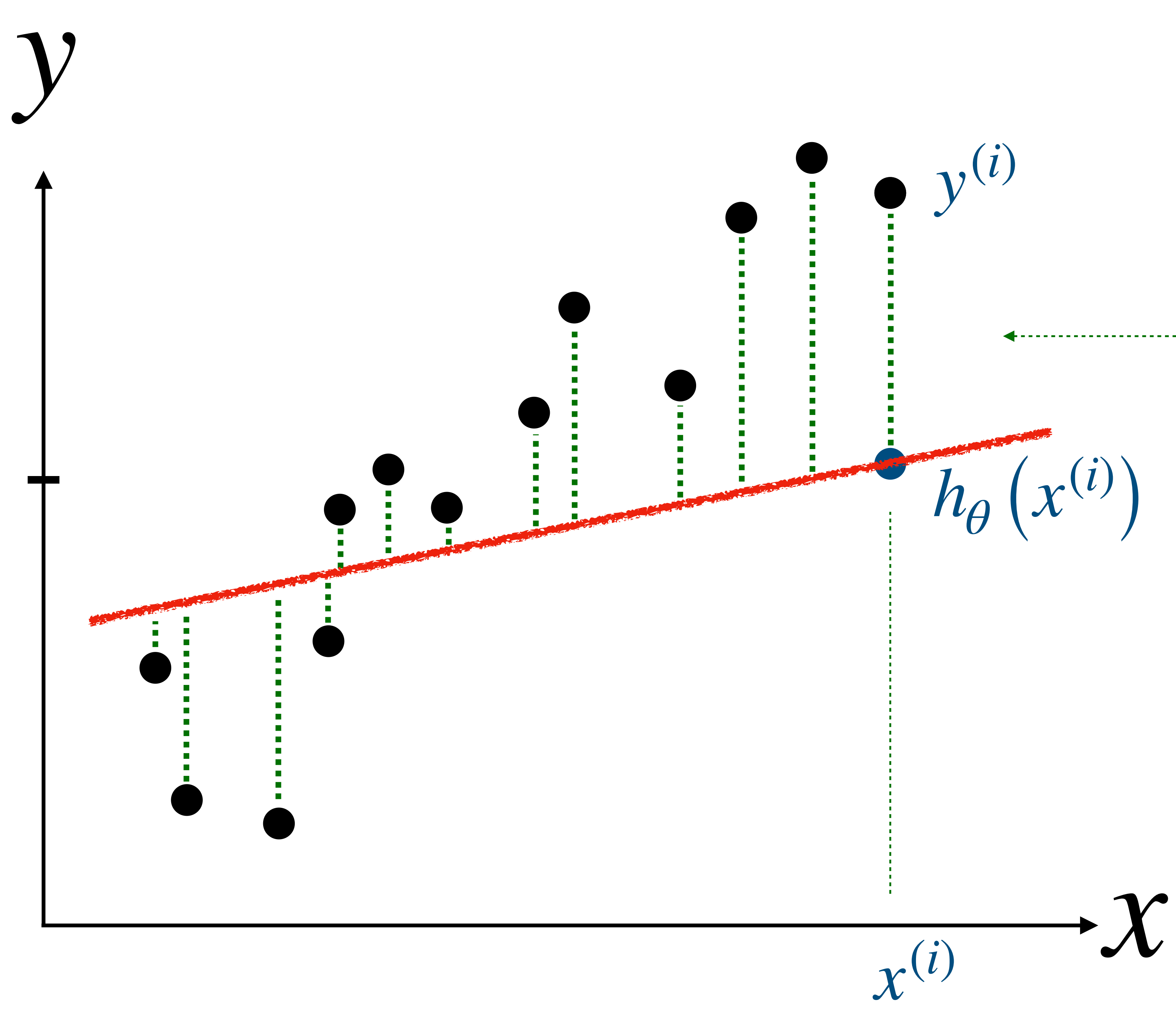
$$h_\theta(\mathbf{x}) = \theta^\top \mathbf{x} = \sum_{i=0}^{d} \theta_i x_i$$

Cost function

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{d} \left(h_\theta\left(x^{(i)}\right) - y^{(i)} \right)^2$$

$$= \frac{1}{2} \sum_{i=1}^{d} \left(\theta^\top \mathbf{x}^{(i)} - y^{(i)} \right)^2$$

Ordinary least squares



distance $\left(h_\theta\left(x^{(i)}\right), y^{(i)} \right)$

$h_\theta\left(x^{(i)}\right) - y^{(i)}$	Residuals
$\left\| h_\theta\left(x^{(i)}\right) - y^{(i)} \right\|$	Absolute loss
$\left(h_\theta\left(x^{(i)}\right) - y^{(i)} \right)^2$	Square loss

Interactive Demo

https://colab.research.google.com/drive/1jEMvm_qlLneIeOFDC5Andr7JstIetVet?usp=sharing

Choose θ to minimize $J(\theta)$

Cost function

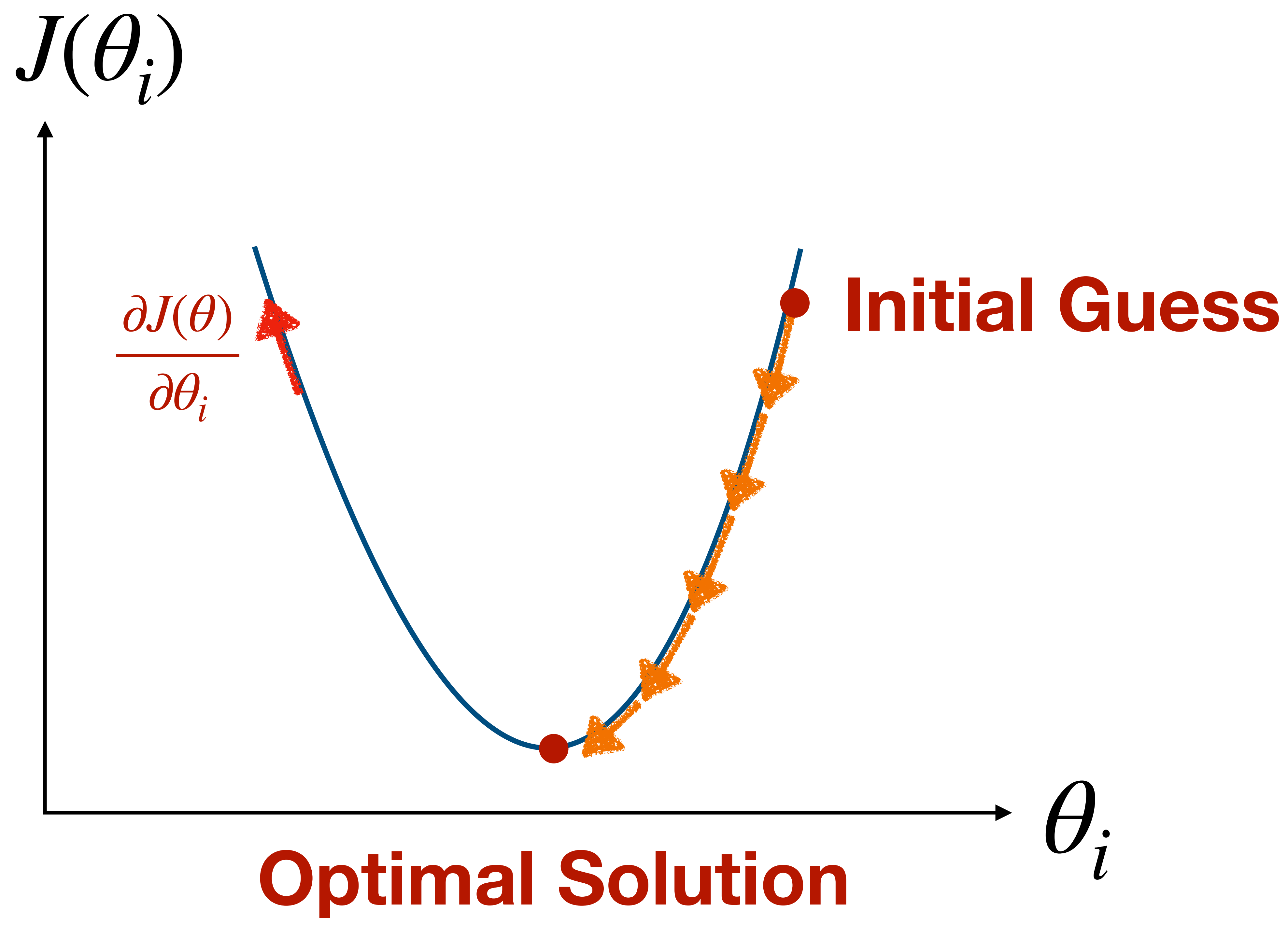
$$J(\theta) = \frac{1}{2}\sum_{i=1}^{d}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

Gradient Descent Update

while not converged:

$$\theta_i := \theta_i - \alpha \frac{\partial J(\theta)}{\partial \theta_i}$$

Learning Rate



Gradient can be computed explicitly

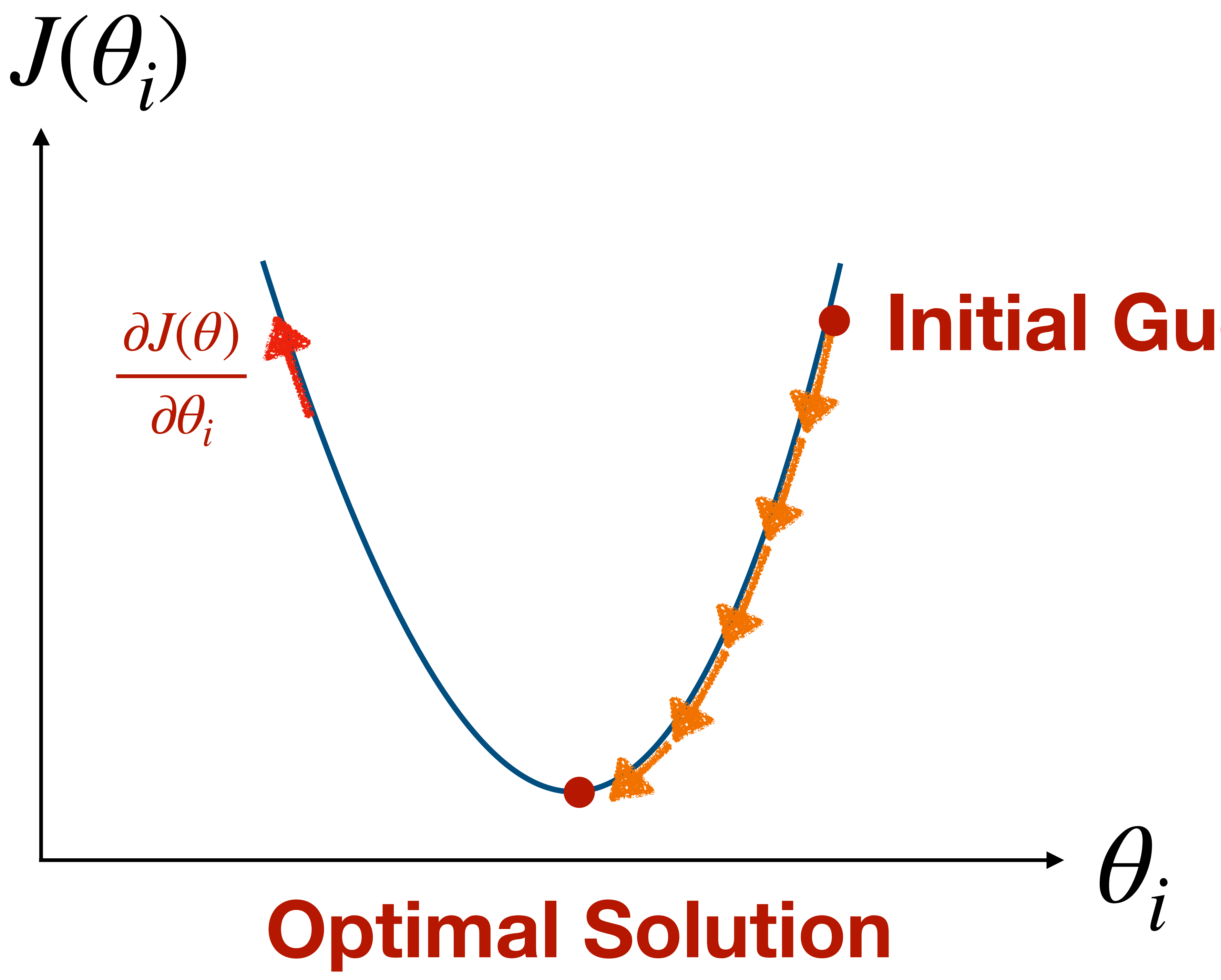
while not converged:

$$\theta_i := \theta_i - \alpha \frac{\partial J(\theta)}{\partial \theta_i}$$

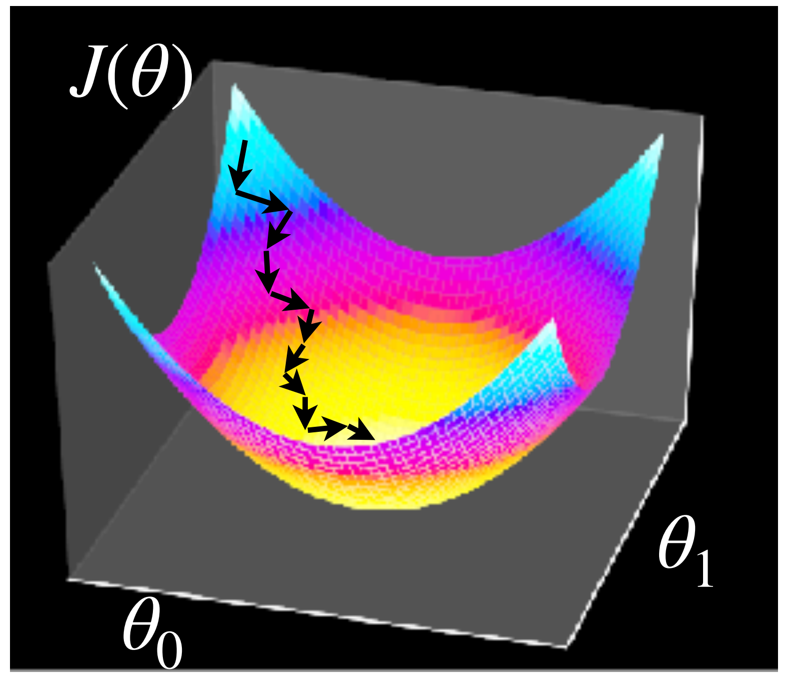
Learning Rate

Derive $\frac{\partial J(\theta)}{\partial \theta_i}$ explicitly, for one (x, y) pair

Assume $y = \theta_0 x + \theta_1$



Least Mean Squares (LMS)

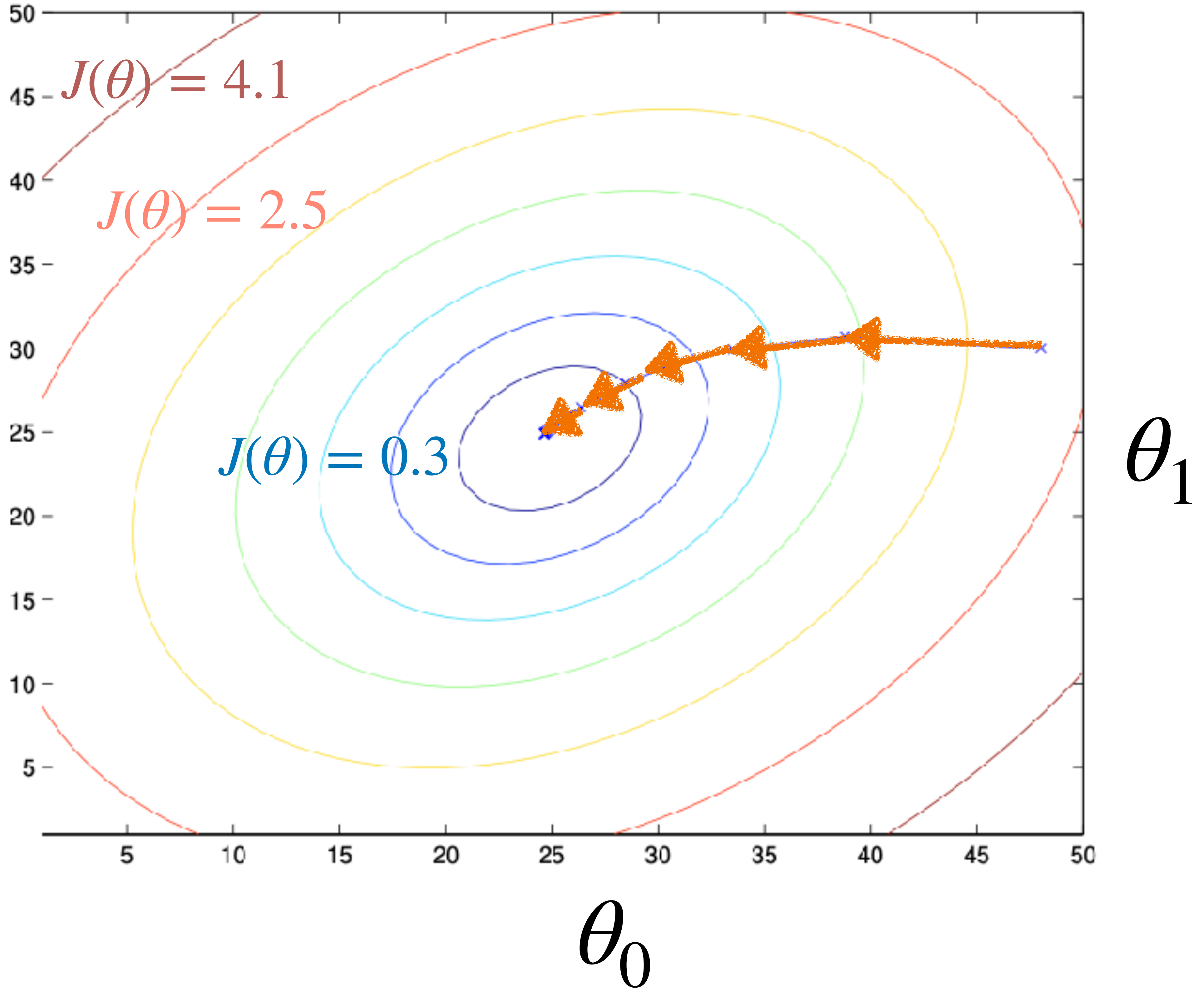


A.K.A **Widrow-Hoff** learning rule

For a single training example $\left(x^{(i)}, y^{(i)}\right)$:

$$\theta_j := \theta_j - \alpha \left(h_\theta \left(x^{(i)}\right) - y^{(i)} \right) x_j^{(i)}$$

Contour Plot



Batch Gradient Descent

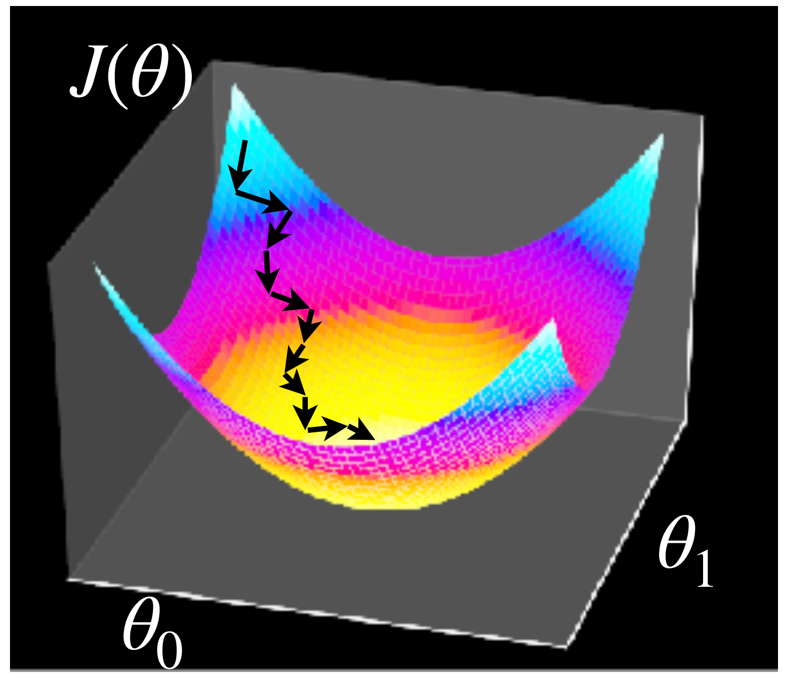
for t = 1...T: (Epochs)

for all parameters j:

$$\theta_j := \theta_j - \alpha \sum_{i=1}^{n} \left(h_\theta \left(x^{(i)}\right) - y^{(i)} \right) x_j^{(i)}$$

Stack and vectorize

Least Mean Squares (LMS)

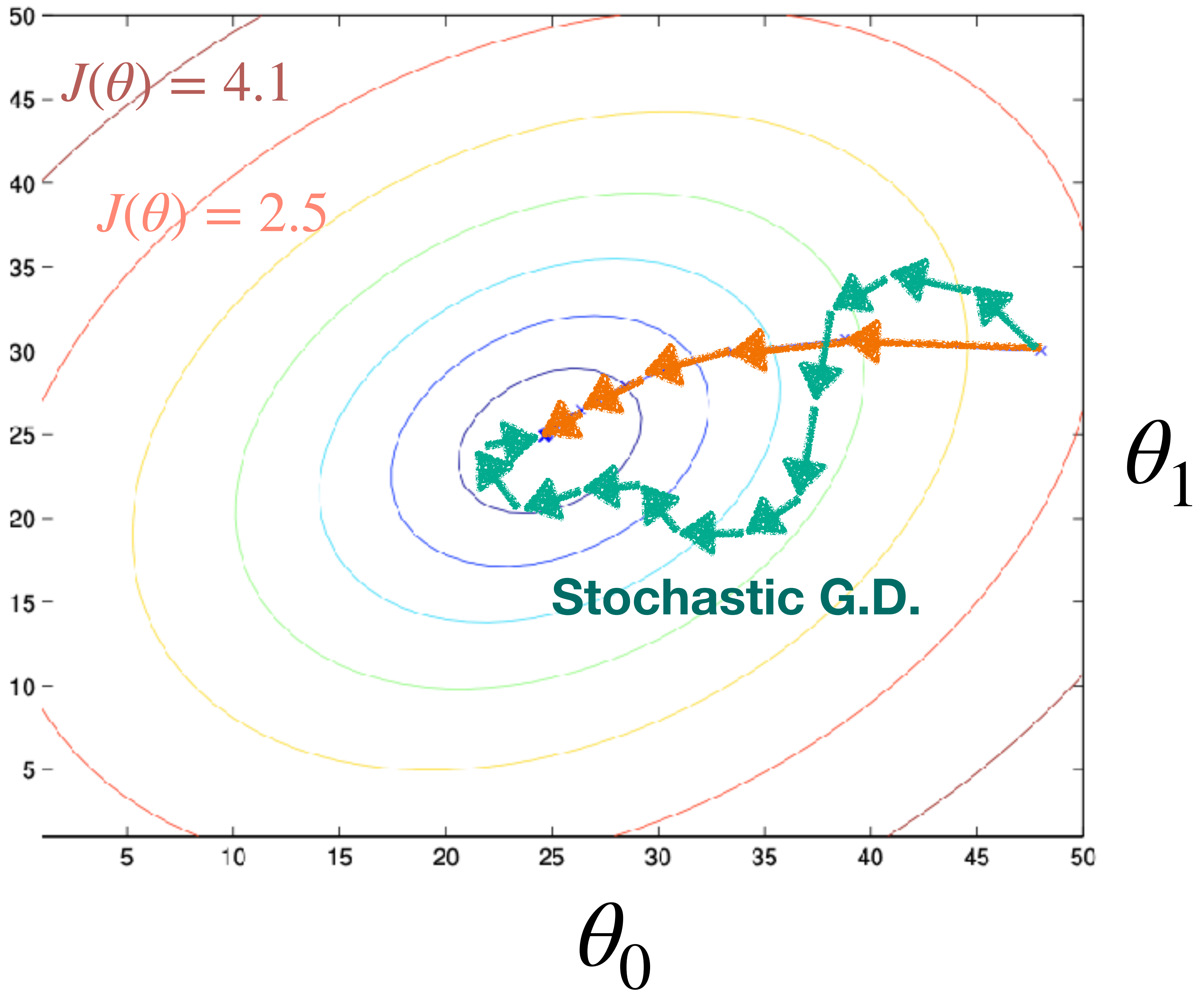


Batch Gradient Descent (vectorized)

for t = 1…T:

$$\theta := \theta - \alpha \sum_{i=1}^{n} \left(h_\theta\left(x^{(i)}\right) - y^{(i)} \right) x^{(i)}$$

Contour Plot



Stochastic Gradient Descent

for t = 1…T:

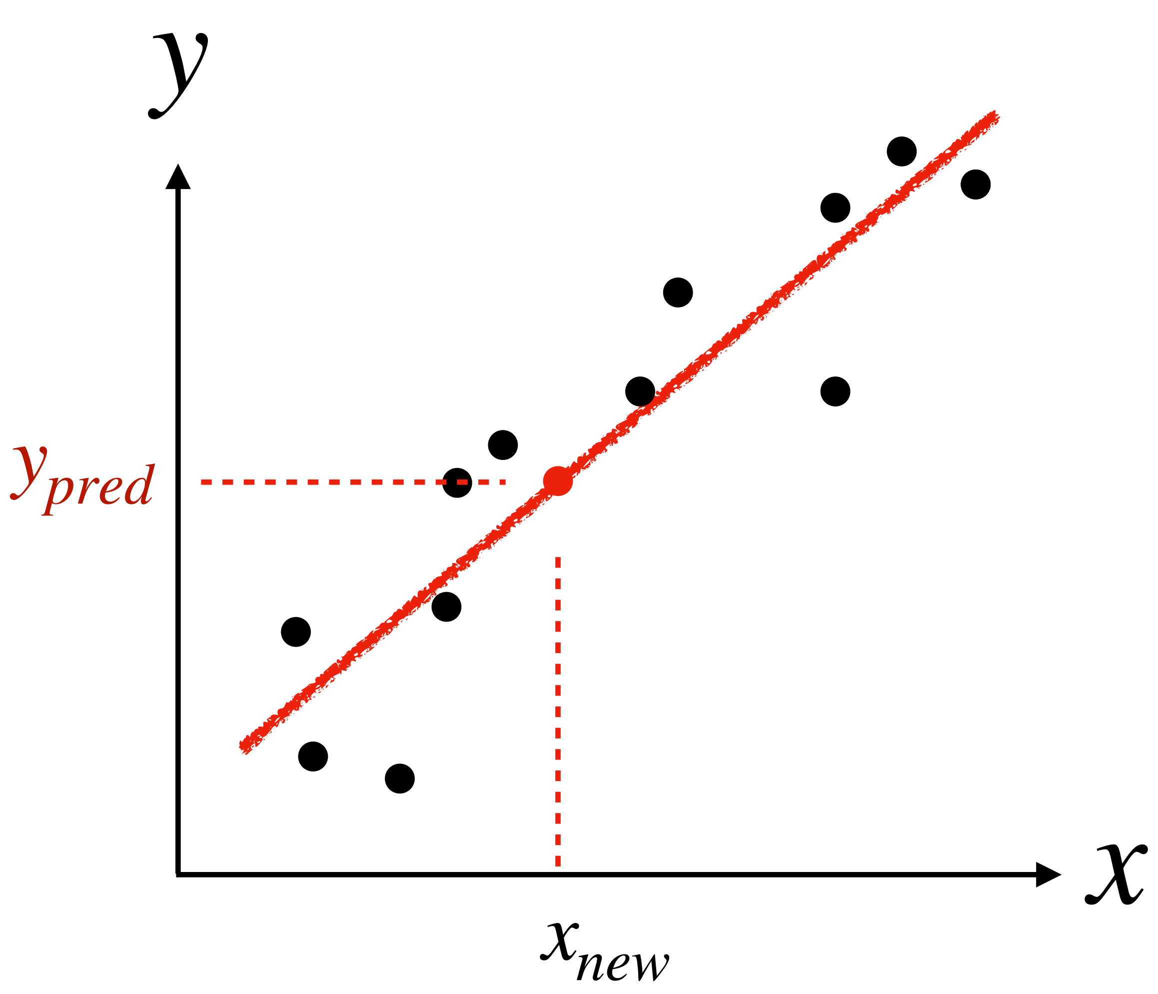
for i = 1…n:

$$\theta := \theta - \alpha \left(h_\theta\left(x^{(i)}\right) - y^{(i)} \right) x^{(i)}$$

Summary

5. Predict unseen data

$$y_{pred} = h_{\hat{\theta}}(x_{new})$$



1. Assume a linear hypothesis

$$h_\theta(\mathbf{x}) = \theta^\top \mathbf{x} = \sum_{i=0}^{d} \theta_i x_i$$

4. Optimal predictor

$$y = h_{\hat{\theta}}(x)$$

$\hat{\theta}$

2. Cost function

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{d} \left(h_\theta \left(x^{(i)} \right) - y^{(i)} \right)^2$$

3. Minimize: Gradient Descent

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

SGD

for t = 1...T:

  for i = 1...n:

$$\theta := \theta - \alpha \left(h_\theta \left(x^{(i)} \right) - y^{(i)} \right) x^{(i)}$$

Can you find the minimum analytically?

Design matrix

$$X = \begin{bmatrix} -- & {x^{(1)}}^\top & -- \\ -- & {x^{(2)}}^\top & -- \\ -- & \vdots & -- \\ -- & {x^{(n)}}^\top & -- \end{bmatrix}$$

Parameters

$$\vec{\theta} = \begin{bmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_m \end{bmatrix}$$

Output

$$\vec{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

Minimize

$$J(\theta) = \frac{1}{2} \| X\theta - \vec{y} \|_2^2$$

$$\longrightarrow \quad \nabla_\theta J(\theta) = 0$$

Normal Equation

$$\theta = \left(X^\top X\right)^{-1} X^\top \vec{y}$$

Feature Engineering

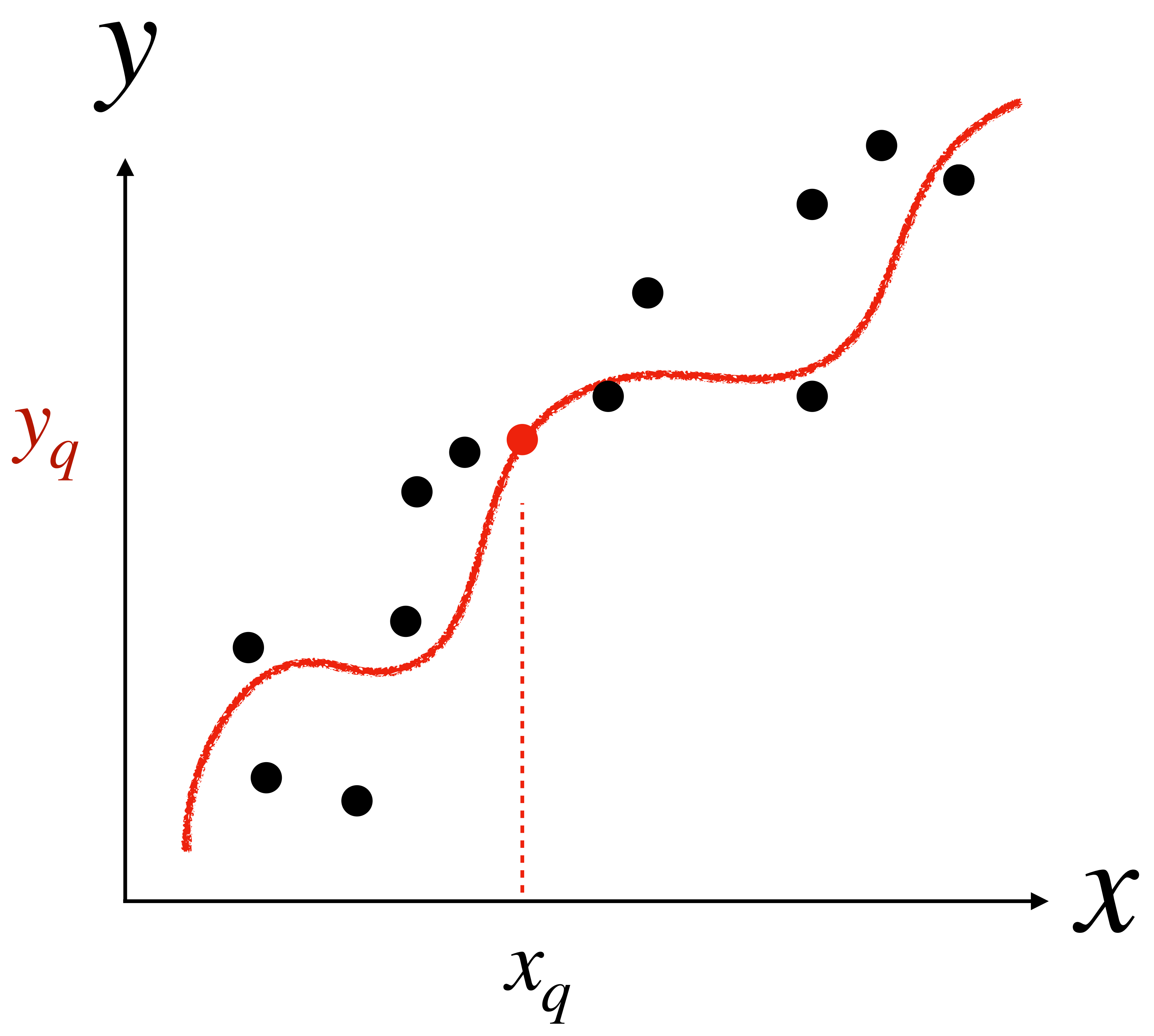
h **is does not have to be linear in** x

Input x	Output y
$x^{(1)}$	$y^{(1)}$
$x^{(2)}$	$y^{(2)}$
$x^{(3)}$	$y^{(3)}$
$x^{(4)}$	$y^{(4)}$

Example: construct a polynomial model

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \ldots$$

Some other function?



$$h_\theta(x) = \underbrace{[\theta_0, \theta_1, \theta_2, \theta_3, \ldots]}_{\theta} \cdot \underbrace{[1, x, x^2, x^3, \ldots]}_{\phi(x)}$$

Feature map

$$h_\theta(x) = \theta^\top \phi(x)$$

Feature Engineering

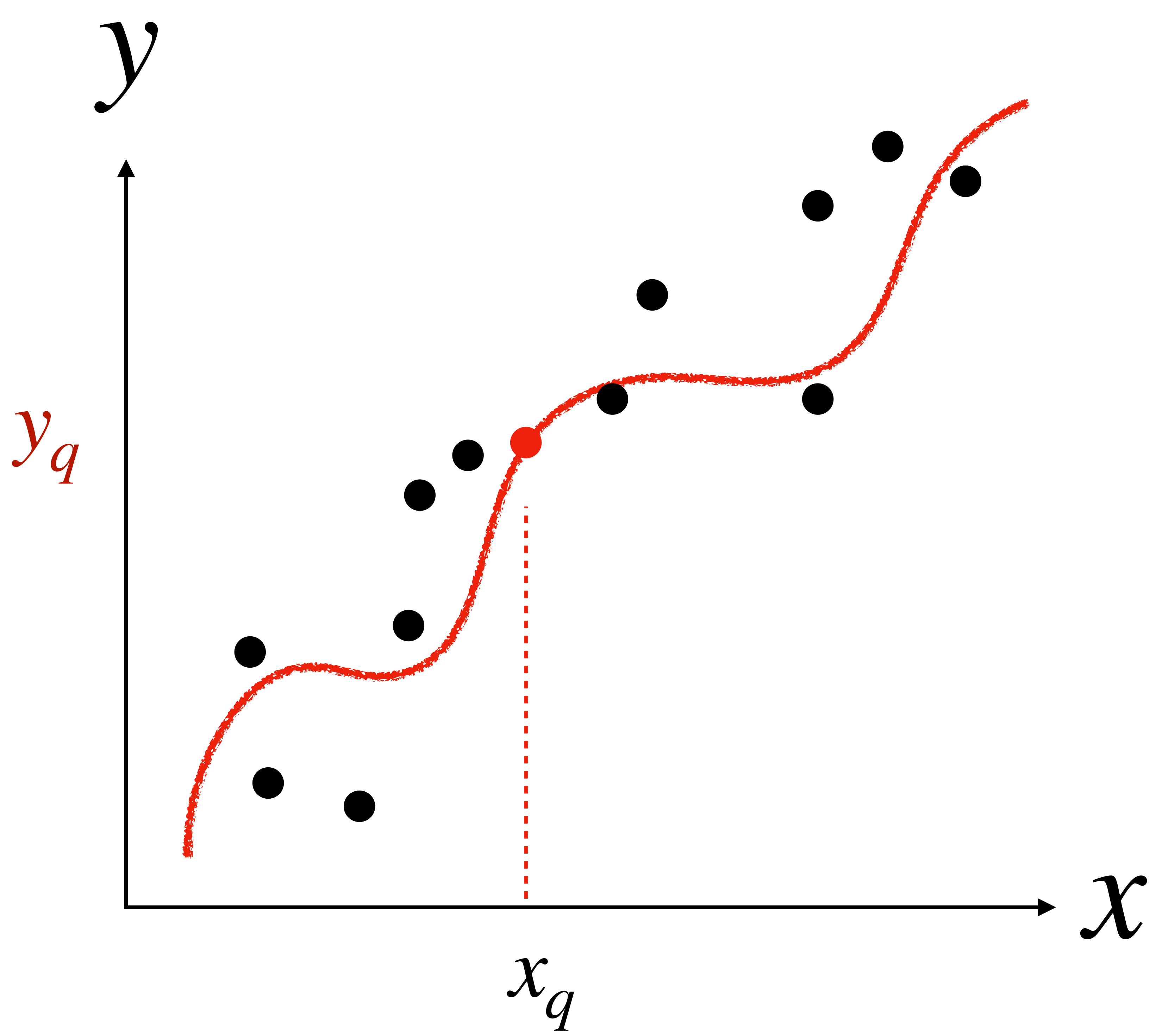
h **is does not have to be linear in** x

Input	Output
x	y
$x^{(1)}$	$y^{(1)}$
$x^{(2)}$	$y^{(2)}$
$x^{(3)}$	$y^{(3)}$
$x^{(4)}$	$y^{(4)}$

Example: construct a polynomial model

$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \dots$$

Some other function?



$$h_\theta(x) = \underbrace{[\theta_0, \theta_1, \theta_2, \theta_3, \dots]}_{\theta} \cdot \underbrace{[1, x, x^2, x^3, \dots]}_{\phi(x)}$$

Feature map

$$h_\theta(x) = \theta^\top \phi(x) = \theta_0 \phi_0(x) + \theta_1 \phi_1(x) + \theta_2 \phi_2(x) + \dots$$

Feature Engineering

A feature map can also **drop features**

Example: construct a polynomial model

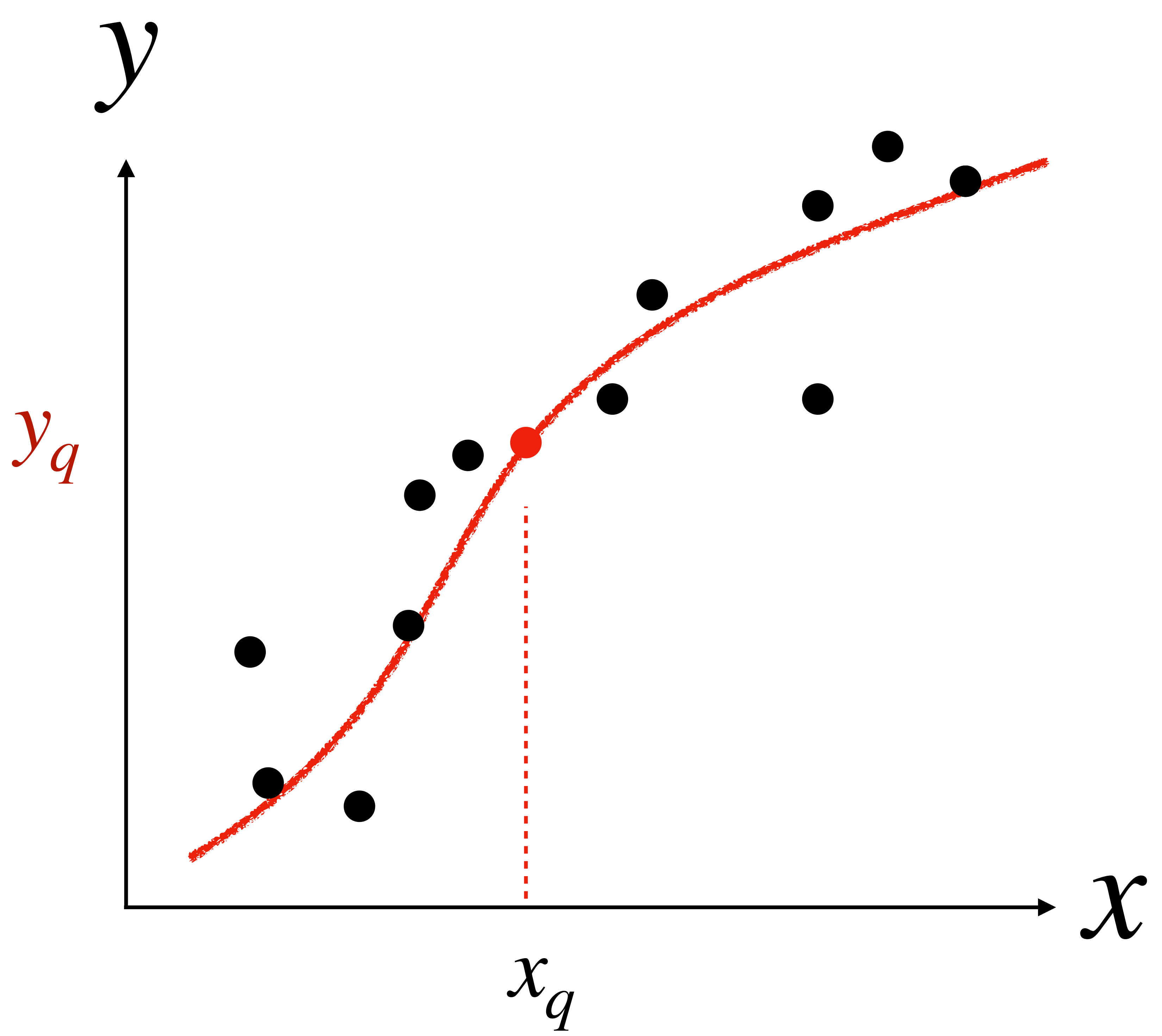
$$h_\theta(x) = \theta_1 x + \theta_3 x^3$$

$$h_\theta(x) = [\theta_1, \theta_3] \cdot [x,\ x^3]$$

$\phi(x)$ *Feature map*

$$h_\theta(x) = \theta^\top \phi(x)$$

Some other function?

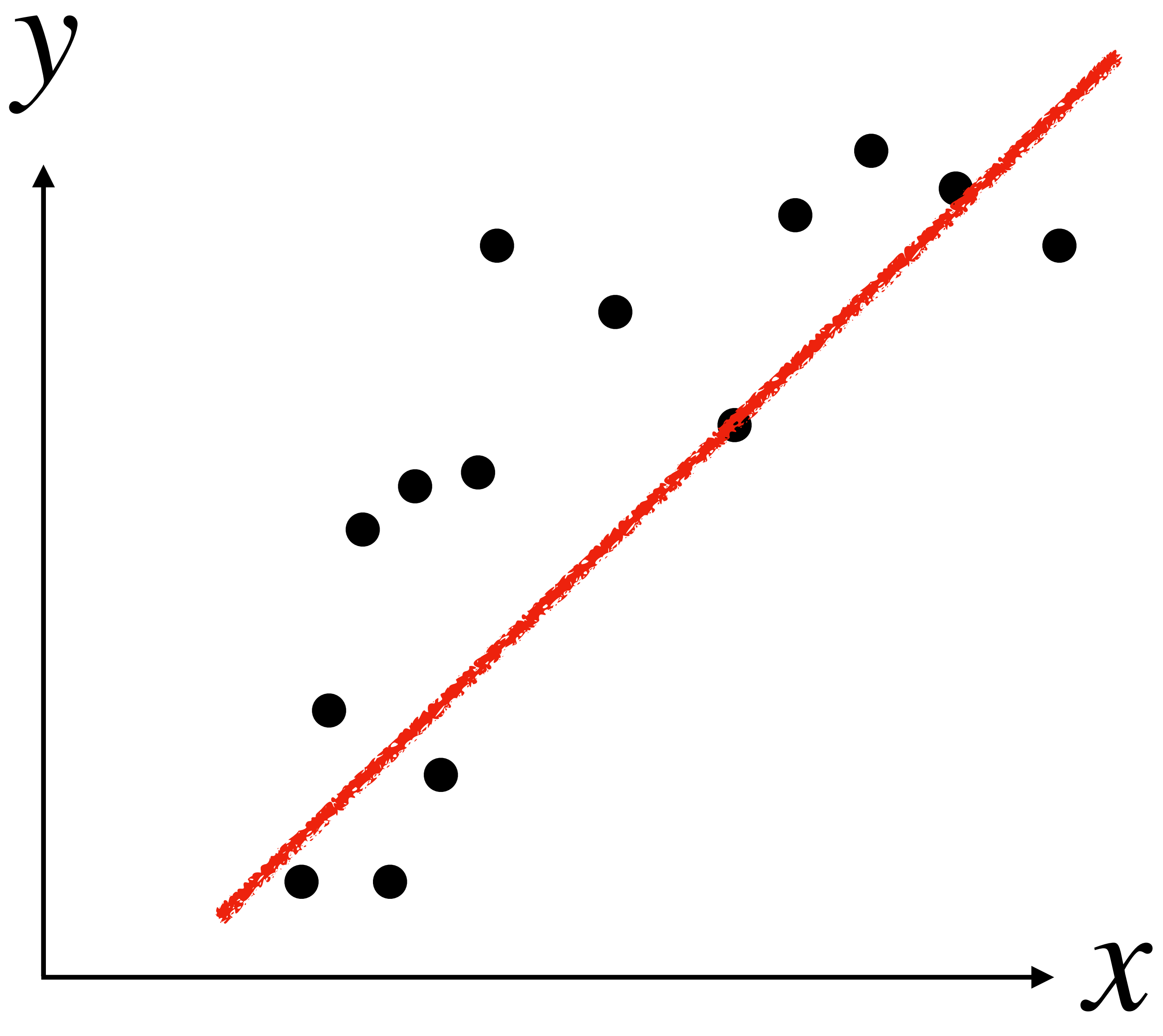


How to choose $\phi(x)$?

How to optimize over $\phi(x)$

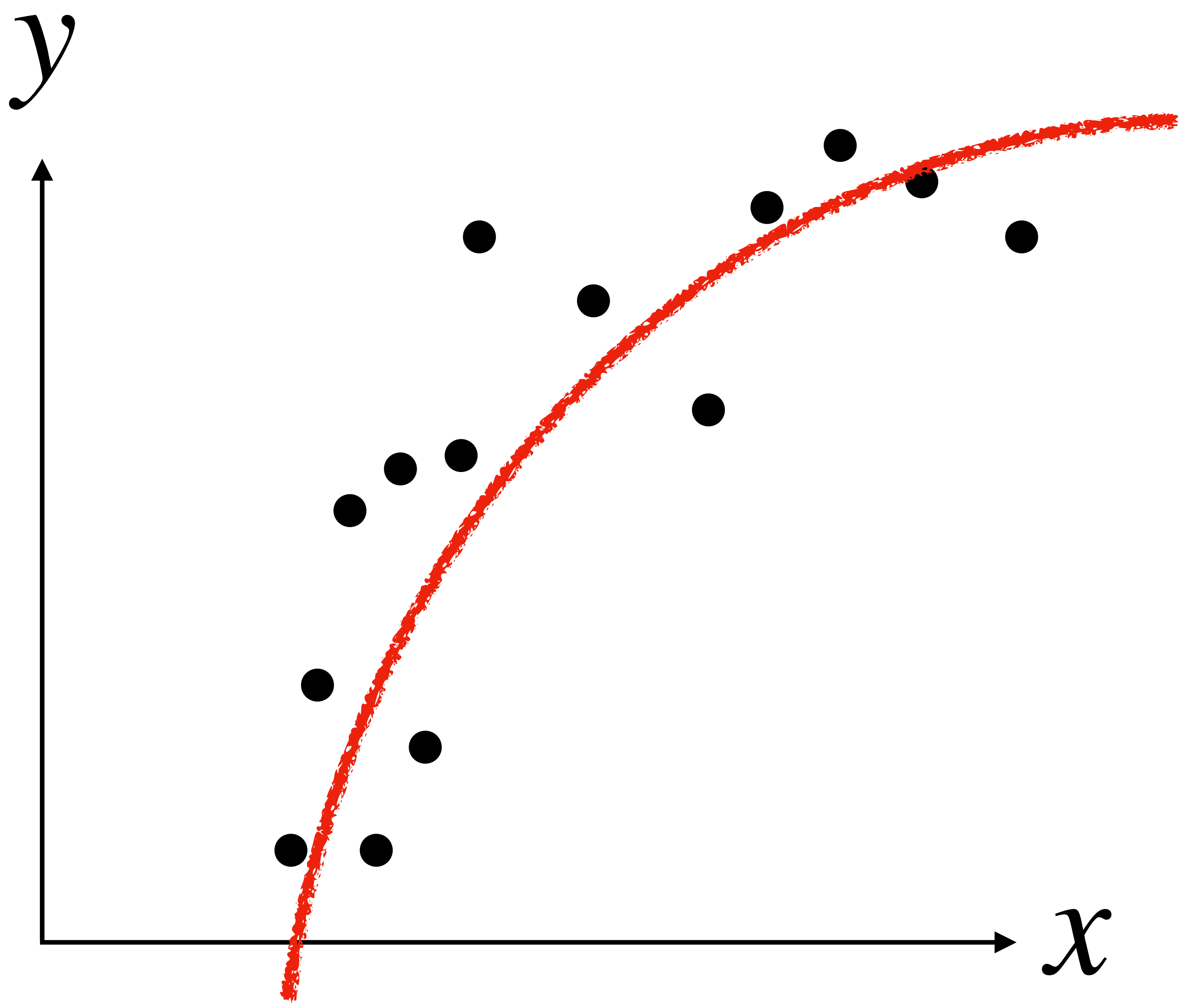
Underfitting

High Bias



$$\phi(x) = [1, x]$$

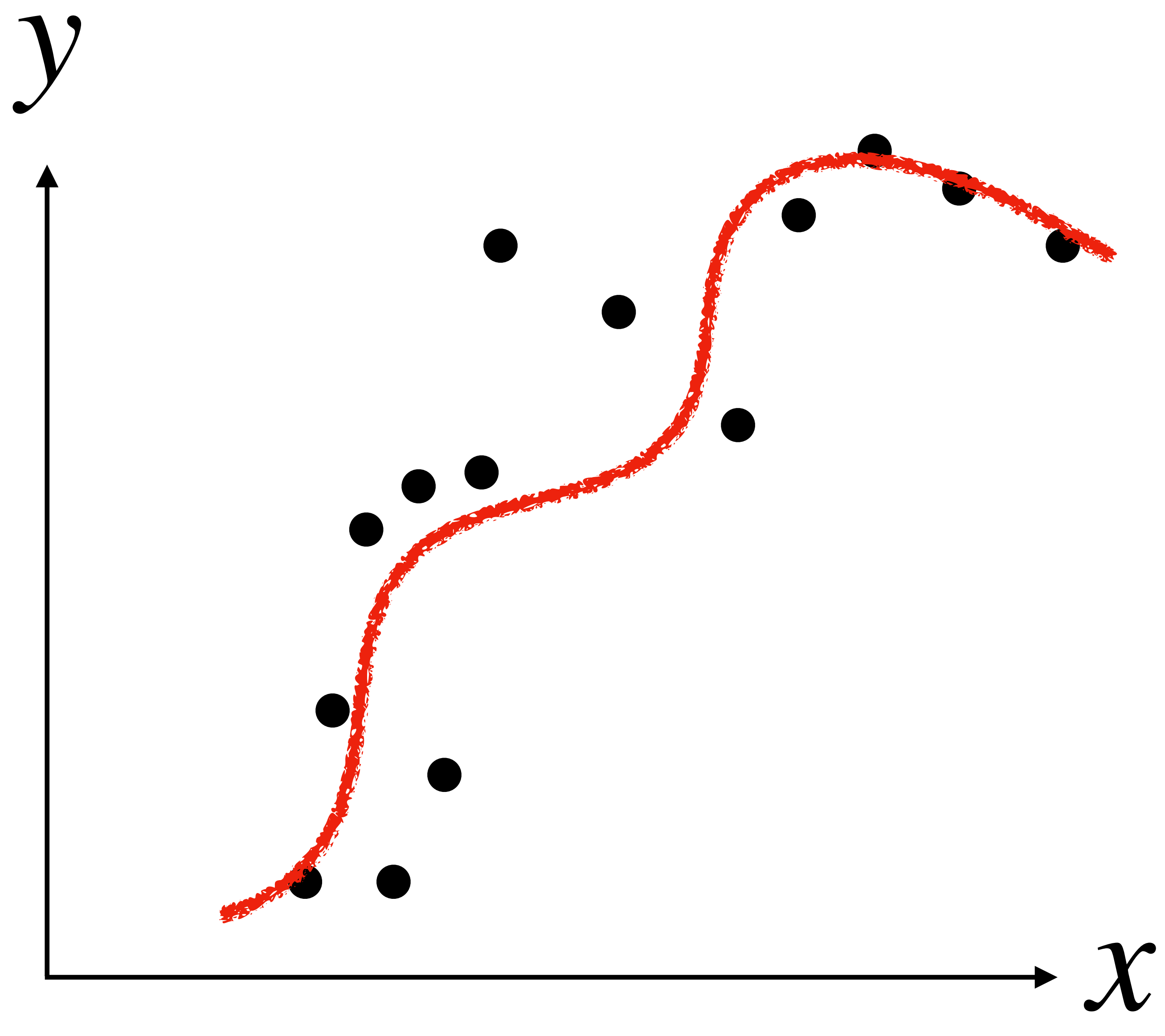
Just right



$$\phi(x) = [1, x, x^2]$$

Overfitting

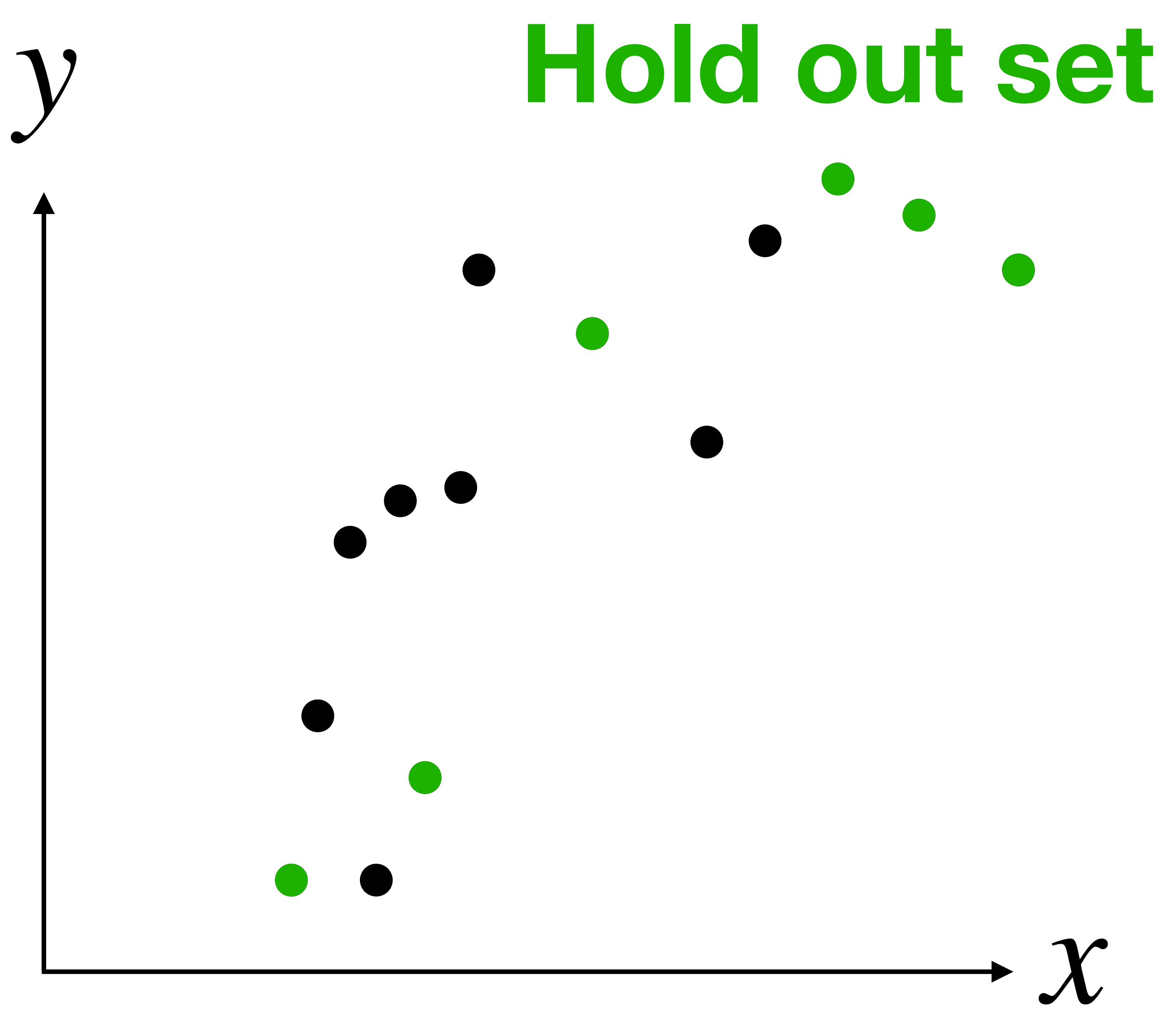
High Variance



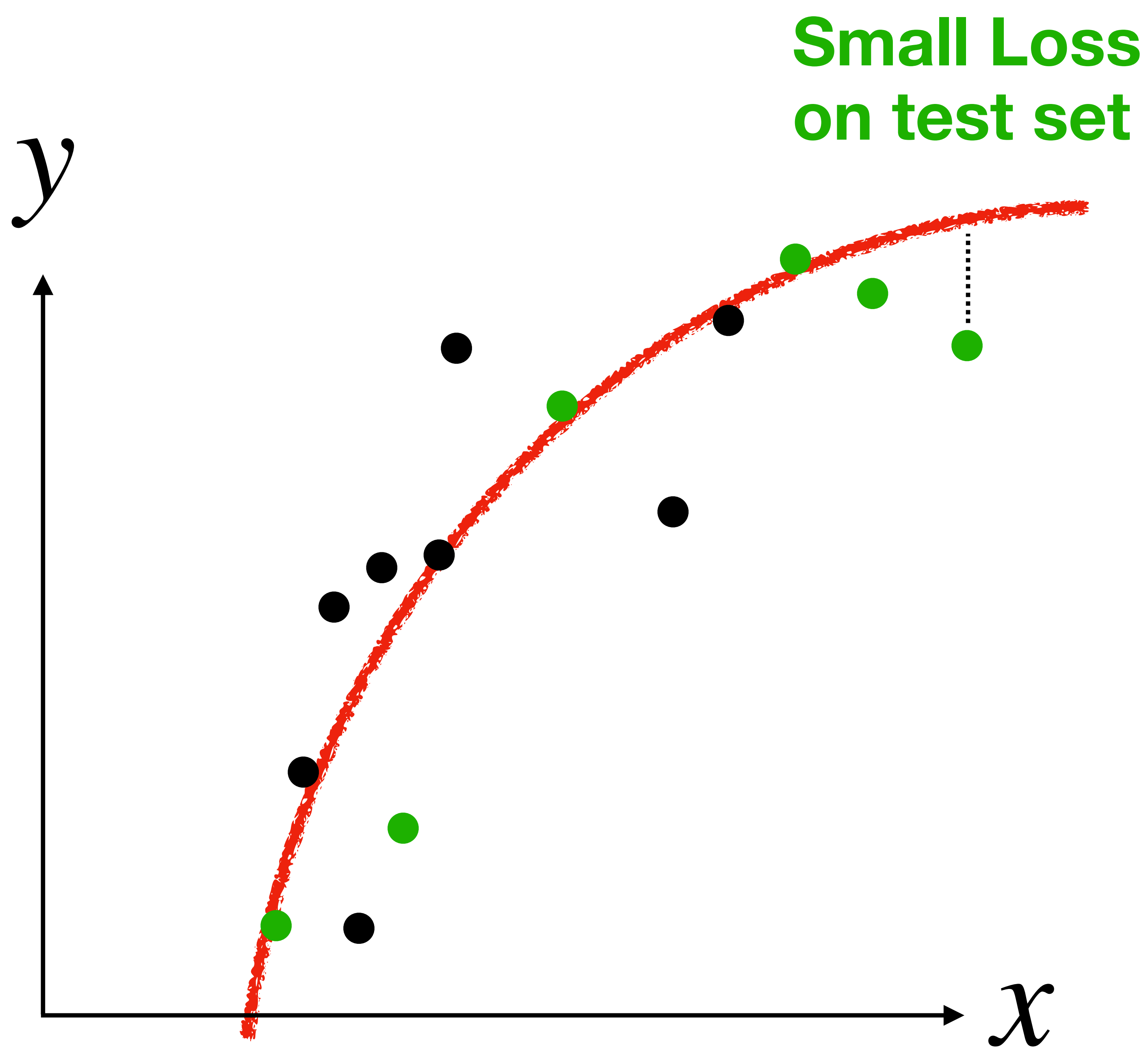
$$\phi(x) = [1, x, x^2, x^3, \ldots]$$

How can we tell if $\phi(\cdot)$ is good?

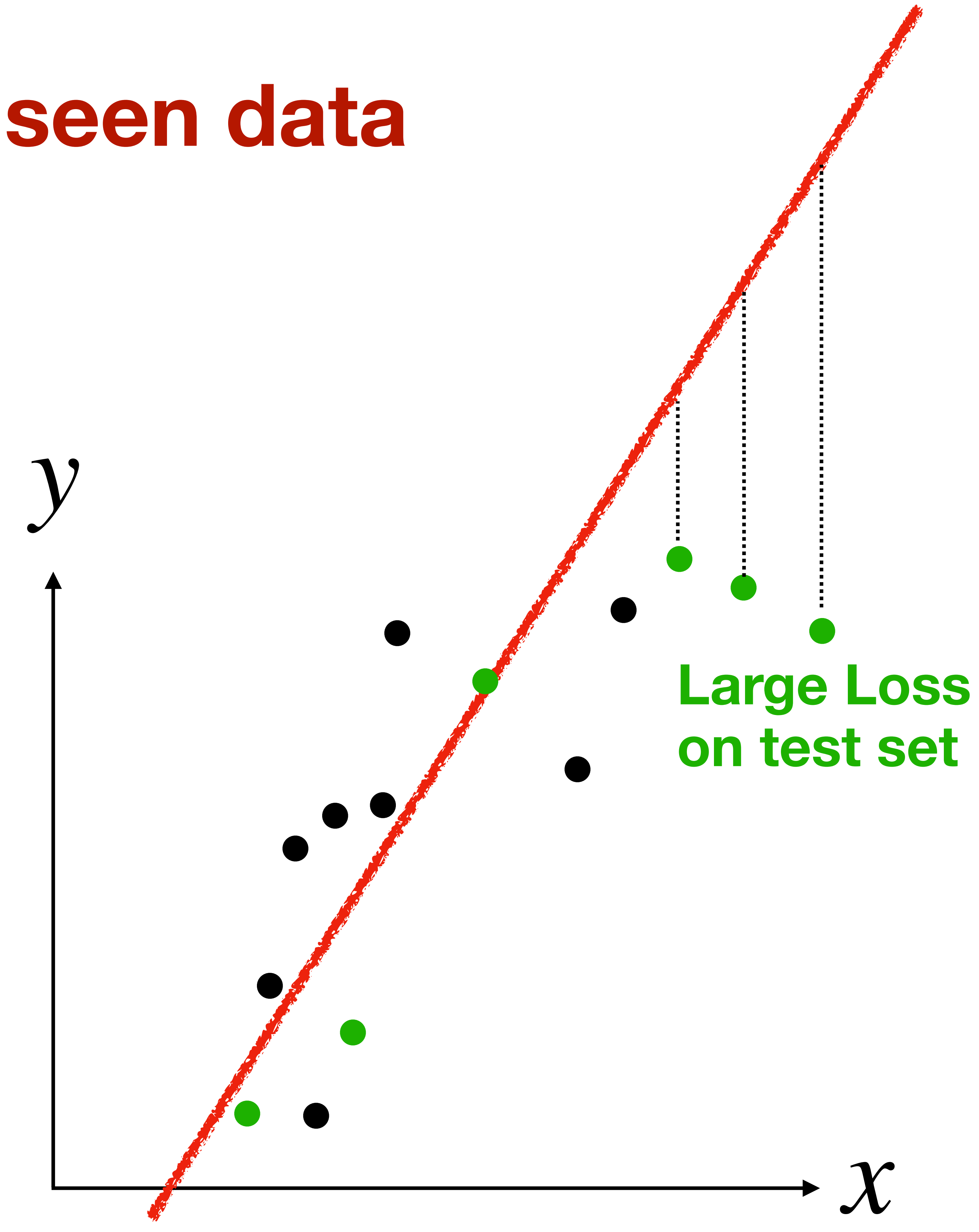
The purpose of Machine Learning is to Generalize to unseen data



Create a test set to evaluate model



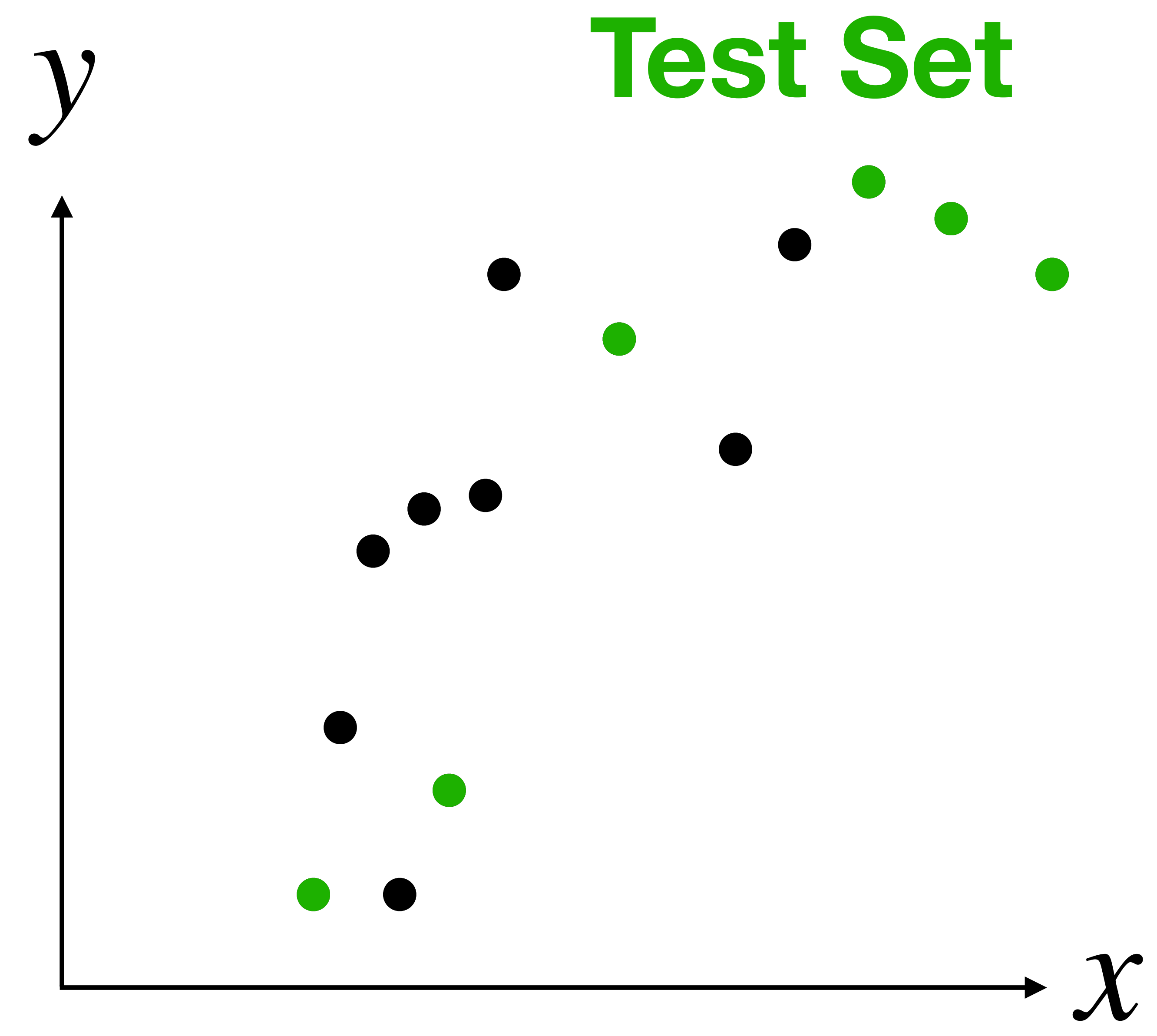
$$\phi(x) = [1, x, x^2]$$



$$\phi(x) = [1, x]$$

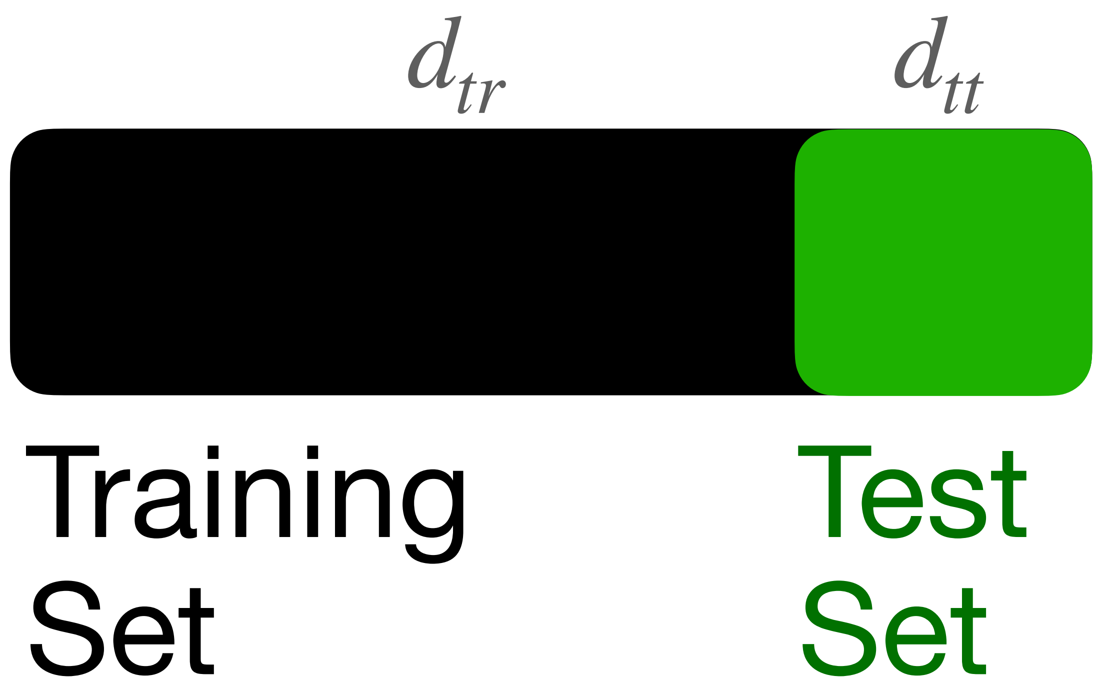
How do we tell that $\phi(\cdot)$ is good?

Define objective functions for each subset



Create a **Test set** to evaluate model

Split data:

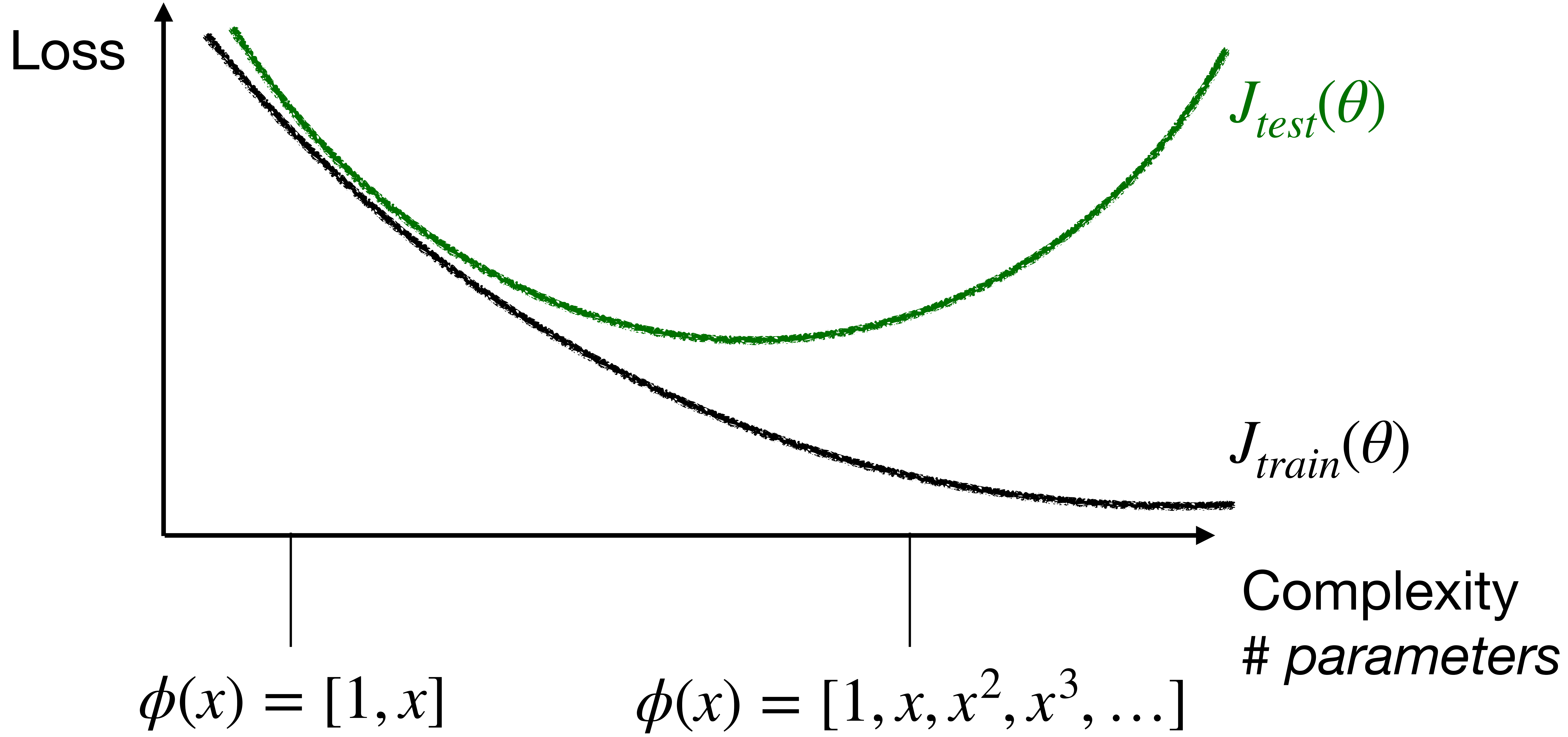


$$J_{train}(\theta) = \frac{1}{2d_{tr}} \sum_{i=1}^{d_{tr}} \left(\theta^\top \phi(x^{(i)}) - y^{(i)}\right)^2$$

$$J_{test}(\theta) = \frac{1}{2d_{tt}} \sum_{i=1}^{d_{tt}} \left(\theta^\top \phi(x^{(i)}) - y^{(i)}\right)^2$$

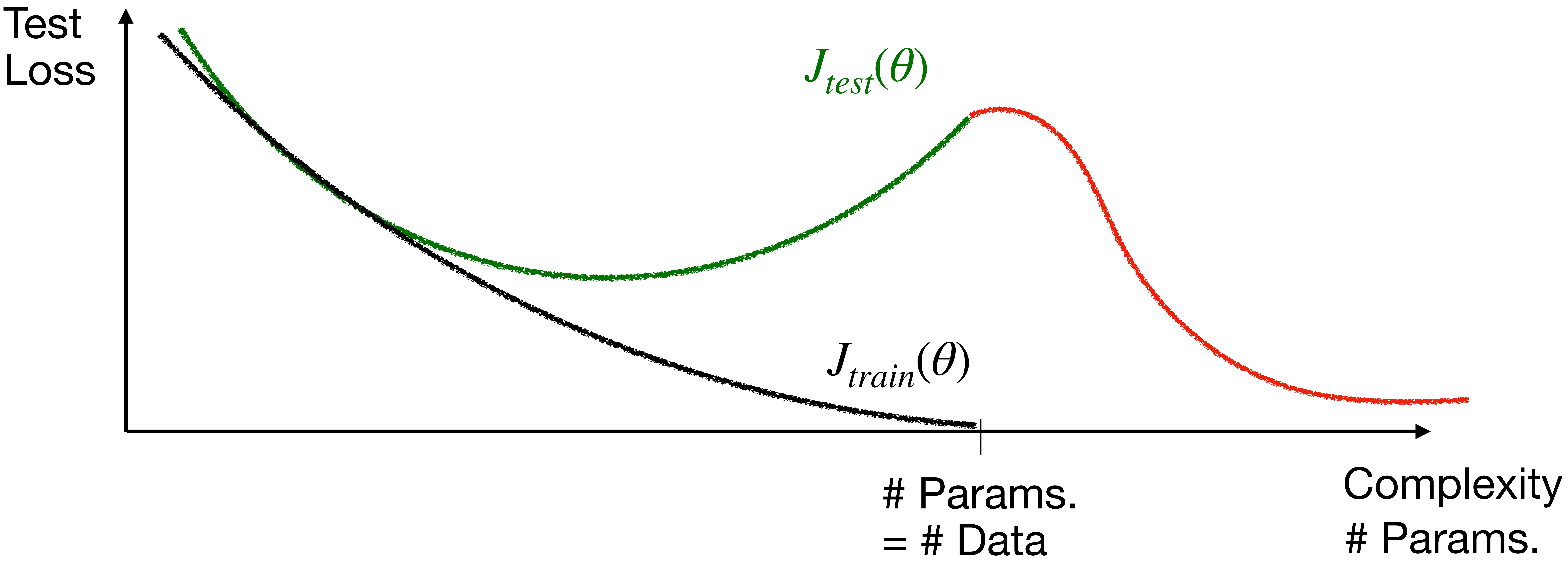
Variance Bias Trade-off

Error as a function of complexity



Double Descent

Model-wise

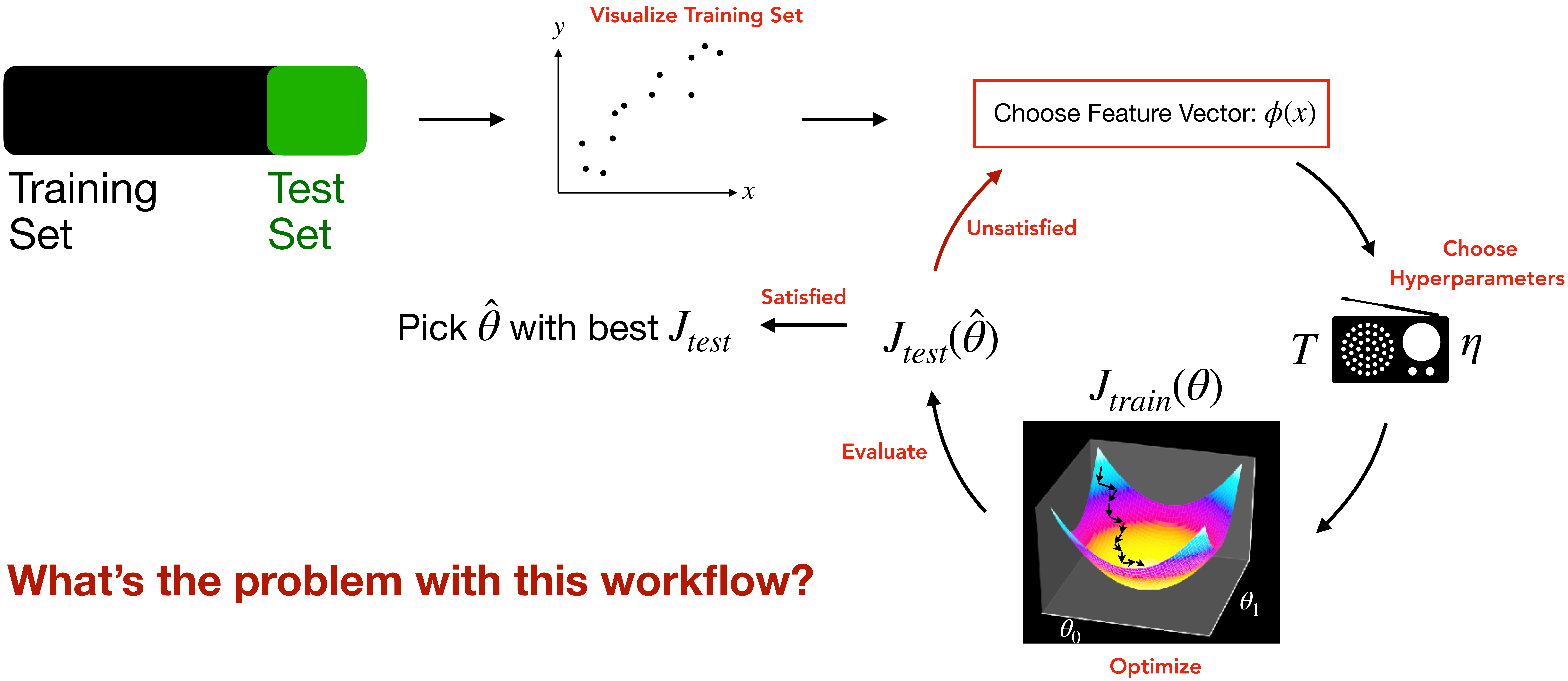


Other Hyperparameters

ϕ is not the only unknown parameter over which we want to optimize

- T: Number of Epochs
- η: Step size
- ϕ: Feature vector

Optimize over ϕ and other hyperparameters

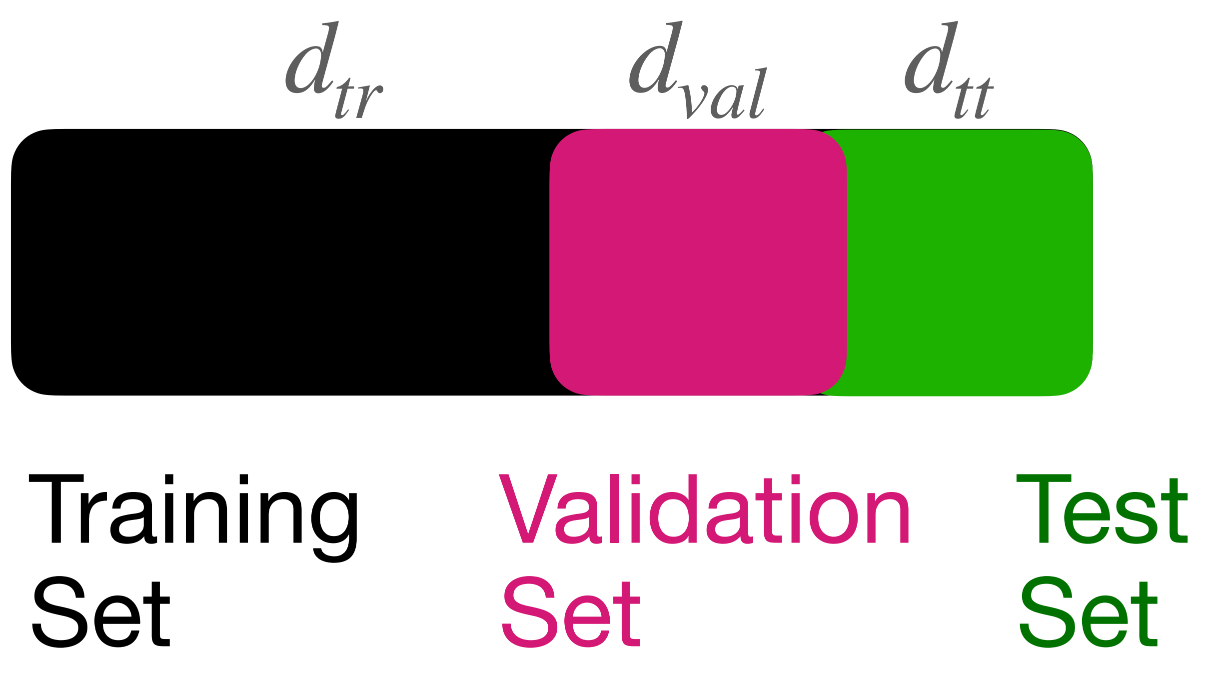


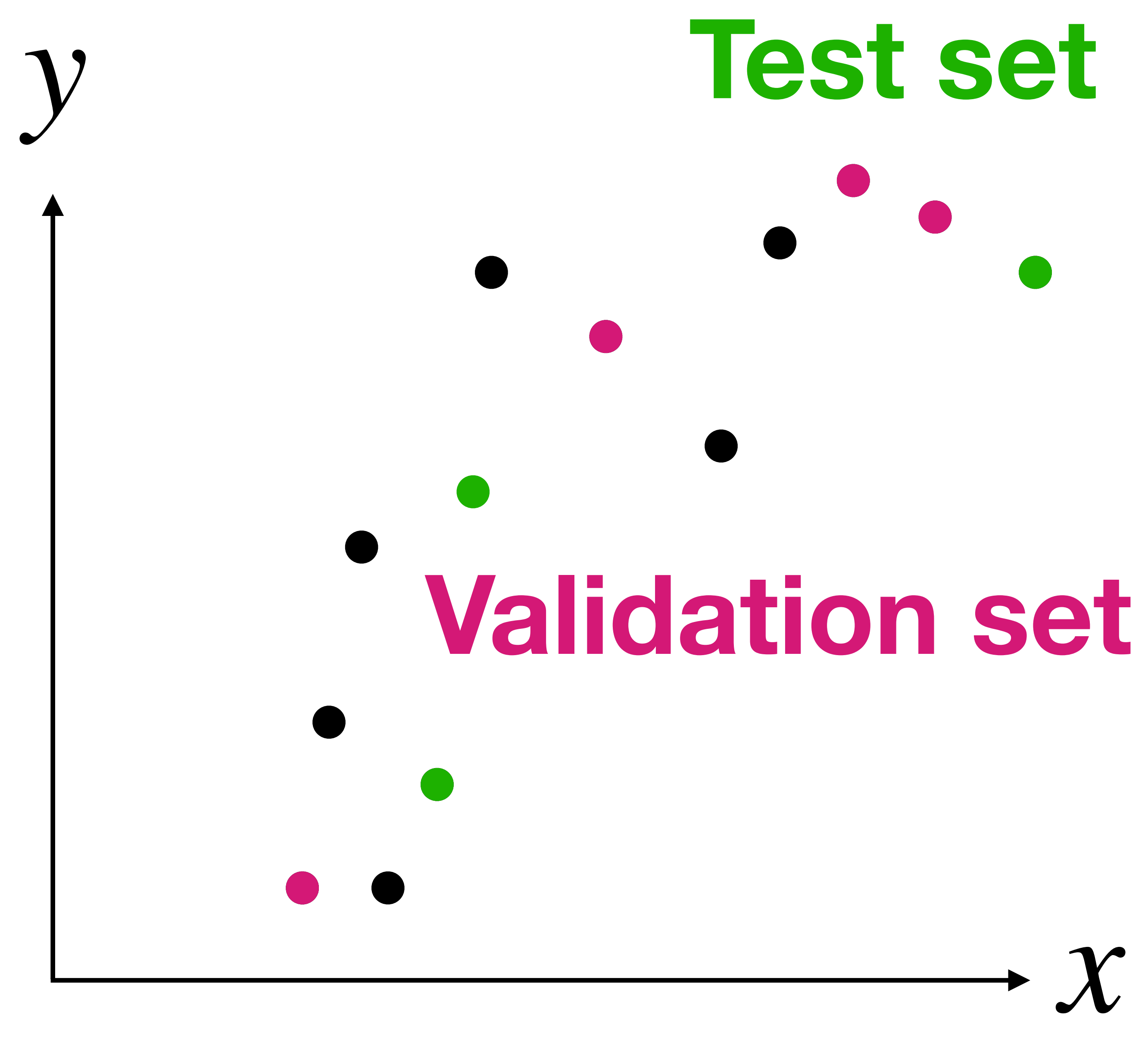
What's the problem with this workflow?

How do we tell that $\phi(\cdot)$ is good?

Define objective functions for each subset

Split data:





Test set: evaluate model **at the end** of hyperparameter optimization

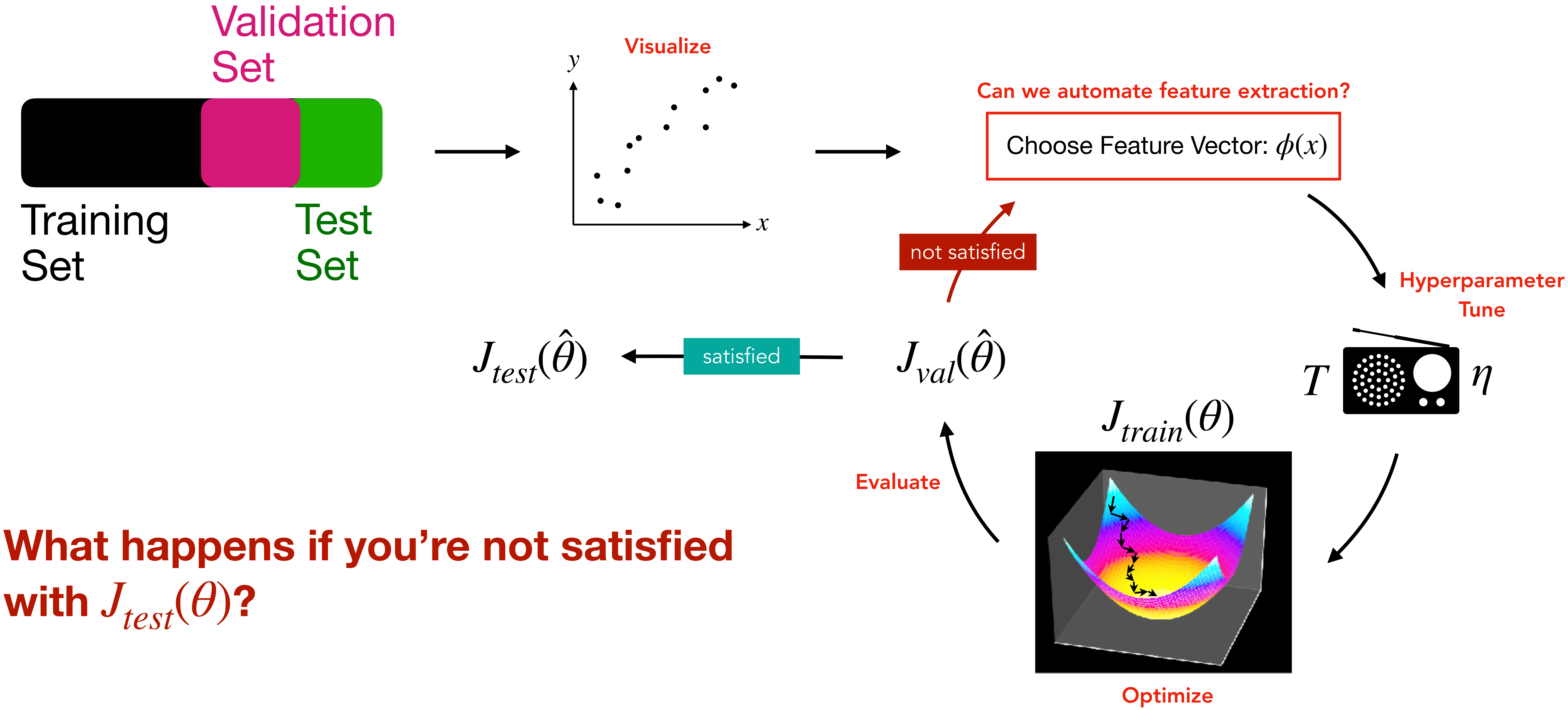
Validation set: evaluation model **during** hyperparameter optimization

$$J_{train}(\theta) = \frac{1}{2d_{tr}} \sum_{i=1}^{d_{tr}} \left(\theta^\top \phi(x^{(i)}) - y^{(i)}\right)^2$$

$$J_{val}(\theta) = \frac{1}{2d_{val}} \sum_{i=1}^{d_{val}} \left(\theta^\top \phi(x^{(i)}) - y^{(i)}\right)^2$$

$$J_{test}(\theta) = \frac{1}{2d_{tt}} \sum_{i=1}^{d_{tt}} \left(\theta^\top \phi(x^{(i)}) - y^{(i)}\right)^2$$

Machine Learning workflow - Cross Validation



What happens if you're not satisfied with $J_{test}(\theta)$?

Remedies to Overfitting

Practical tips to decrease overfitting

- Make the model simpler if it's overfitting, and more complex if it's underfitting
  - **Recursive Feature Elimination:** start with all features and drop them one by one while tracking the loss
  - Get rid of features that you think are irrelevant in predicting the desired output
- Add a regularization term that makes the hypothesis class smaller

$$J_{reg}(\theta) = J(\theta) + \lambda R(\theta)$$

Regularization

Force fitting parameters to be smaller - ‘shrink’ hypothesis class

$$h_\theta(x) = 100.2 + 50.6x + 70.4x^2 + 1345x^3 + 200.3x^4$$

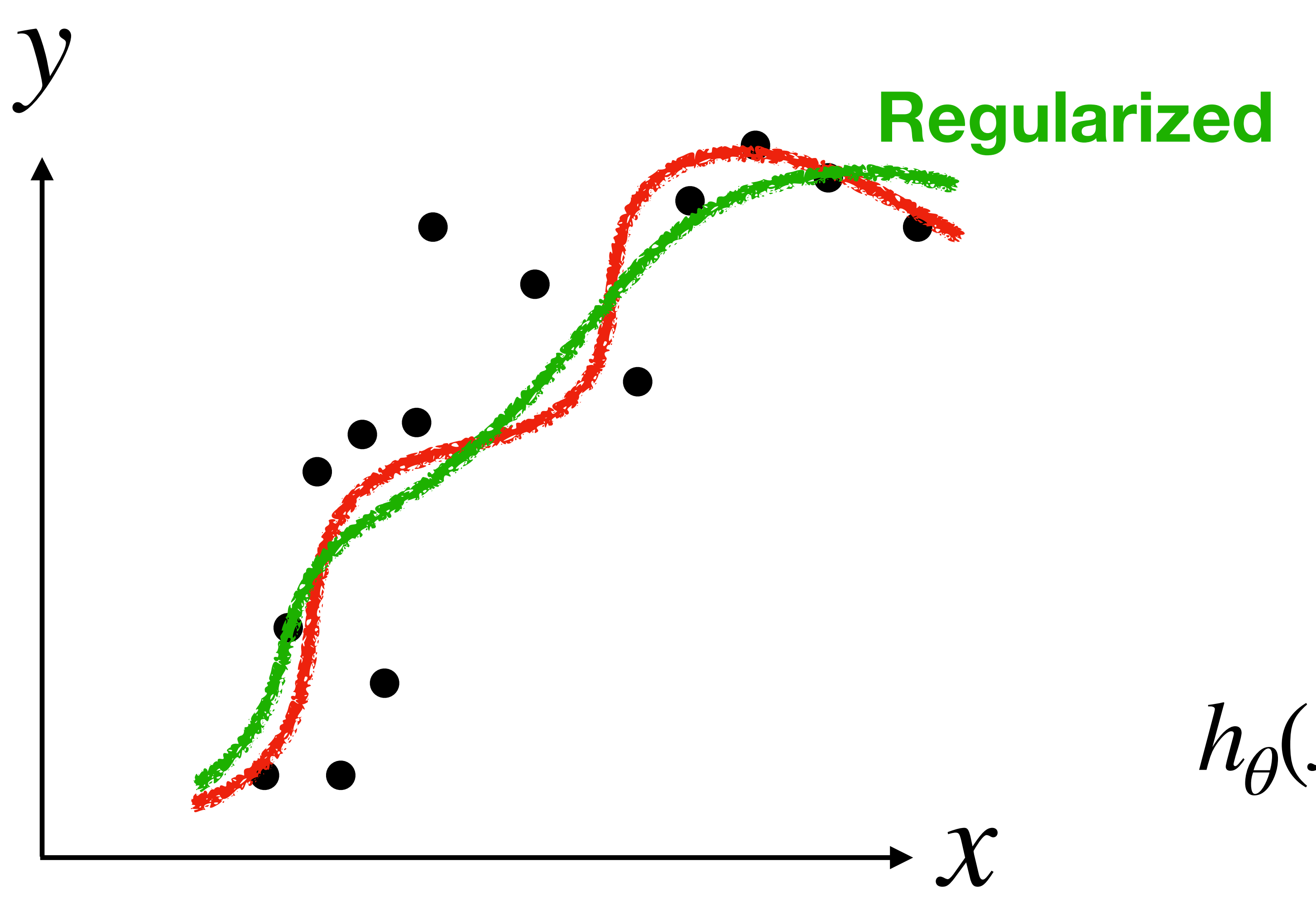
$$J_{reg}(\theta) = J(\theta) + \lambda\, R(\theta)$$

L1 Regularization

$$R(\theta) = \|\theta\|_1$$

$$h_\theta(x) = 5.1x + 7.2x^2 + 3.3x^4$$

Less coefficients



L2 Regularization

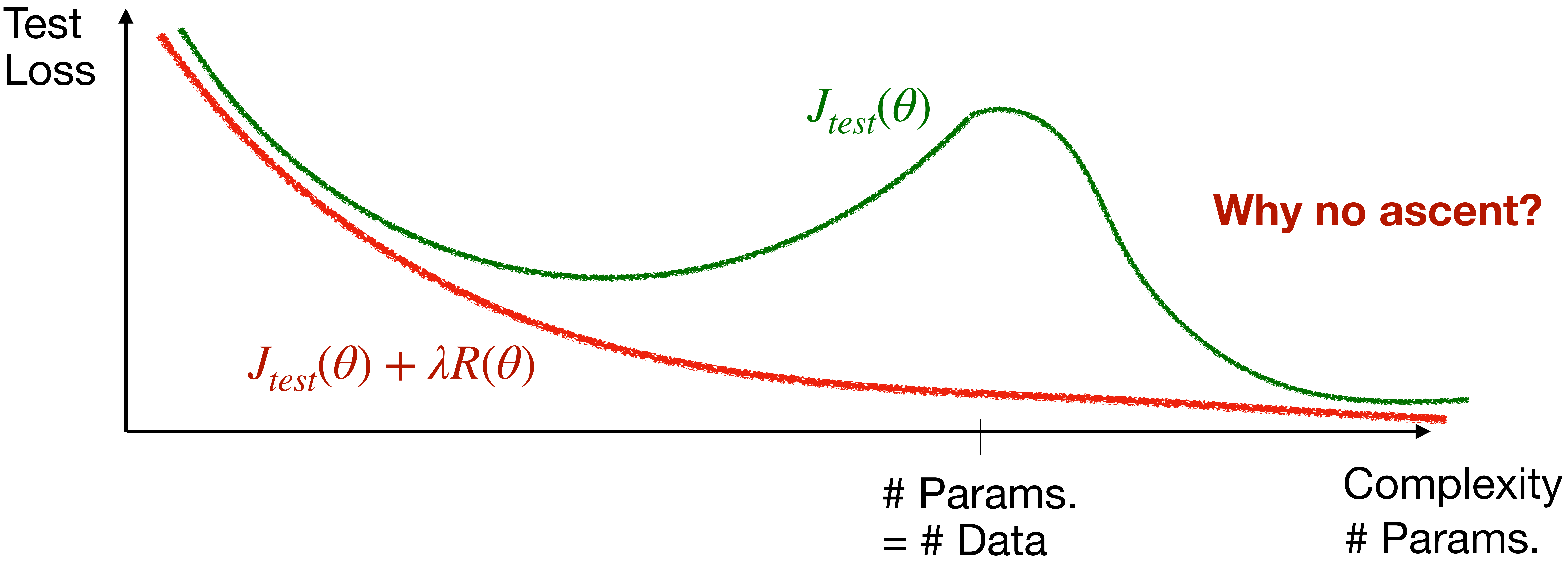
$$R(\theta) = \|\theta\|_2$$

$$h_\theta(x) = .1 + 5.2x + 7.4x^2 + .05x^3 + 2.3x^4$$

Smaller coefficients

Double Descent

Regularization solves the problem with large parameters

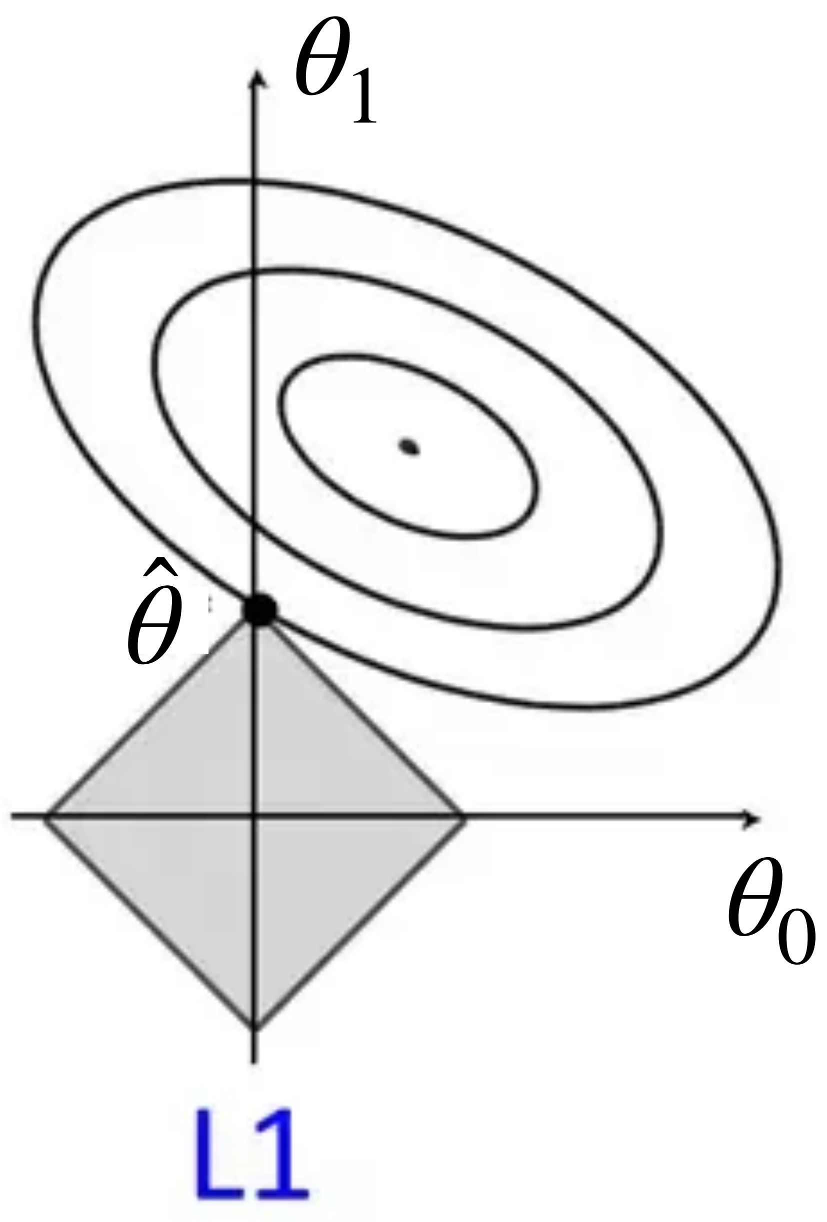


Regularization

Force fitting parameters to be smaller - 'shrink' hypothesis class

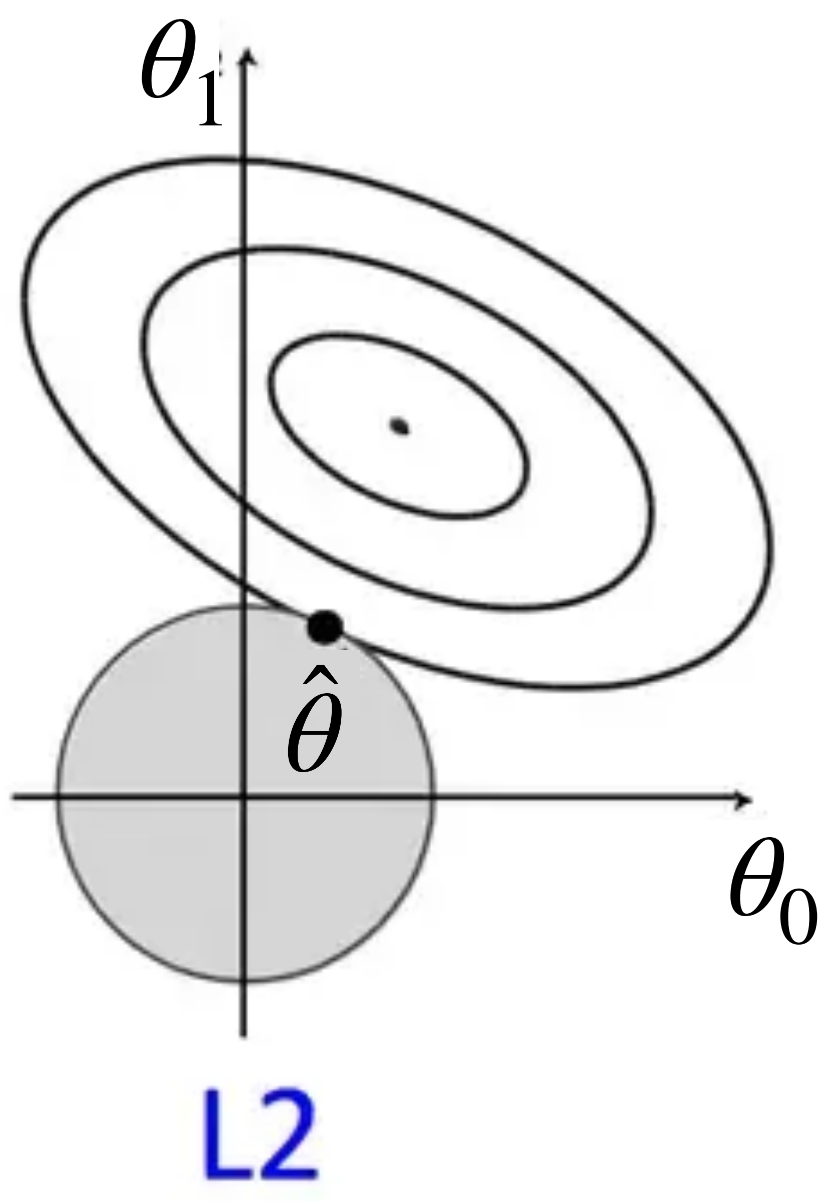
L1 Regularization

$$R(\theta) = ||\theta||_1$$



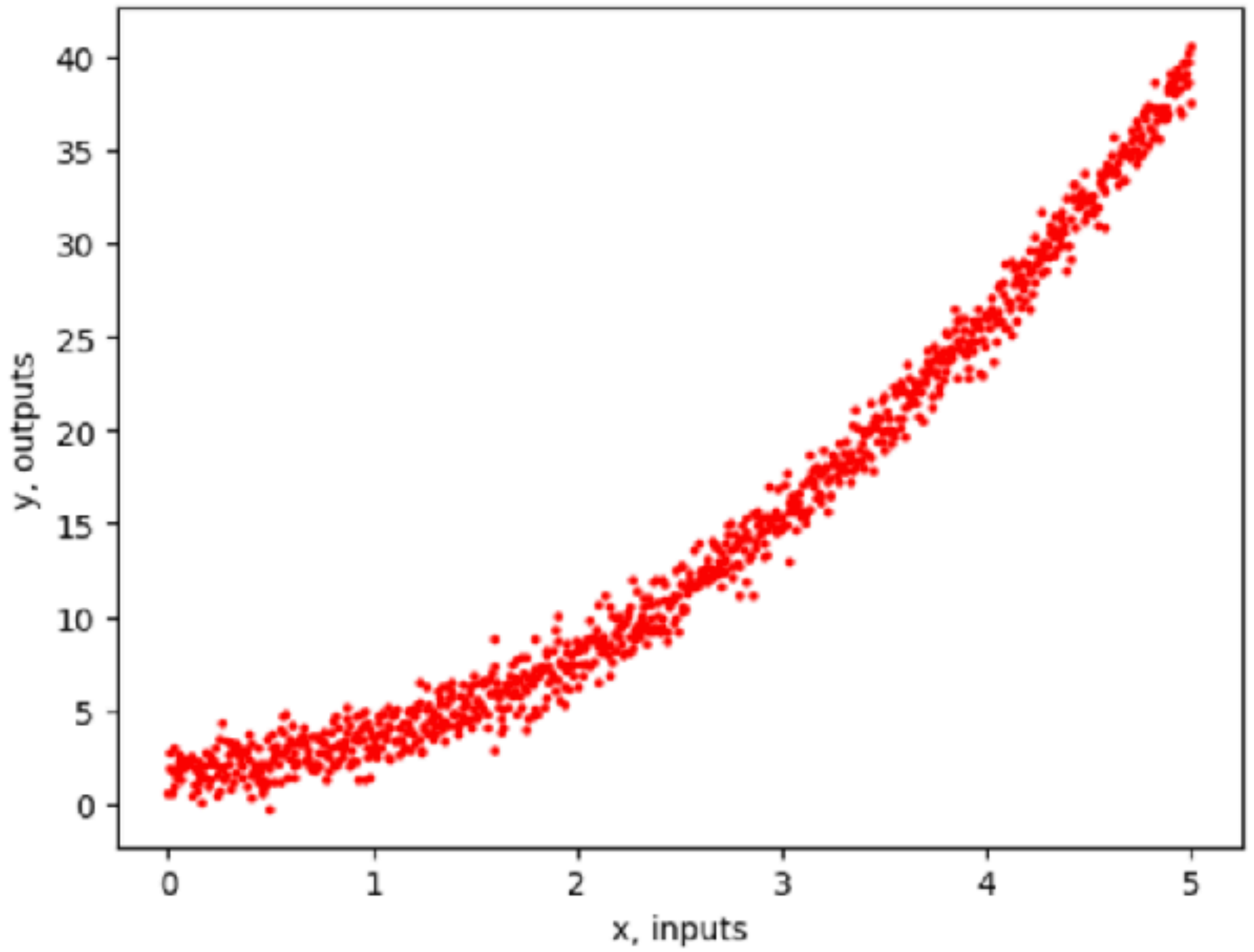
L2 Regularization

$$R(\theta) = ||\theta||_2$$



Create synthetic data

```
# synthetic parameters
num_points = 1000
var = 1
a = 1.5
b = 2

# generate data
x = np.linspace(0, 5, num_points)
y = 1.5 * x**2 + b + var * np.random.normal(0, 1, num_points)
```



Feature engineering (design matrix)

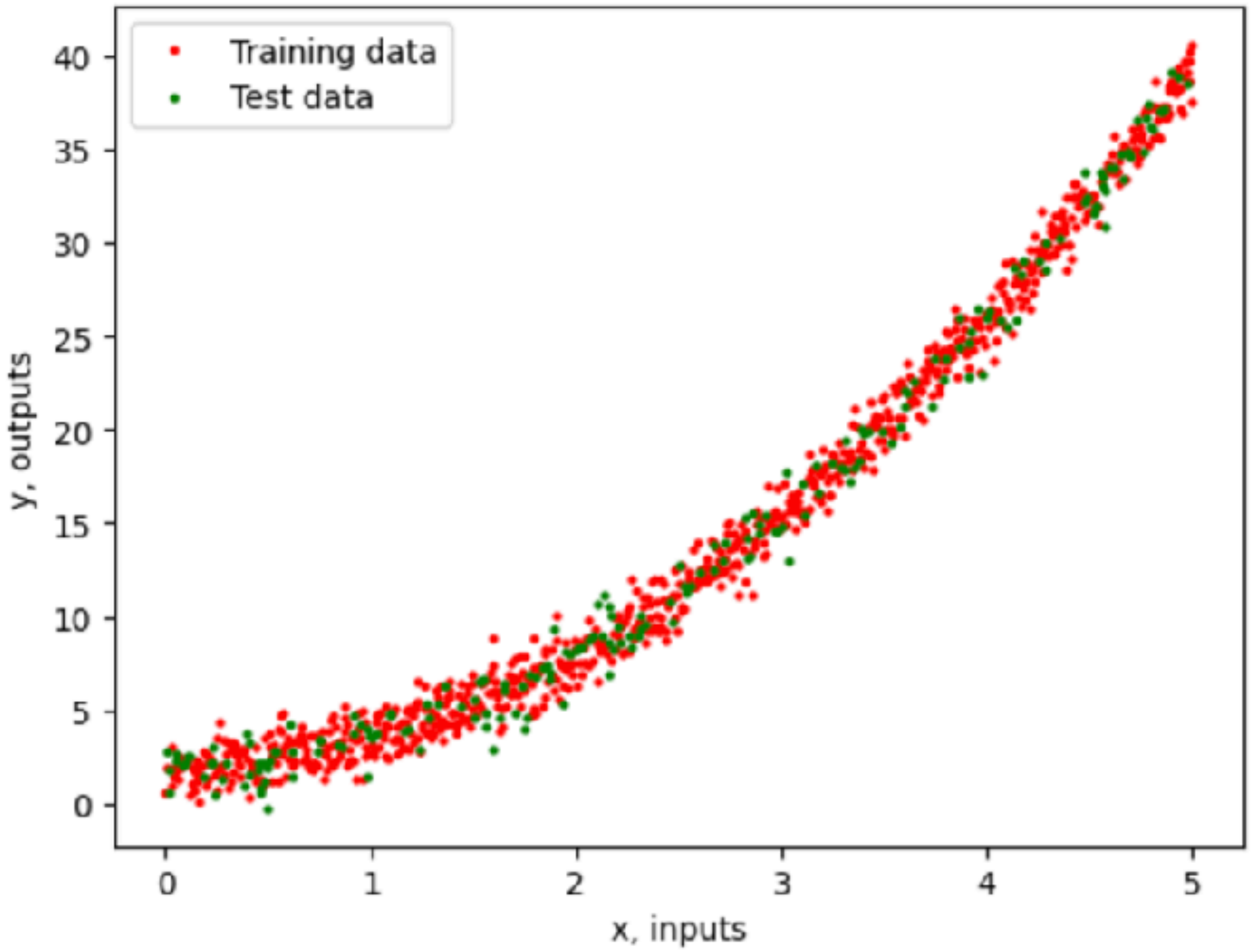
```python
# Create features

def design_matrix(x, degree):
    X = np.zeros((len(x), degree+1))
    for i in range(X.shape[1]):
        X[:, i] = x**i
    return X


degree = 2
X = design_matrix(x, degree)
y = y.reshape(-1, 1)
```

Shuffle and split

```
# Split data

n_train = int(0.8 * num_points)
n_test = num_points - n_train

shuff_index = np.random.permutation(num_points)
X_shuffle = X[shuff_index]
y_shuffle = y[shuff_index]

X_train = X_shuffle[:n_train]
X_test = X_shuffle[n_train:]
y_train = y_shuffle[:n_train]
y_test = y_shuffle[n_train:]
```

Visualize (training set)

```
# Plot training data
fig = plt.figure()
plt.plot(X_train[:, 1], y_train, 'ro', ms=2, label='Training data')
plt.plot(X_test[:, 1], y_test, 'go', ms=2, label='Test data')
plt.xlabel('x, inputs')
plt.ylabel('y, outputs')
plt.legend()
plt.show()
```



Define cost function and Gradient Descent

Cost function

```
def cost_function(X, y, theta):
    m = len(y)
    return 1/(2*m) * np.sum((X @ theta - y)**2)
```

Gradient Descent Function

```
def gradient_descent(X, y, theta, learning_rate, num_iters):
    m = len(y)
    J_history = np.zeros(num_iters)
    for i in range(num_iters):
        theta = theta - (learning_rate/m) * X.T @ (X @ theta - y)
        J_history[i] = cost_function(X, y, theta)
    return theta, J_history
```

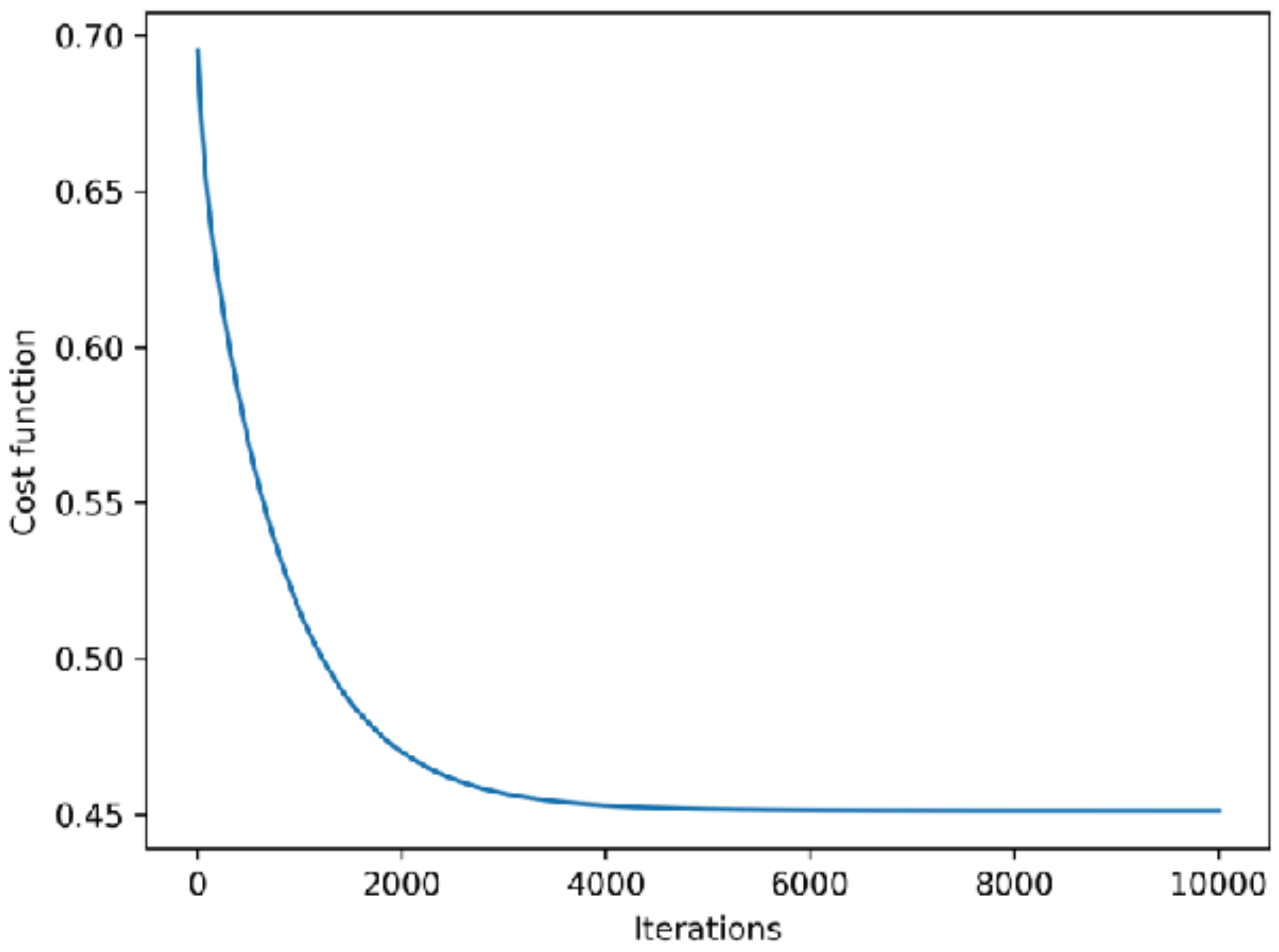
Gradient Descent Update

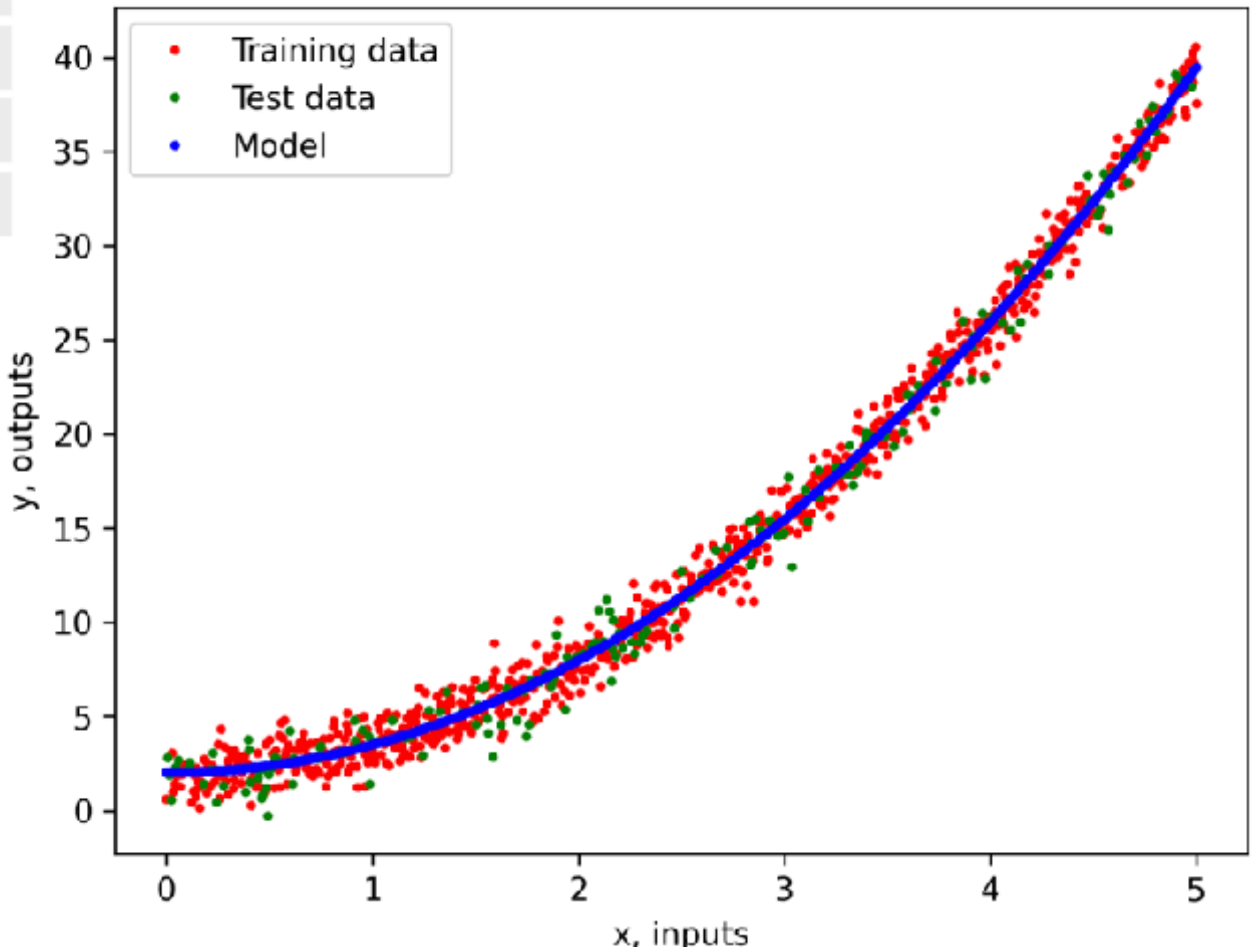
```
theta = np.random.randn(degree+1, 1)
learning_rate = 0.01
num_iters = 10000
theta, J_history = gradient_descent(X_train, y_train, theta, learning_rate, num_iters)
```

```
theta
✓ 0.0s
array([[ 2.04211351],
       [-0.02468485],
       [ 1.50370819]])
```

Plot result

```
# plot comparison
fig = plt.figure()
plt.plot(X_train[:, 1], y_train, 'ro', ms=2, label='Training data')
plt.plot(X_test[:, 1], y_test, 'go', ms=2, label='Test data')
plt.plot(X_train[:, 1], X_train @ theta, 'bo', ms=2, label='Model')
plt.xlabel('x, inputs')
plt.ylabel('y, outputs')
plt.legend()
plt.show()
```





Plot result

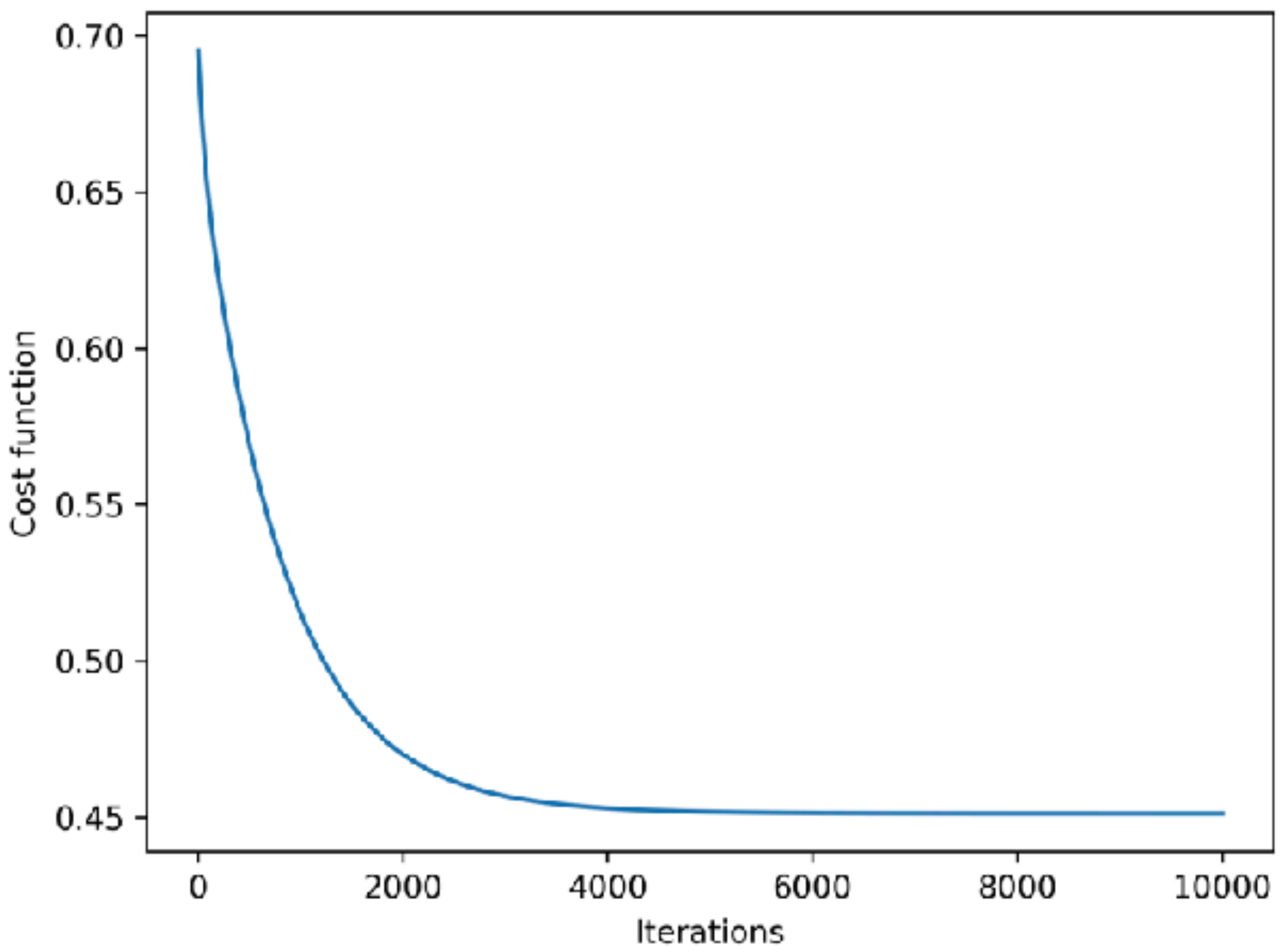
```
# plot comparison
fig = plt.figure()
plt.plot(X_train[:, 1], y_train, 'ro', ms=2, label='Training data')
plt.plot(X_test[:, 1], y_test, 'go', ms=2, label='Test data')
plt.plot(X_train[:, 1], X_train @ theta, 'bo', ms=2, label='Model')
plt.xlabel('x, inputs')
plt.ylabel('y, outputs')
plt.legend()
plt.show()
```

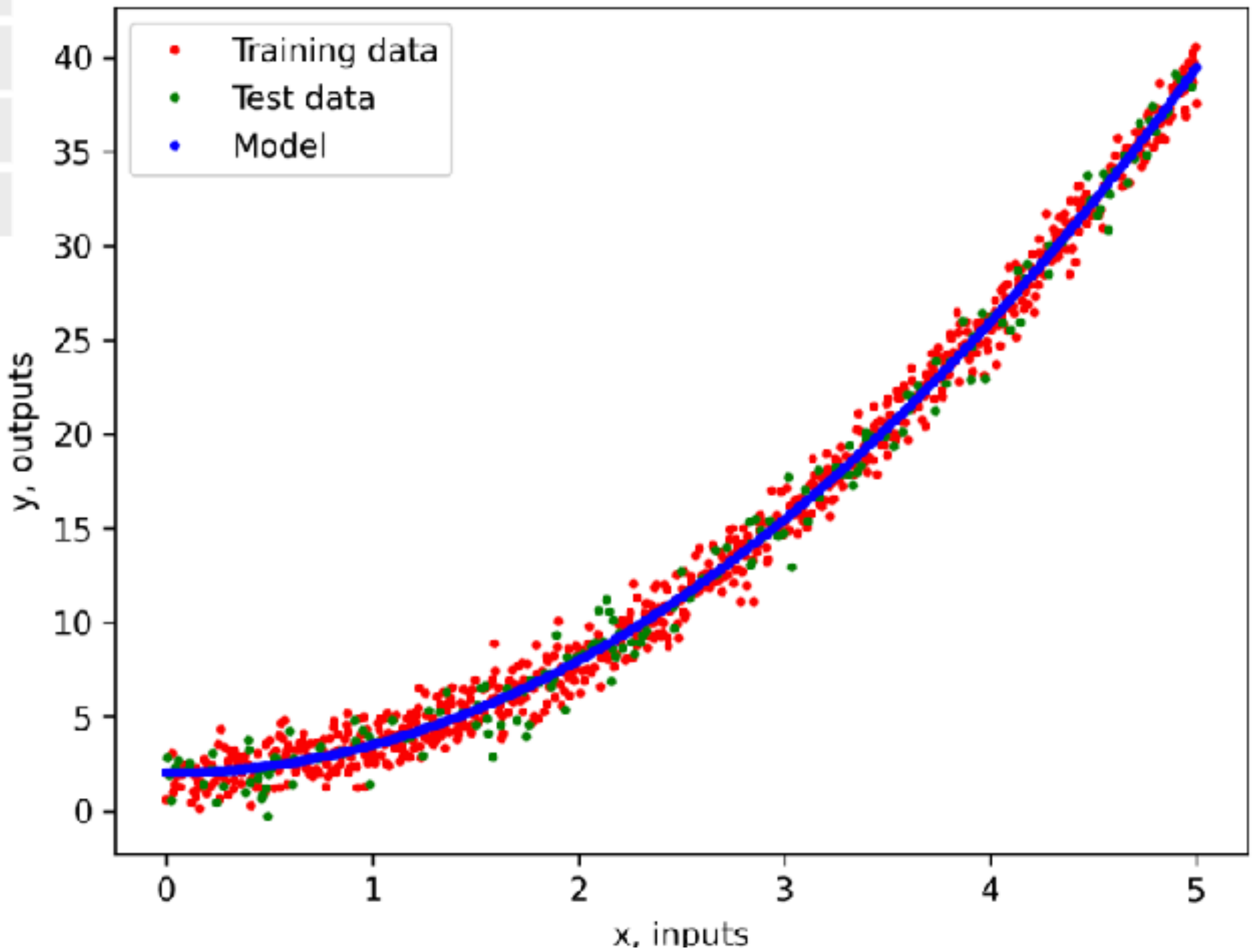
Train and Test loss Comparison

```
test_loss = cost_function(X_test, y_test, theta)
train_loss = cost_function(X_train, y_train, theta)

print(f'Test loss: {test_loss}')
print(f'Train loss: {train_loss}')
```

✓ 0.0s

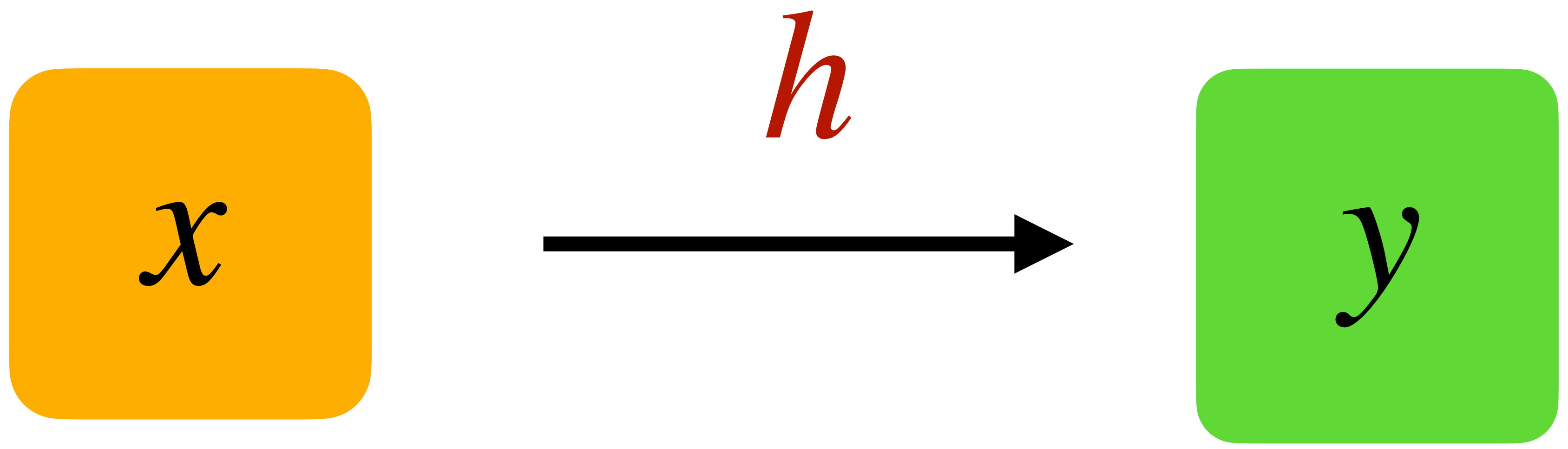
```
Test loss: 0.508970692715051
Train loss: 0.4511700483353495
```





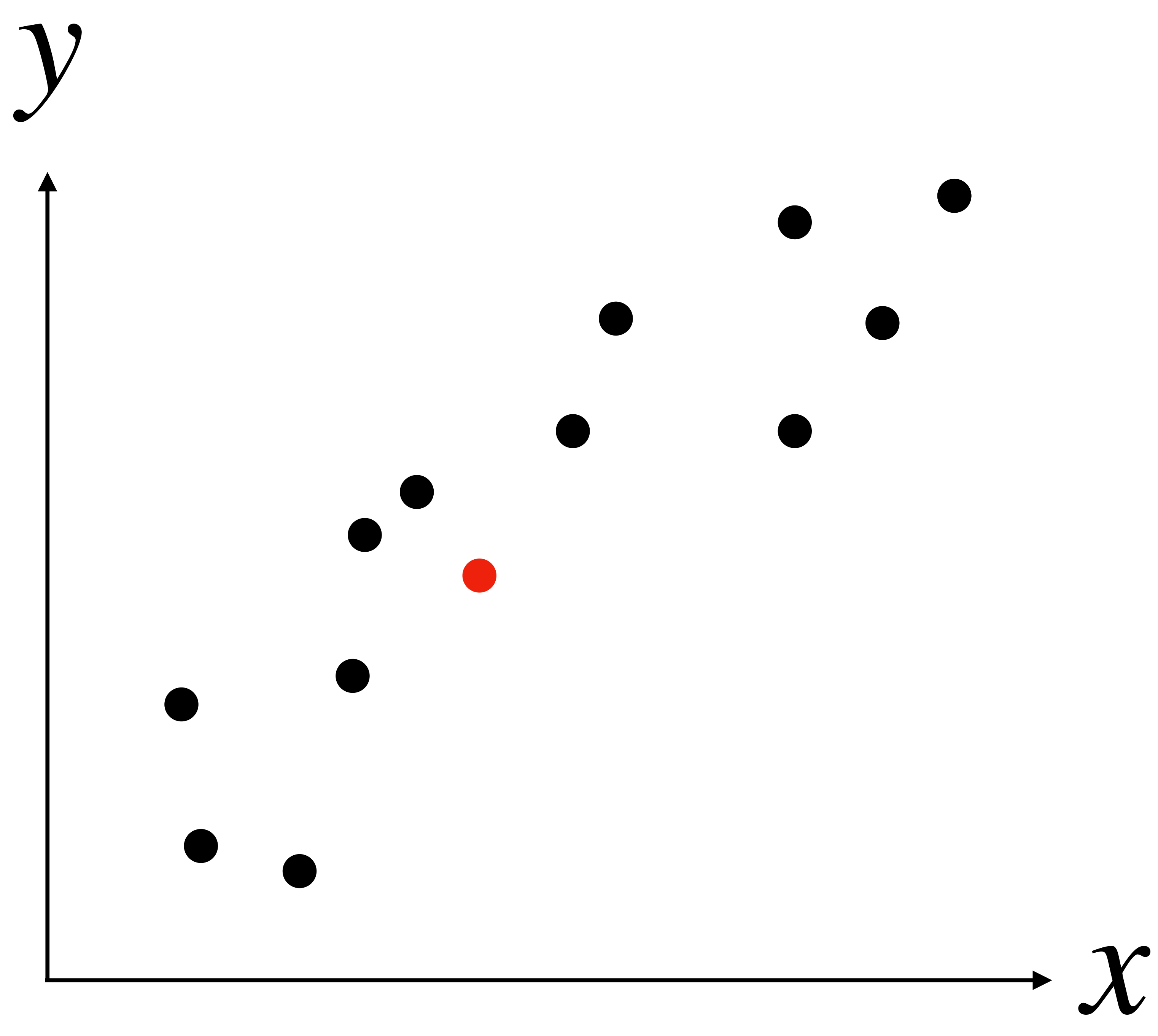
Given new input, what's the output?

Assuming $y \in \mathbb{R}$

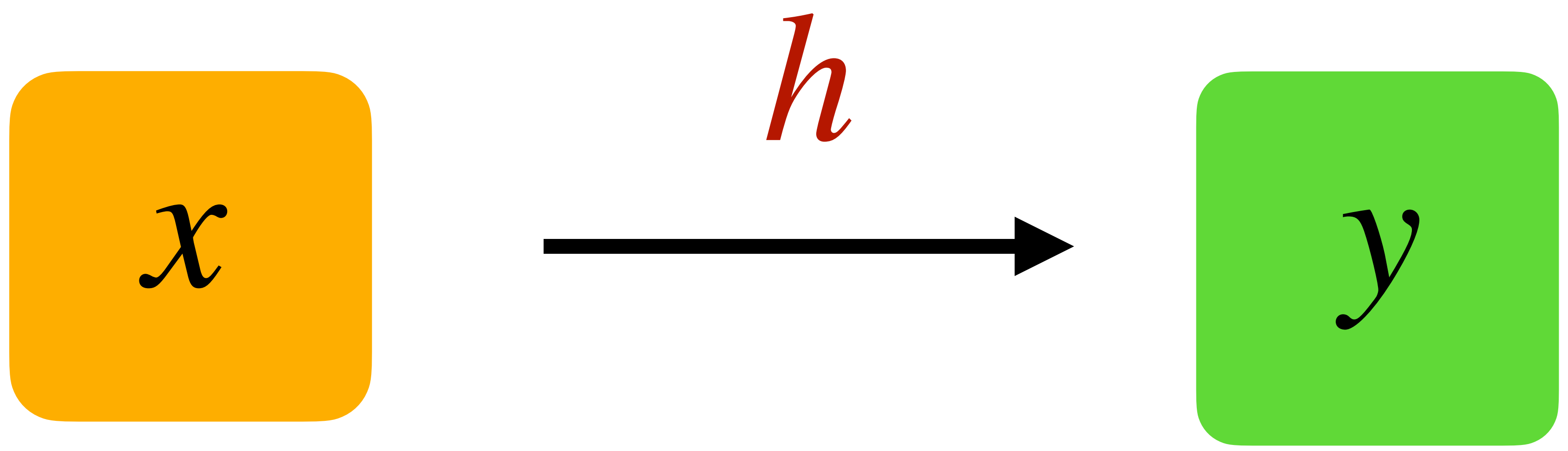


Given the data,
find a **function** h,
that predicts y, given x

$$\mathbf{y} = h(\mathbf{x})$$



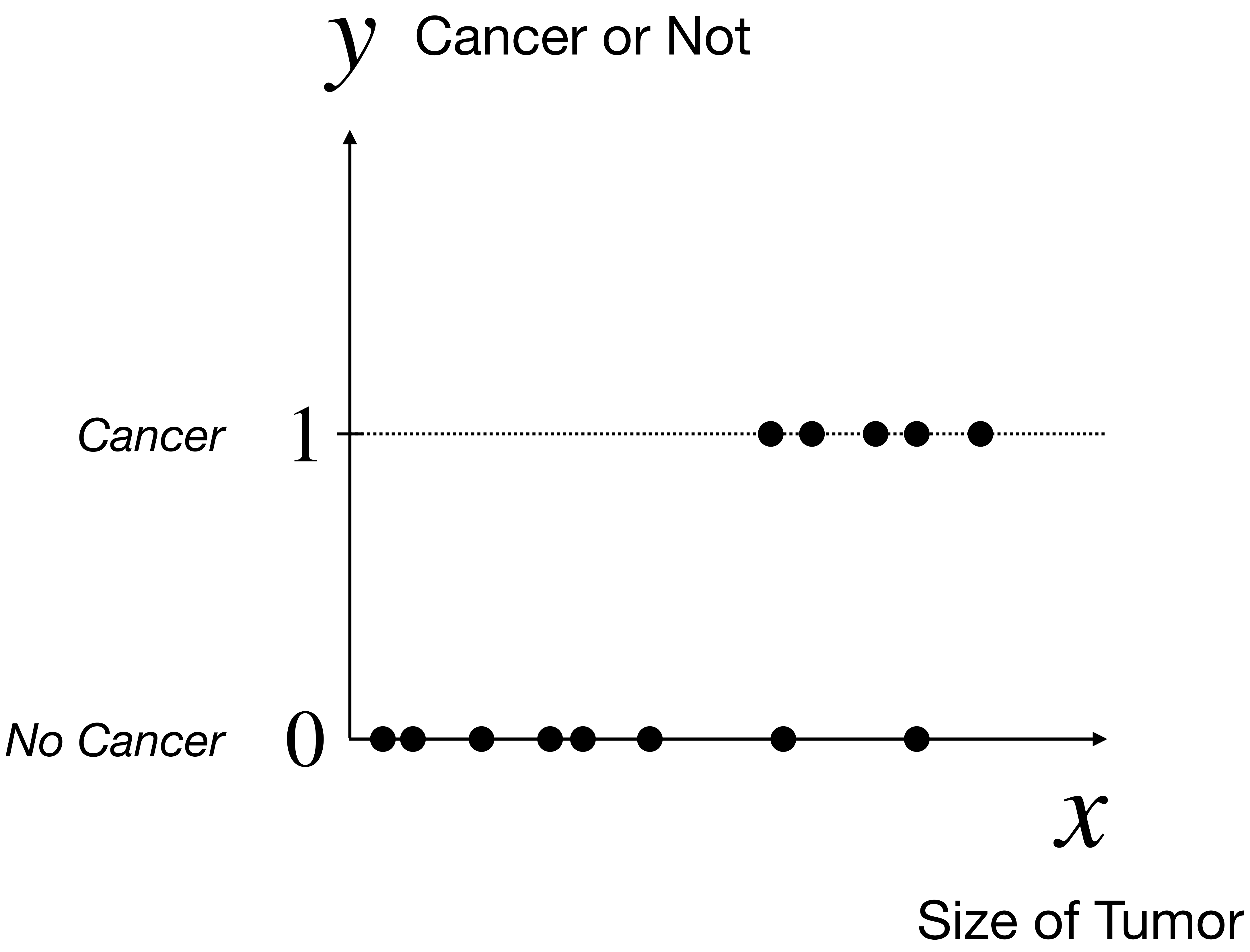
What if y is a label?



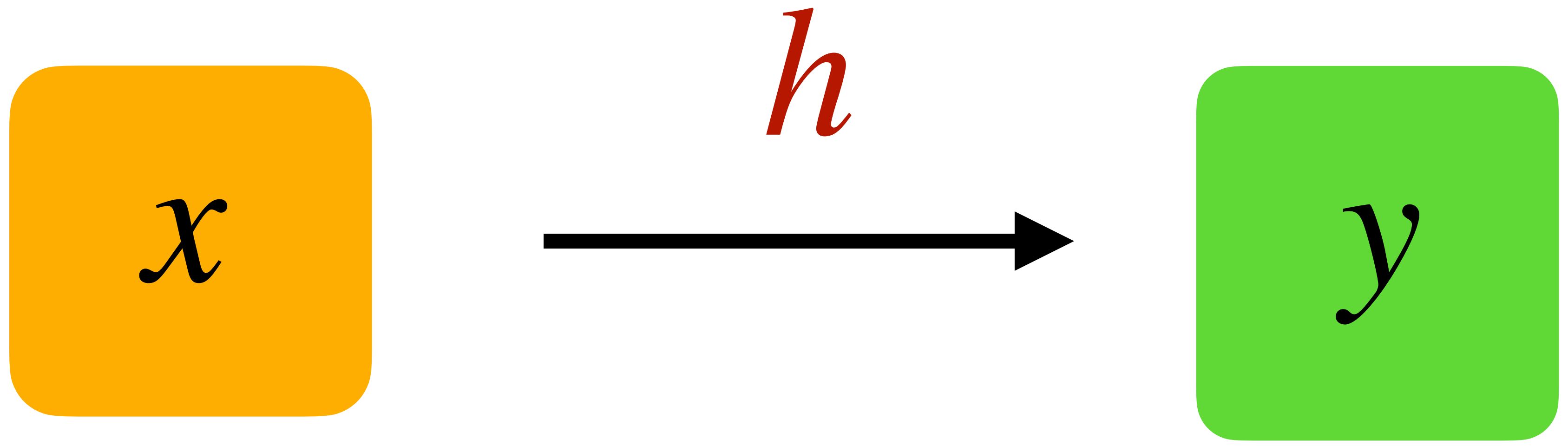
Given the data,
find a **function** h,
that predicts y, given x

$$\mathbf{y} = h(\mathbf{x})$$

$$y \in [0,1]$$



What if y is a label?

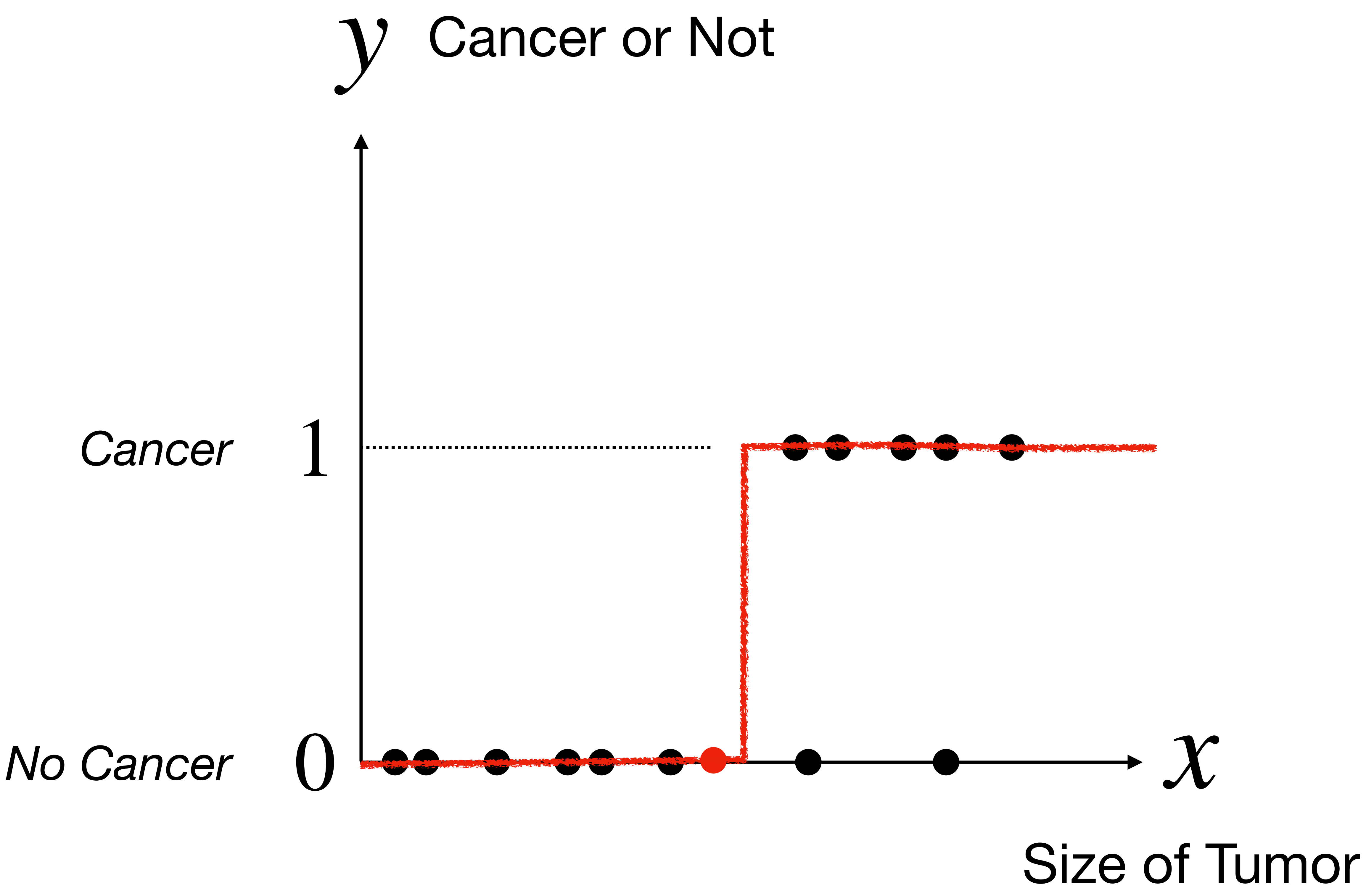


Given the data,
find a **function** h,
that predicts y, given x

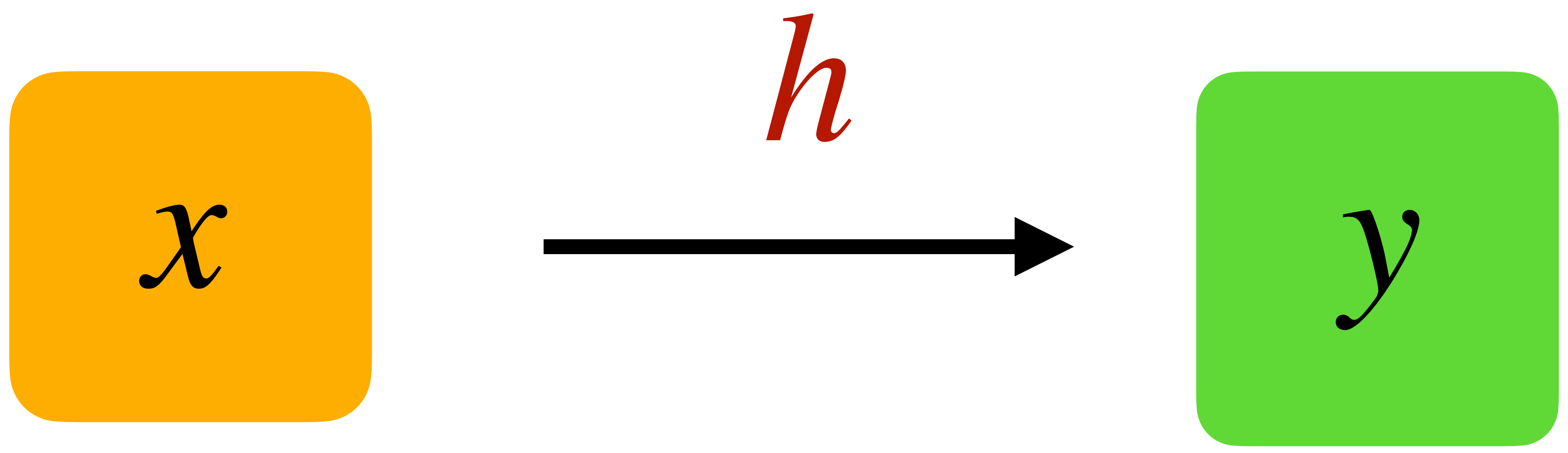
$$\mathbf{y} = h(\mathbf{x})$$

$$y \in [0,1]$$

A step function, or threshold



What if y is a label?

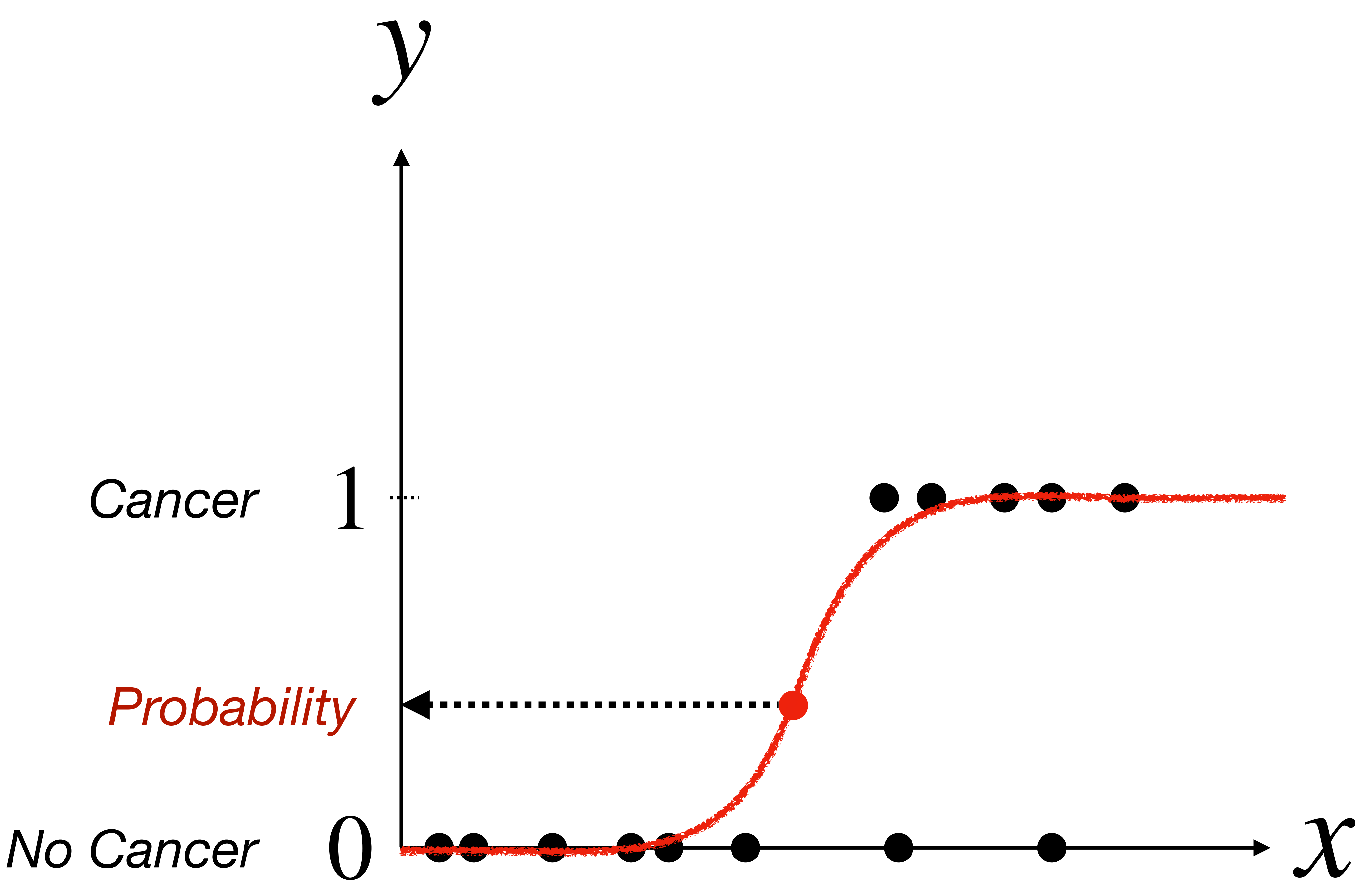


Given the data,
find a **function** h,
that predicts y, given x

$$\mathbf{y} = h(\mathbf{x})$$

$$y \in [0,1]$$

A smooth function that returns probability of occurrence

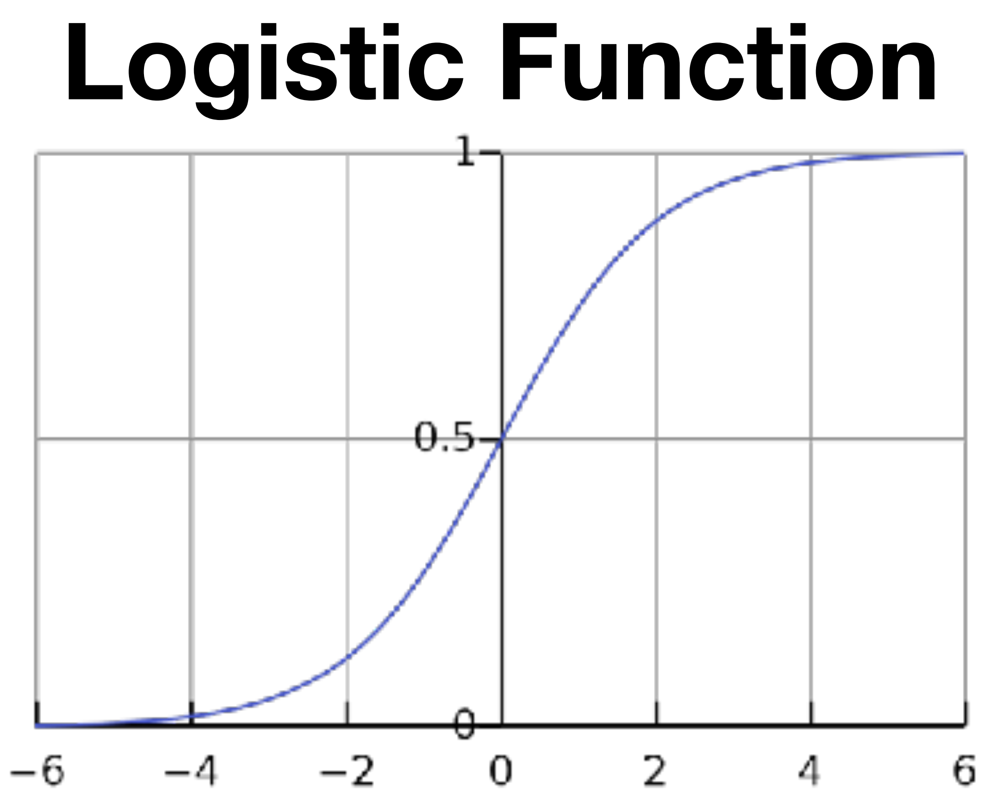


What if y is a label?

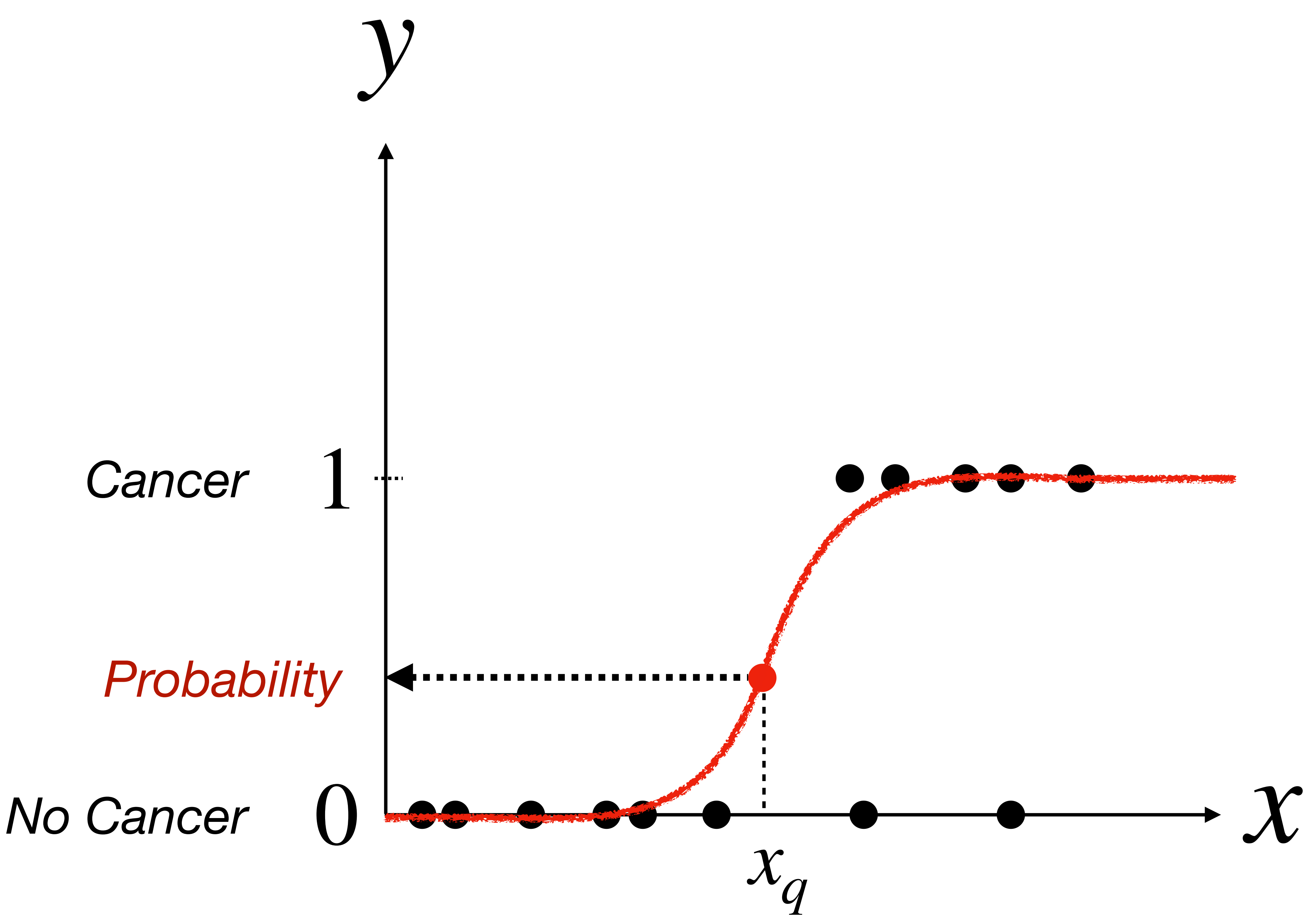
$$y = h_\theta(x) \quad \& \quad y \in [0,1]$$

A **smooth** function that returns **probability of occurrence**

$$y = \frac{1}{1 + e^{-x}}$$



$$h_\theta(x) = \frac{1}{1 + e^{-(\theta_0 + \theta_1 x)}}$$



What if y is a label?

A **smooth** function that returns **probability of occurrence**

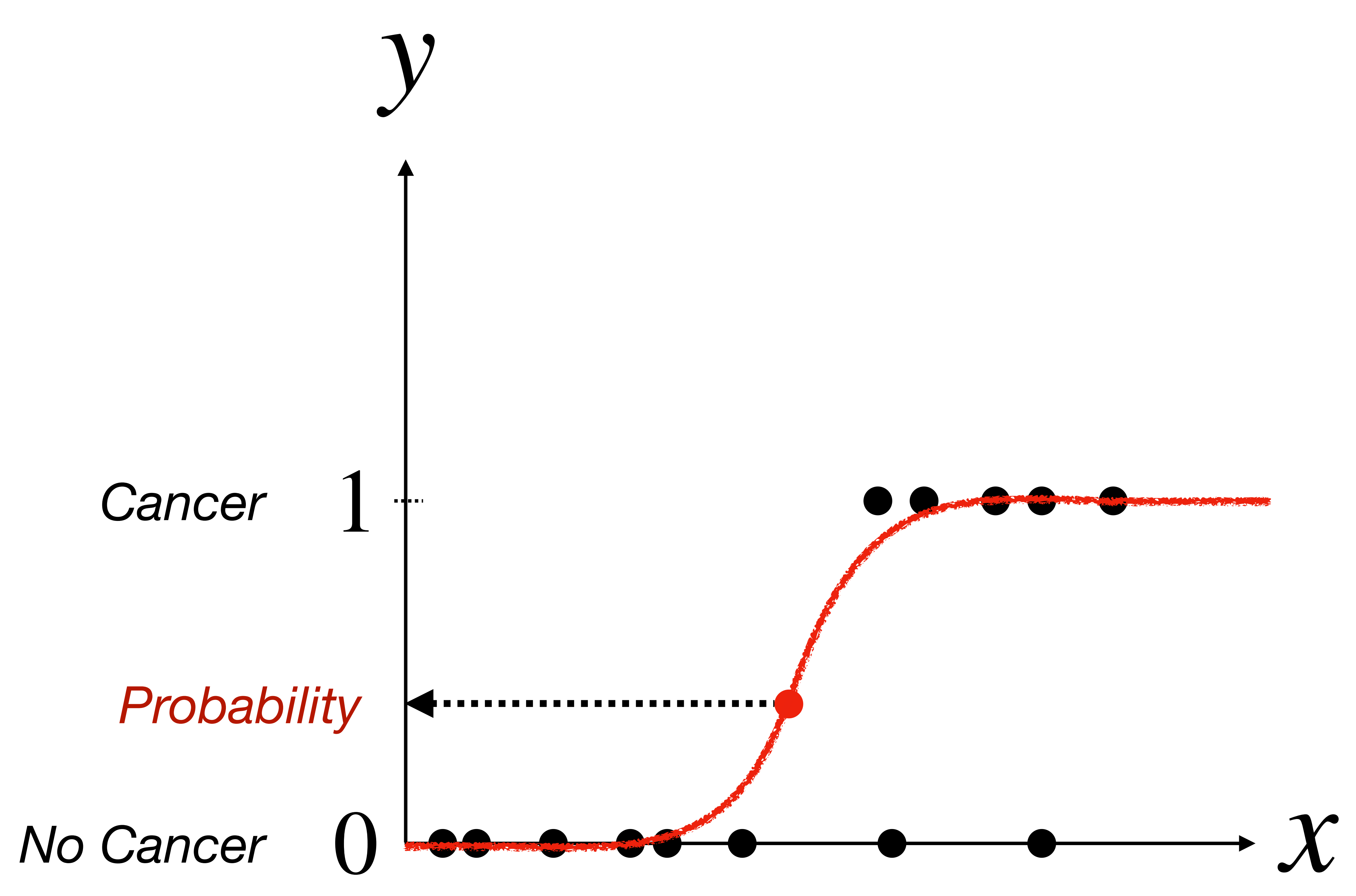
$$y = h_\theta(x) \quad \& \quad y \in [0,1]$$

$$h_\theta(x) = \frac{1}{1 + e^{-(\theta^\top x)}}$$

For $x \in \mathbb{R}^n$

Where $\theta^\top x = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots$

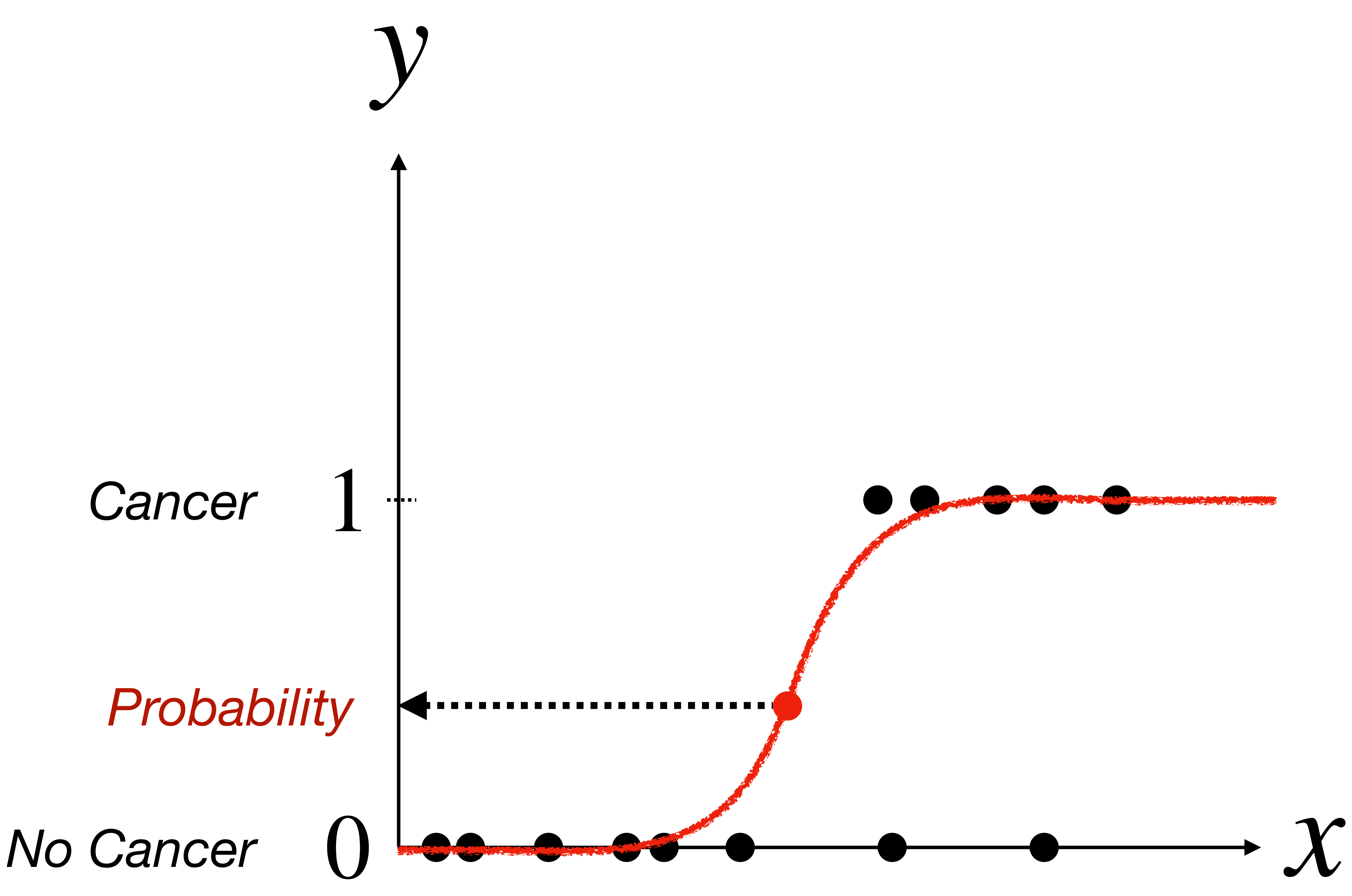
$$\theta = [\theta_0, \theta_1, \ldots]$$
$$x = [x_0, x_1, \ldots]$$



What if y is a label?

$$y = h_\theta(x) \quad \& \quad y \in [0,1]$$

$$h_\theta(x) = \frac{1}{1 + e^{-(\theta^\top x)}}$$

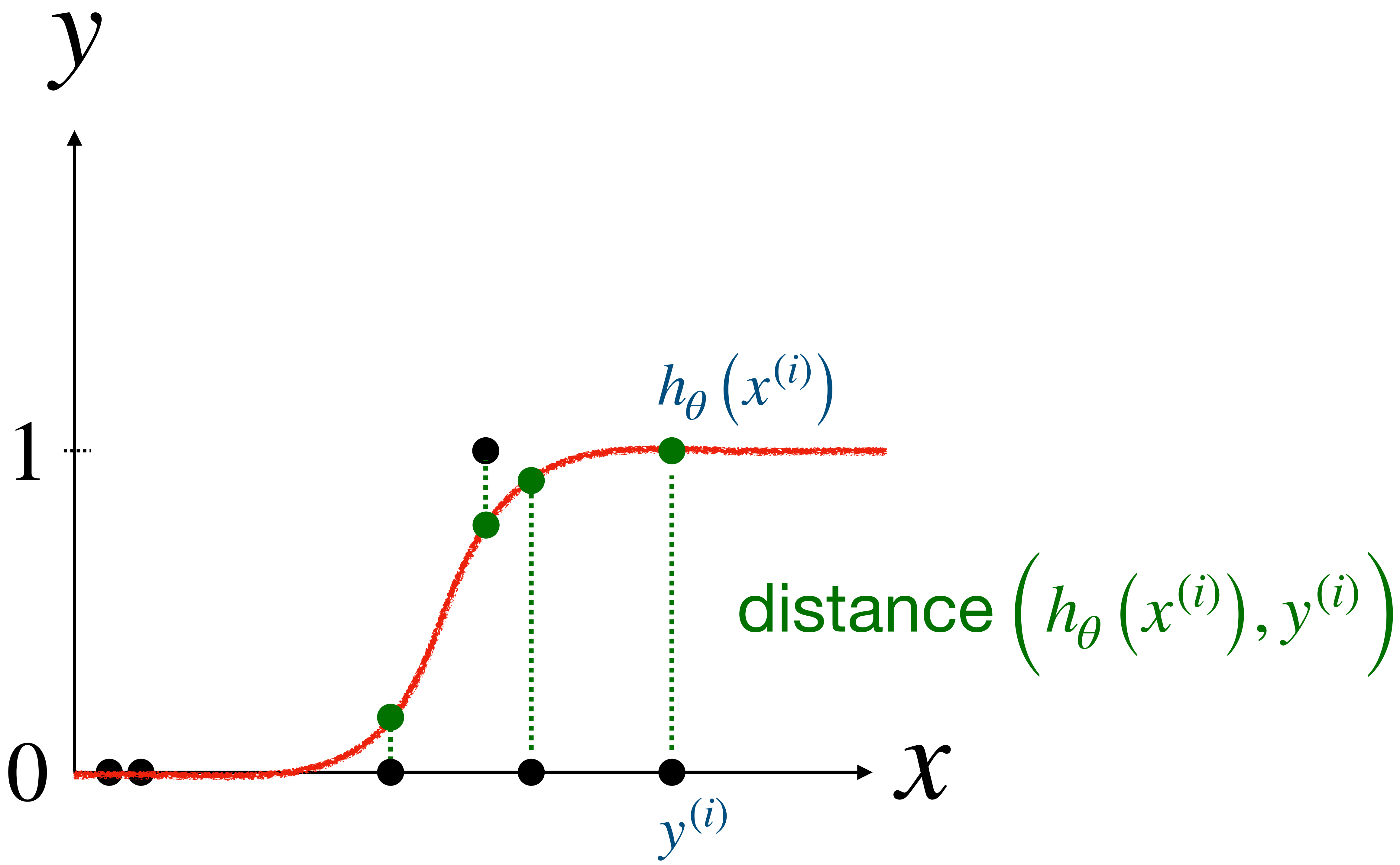


1. **Define a predictor:** the logistic function ✅
2. **Define a loss:** distance between function and data ❓
3. **Optimize loss**
4. **Test model**

Logistic Regression

$$y = h_\theta(x)$$

$$h_\theta(x) = \frac{1}{1 + e^{-(\theta^\top x)}} = g\left(\theta^\top x\right)$$



Linear predictor
negative log-likelihood or OLS

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{d} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

Logistic predictor
Binary-cross entropy loss

$$\mathcal{L}(\theta) = \sum_{i=1}^{n} y^{(i)} \log h_\theta\left(x^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_\theta\left(x^{(i)}\right)\right)$$

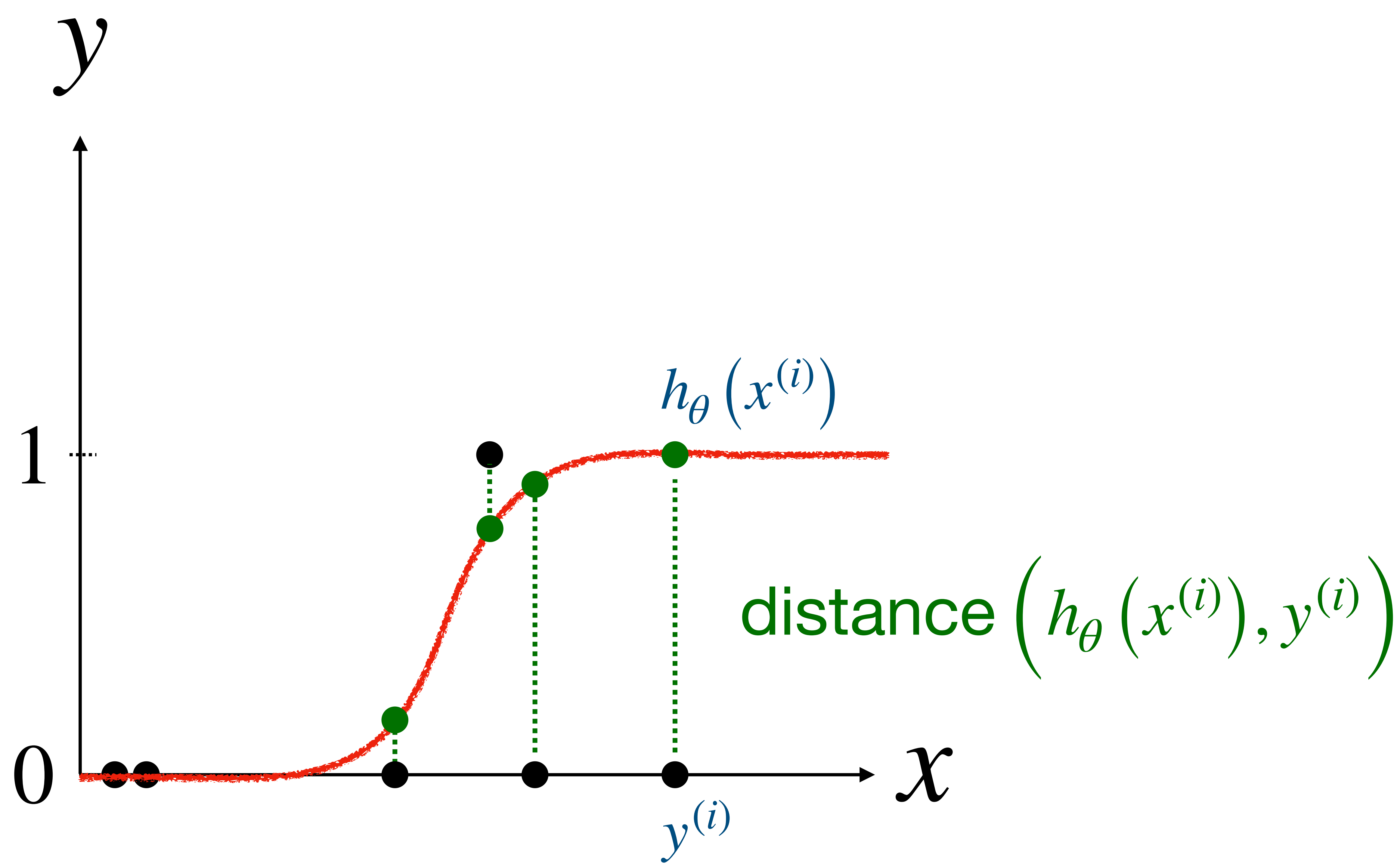
Compute gradient $\nabla \mathcal{L}(\theta)$

Gradient descent → Done!

Logistic Regression

$$y = h_\theta(x)$$

$$h_\theta(x) = \frac{1}{1 + e^{-\left(\theta^\top x\right)}} = g\left(\theta^\top x\right)$$



Linear predictor
negative log-likelihood or OLS

$$J(\theta) = \frac{1}{2}\sum_{i=1}^{d}\left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right)^2$$

Why not use an ordinary least squares loss?

Probabilistic Interpretation of Linear Regression

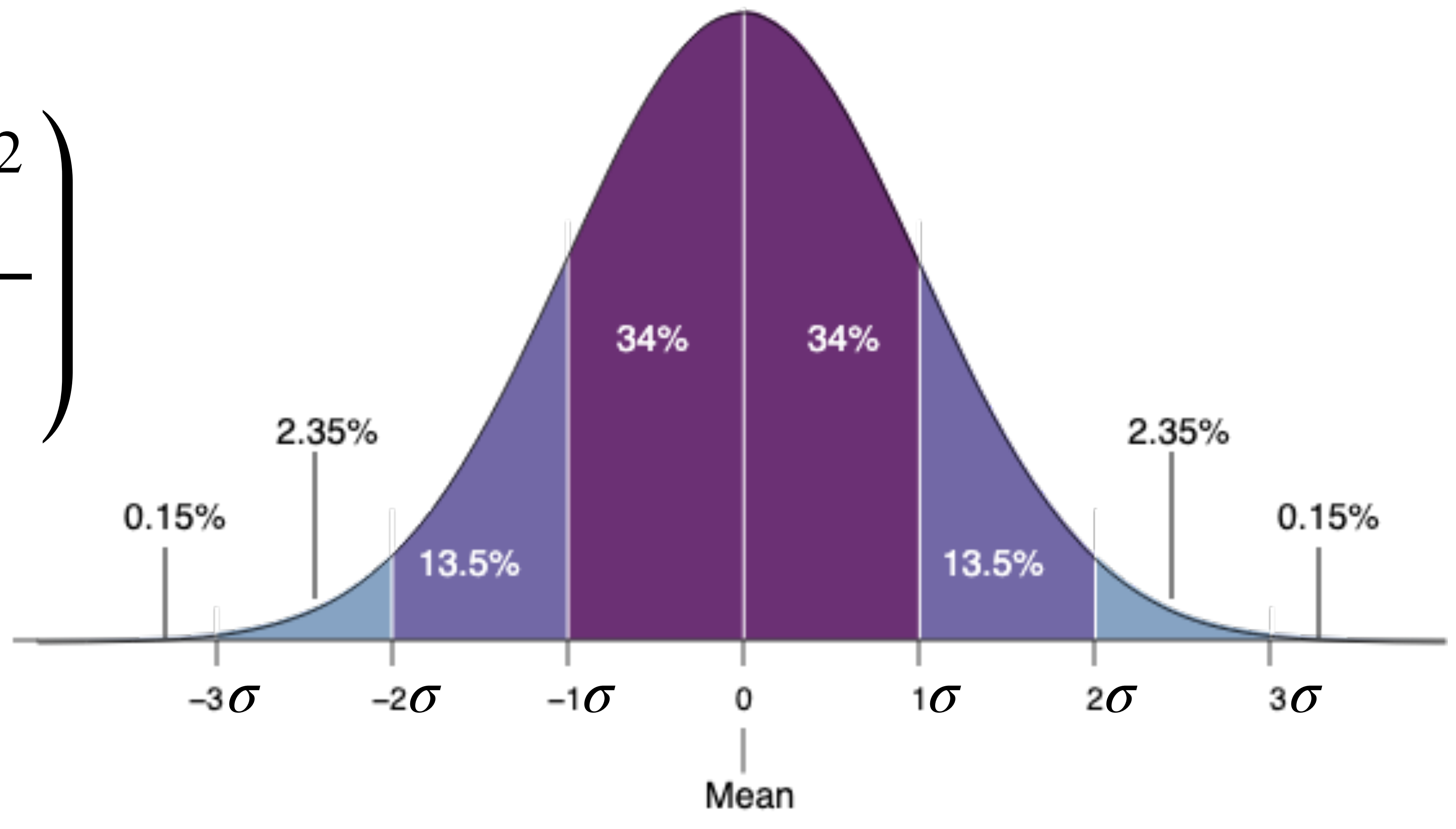
Assume noise is normally distributed around model

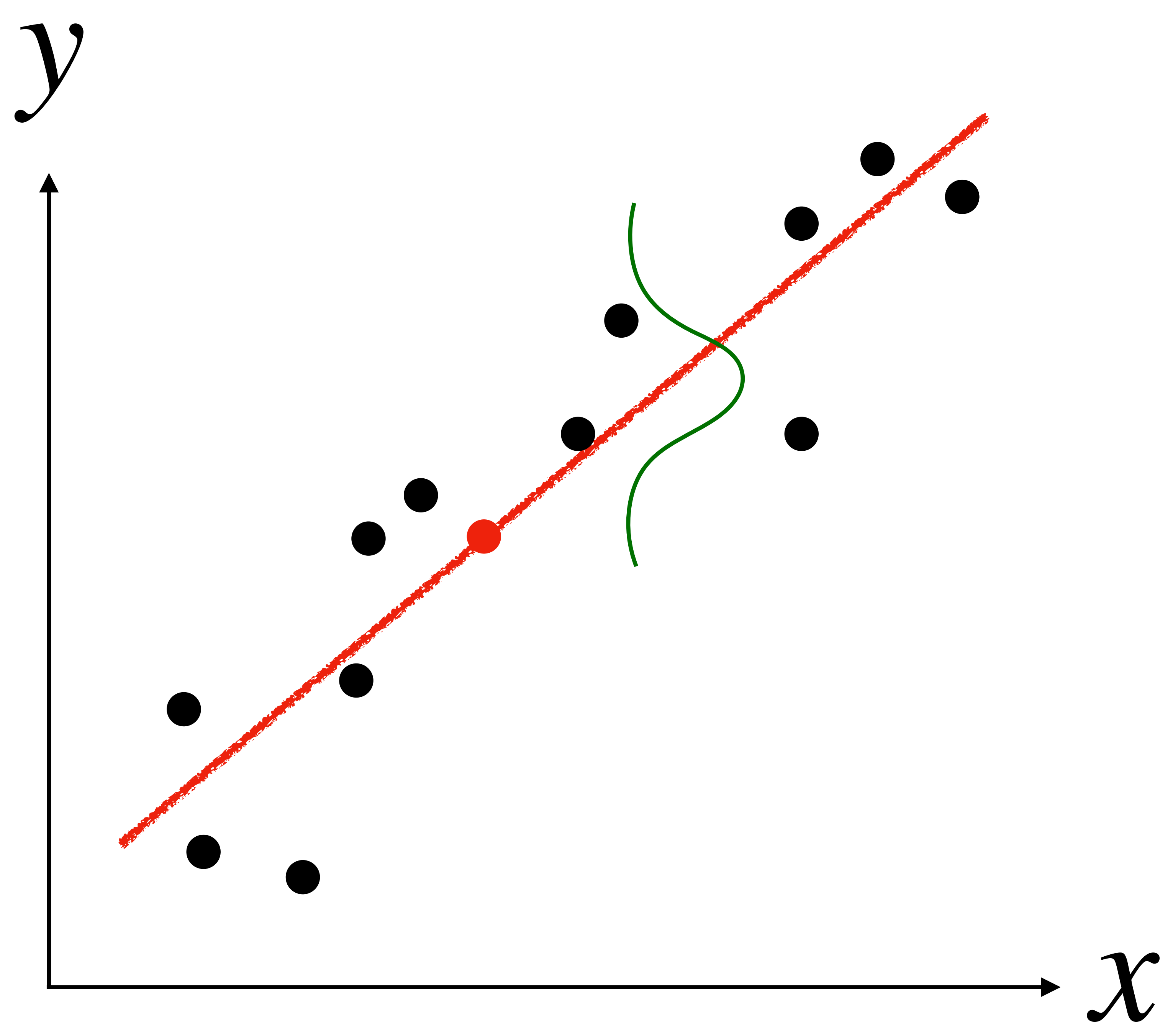
$$y^{(i)} = \theta^\top x^{(i)} + \varepsilon^{(i)}$$

Normally distributed

$$\mathcal{N}\left(0, \sigma^2\right)$$

$$p\left(\varepsilon^{(i)}\right) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(\varepsilon^{(i)}\right)^2}{2\sigma^2}\right)$$



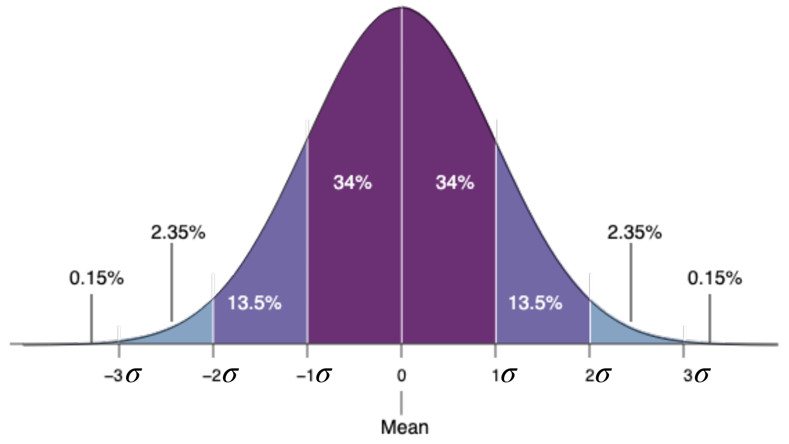


Probabilistic Interpretation

Assume noise is normally distributed around model

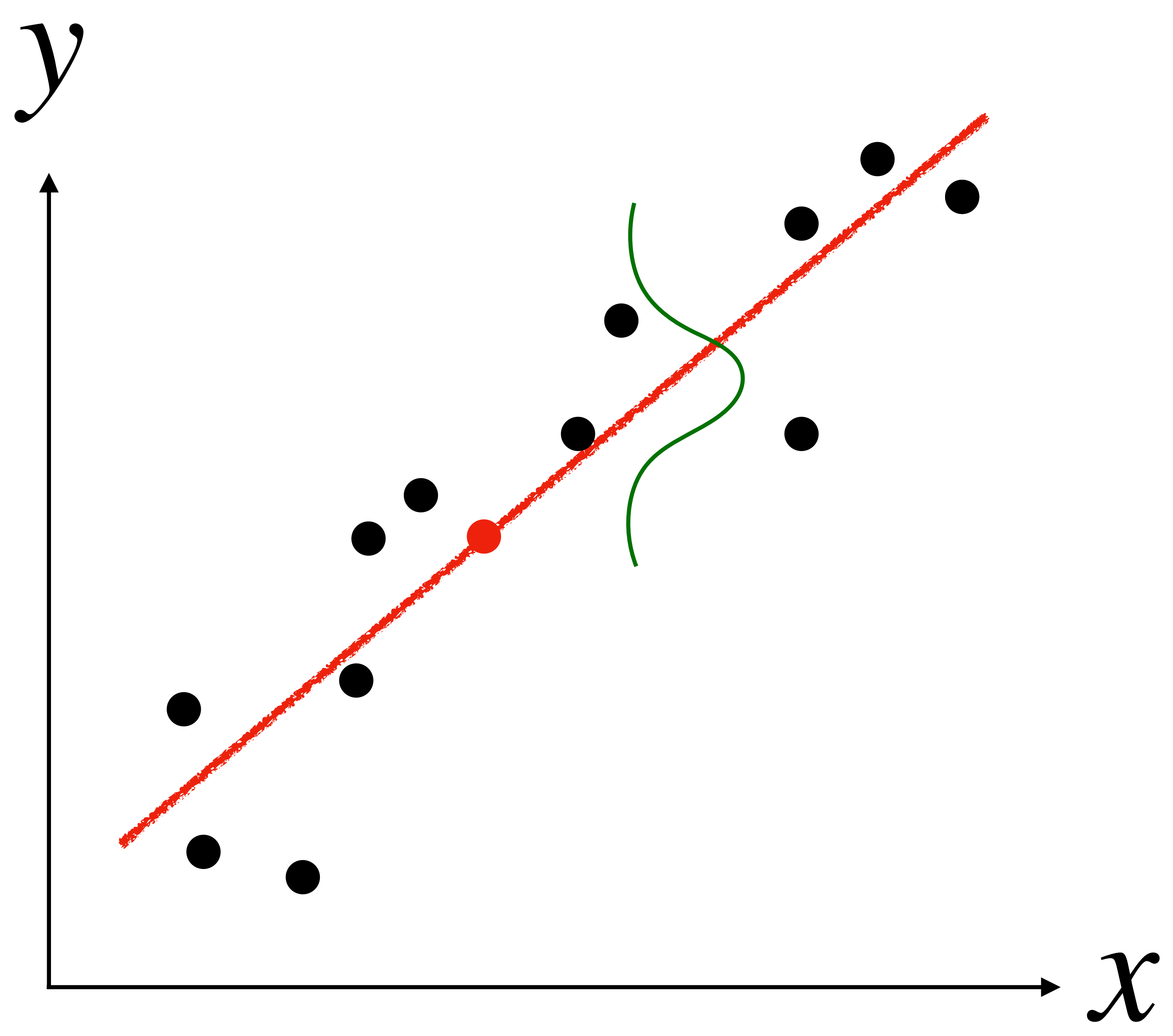
$$y^{(i)} = \theta^{\top} x^{(i)} + \varepsilon^{(i)}$$

$\mathcal{N}\left(0, \sigma^2\right)$



$$p\left(\varepsilon^{(i)}\right) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(\varepsilon^{(i)}\right)^2}{2\sigma^2}\right)$$

$$p\left(y^{(i)} \mid x^{(i)}; \theta\right) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^{\top} x^{(i)}\right)^2}{2\sigma^2}\right)$$

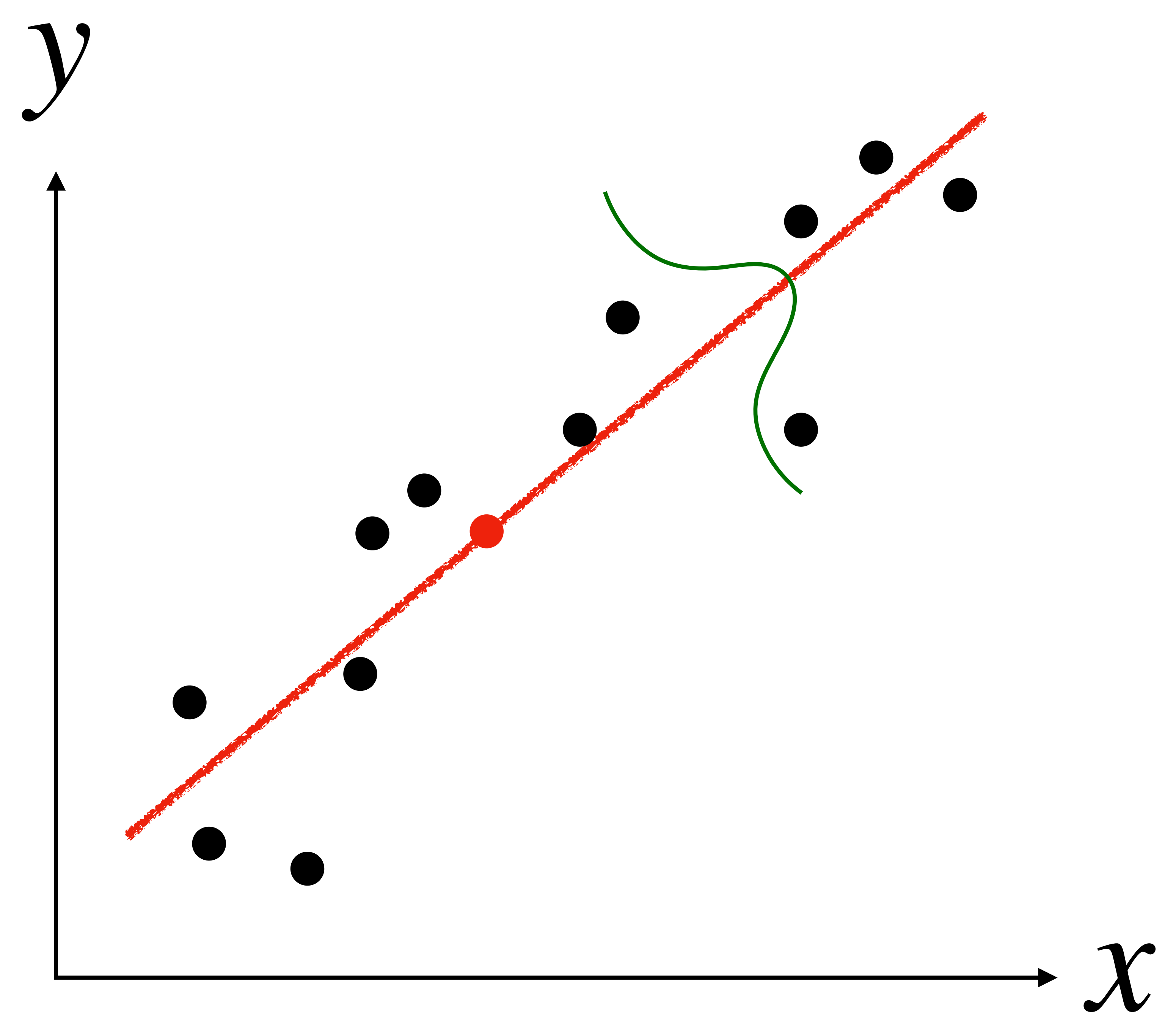


Likelihood of output given input

$$L(\theta) = \prod_{i=1}^{n} p\left(y^{(i)} \,|\, x^{(i)}; \theta\right)$$

Independent and Identically Distributed (IID)

$$= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^\top x^{(i)}\right)^2}{2\sigma^2}\right)$$



Log-likelihood

$$\mathscr{L}(\theta) = \log L(\theta)$$

$$= \log \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^\top x^{(i)}\right)^2}{2\sigma^2}\right)$$

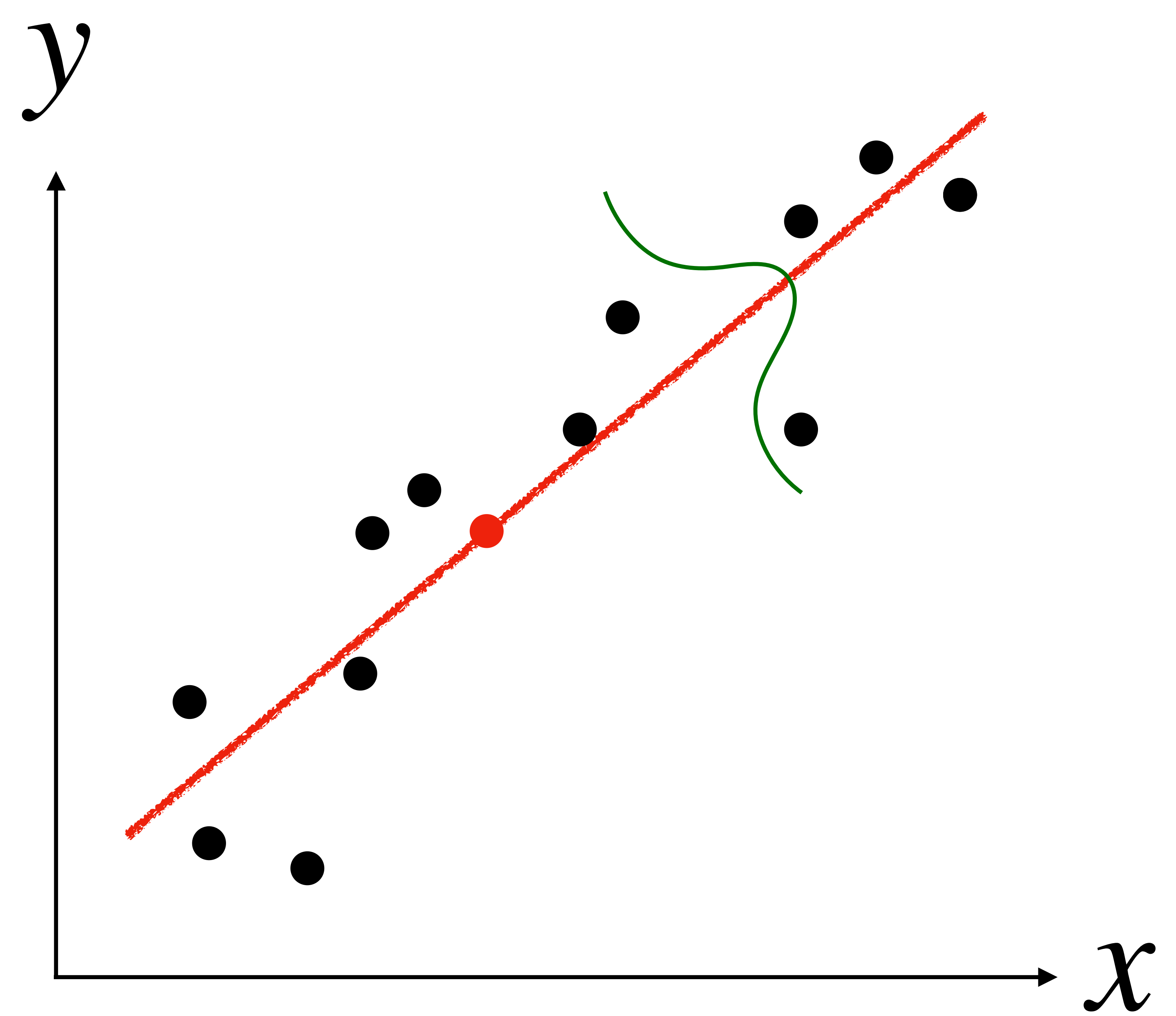
$$= \sum_{i=1}^{n} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^\top x^{(i)}\right)^2}{2\sigma^2}\right) = n \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} \left(y^{(i)} - \theta^\top x^{(i)}\right)^2$$

Maximize Log-likelihood

$$\mathcal{L}(\theta) = \log L(\theta)$$

$$= \sum_{i=1}^{n} \log \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{\left(y^{(i)} - \theta^\top x^{(i)}\right)^2}{2\sigma^2}\right)$$

$$= n \log \frac{1}{\sqrt{2\pi}\sigma} - \frac{1}{2\sigma^2} \sum_{i=1}^{n} \left(y^{(i)} - \theta^\top x^{(i)}\right)^2$$



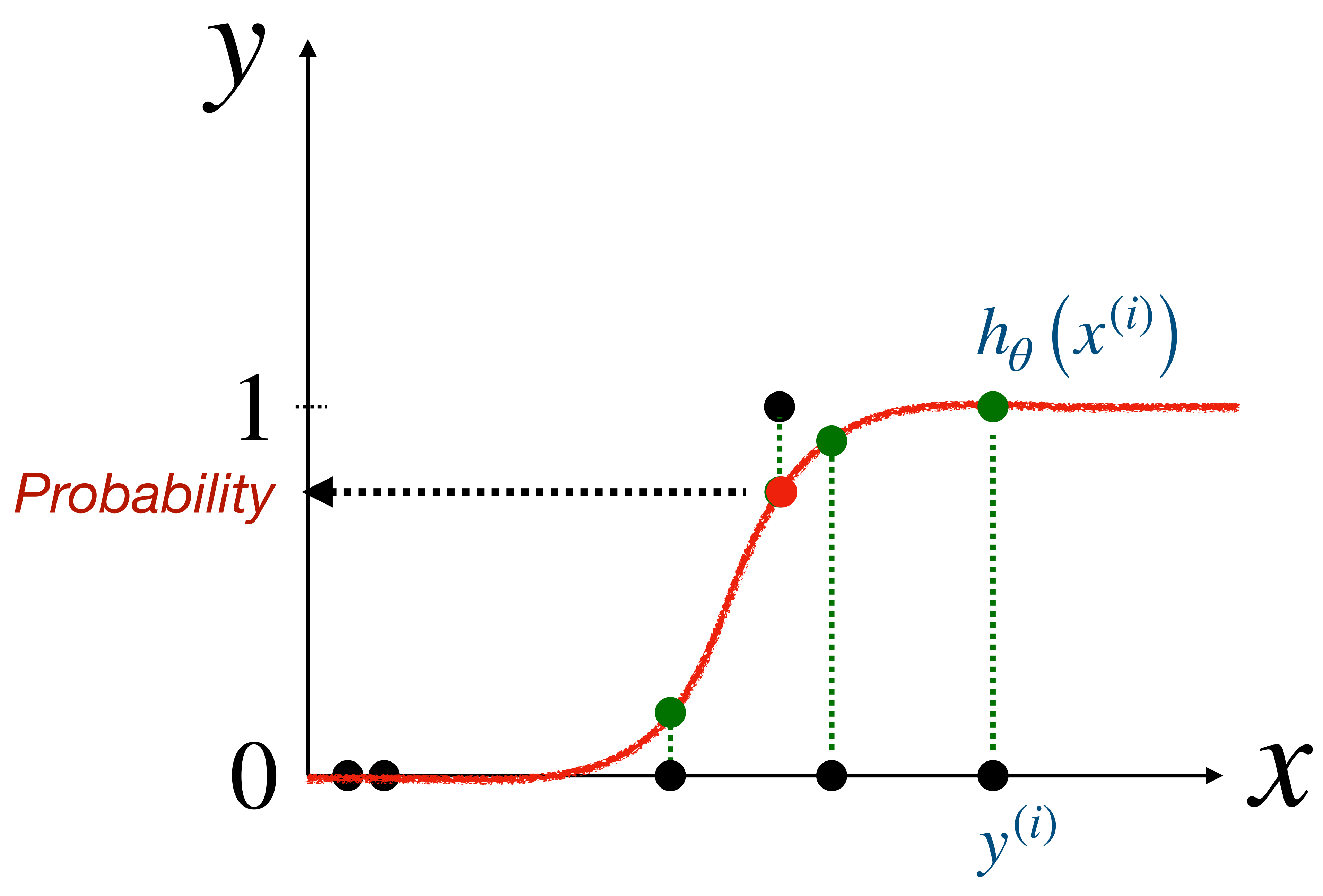
Maximize $\mathcal{L}(\theta)$ $\longrightarrow$ **Minimize** $\frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - \theta^\top x^{(i)}\right)^2$

What if the noise is not Gaussian?

Why not Least Squares?

$$y = h_\theta(x)$$

$$h_\theta(x) = \frac{1}{1 + e^{-\left(\theta^\top x\right)}} = g\left(\theta^\top x\right)$$



Probability of output given input

$$P\left(y = 1 \,\middle|\, x; \theta\right) = h_\theta(x)$$

$$P\left(y = 0 \,\middle|\, x; \theta\right) = 1 - h_\theta(x)$$

→

True label

$$p(y \,|\, x; \theta) = \left(h_\theta(x)\right)^{y} \left(1 - h_\theta(x)\right)^{1-y}$$

Likelihood!

For Bernoulli Distributed Noise

Bernoulli Distribution

Properties [edit]

If X is a random variable with a Bernoulli distribution, then:

$$\Pr(X=1) = p = 1 - \Pr(X=0) = 1 - q.$$

The probability mass function f of this distribution, over possible outcomes *k*, is

$$f(k;p) = \begin{cases} p & \text{if } k=1, \\ q = 1-p & \text{if } k=0. \end{cases}$$ [3]

This can also be expressed as

$$f(k;p) = p^k (1-p)^{1-k} \quad \text{for } k \in \{0,1\}$$

or as

$$f(k;p) = pk + (1-p)(1-k) \quad \text{for } k \in \{0,1\}.$$

The Bernoulli distribution is a special case of the binomial distribution with $n = 1$.[4]

Define Log-likelihood

Likelihood

$$p(y \mid x; \theta) = \left(h_\theta(x)\right)^{y} \left(1 - h_\theta(x)\right)^{1-y}$$

for all (x, y) pair

$$L(\theta) = \prod_{i=1}^{n} p\left(y^{(i)} \mid x^{(i)}; \theta\right)$$

$$= \prod_{i=1}^{n} h_\theta\left(x^{(i)}\right)^{y^{(i)}} \left(1 - h_\theta(x^{(i)})\right)^{1-y^{(i)}}$$

log

$$\mathscr{L}(\theta) = \sum_{i=1}^{n} y^{(i)} \log h_\theta\left(x^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_\theta\left(x^{(i)}\right)\right)$$

Maximize Log-likelihood

$$\mathscr{L}(\theta) = \sum_{i=1}^{n} y^{(i)} \log h_\theta\left(x^{(i)}\right) + \left(1 - y^{(i)}\right) \log\left(1 - h_\theta\left(x^{(i)}\right)\right)$$

Update rule

while not converged:

$$\theta := \theta + \alpha \nabla_\theta \mathscr{L}(\theta)$$

→ **Derive**

Gradient Descent

for t = 1…T:

$$\theta := \theta - \alpha \sum_{i=1}^{n} \left(h_\theta\left(x^{(i)}\right) - y^{(i)}\right) x^{(i)}$$

Same as linear regression

Generalized Linear Models

Gaussian Distribution → Linear Regression

Bernoulli Distribution → Logistic Regression

Update rule

$$\theta := \theta - \alpha \sum_{i=1}^{n} \left(h_\theta \left(x^{(i)} \right) - y^{(i)} \right) x^{(i)}$$

Exponential Family

Family of distributions for which we can derive the same update rule

Assumption: $p(y \mid x; \theta)$ is an exponential family

$$p(y; \eta) = b(y) \exp\left\{\eta^\top y - a(\eta)\right\}$$

Data ← y

Parameters ← η

- $b(y)$ is called the base measure (not depend on η)
- $a(\eta)$ is called the log partition function (not depend on y)
- $a(\eta)$, y and $b(y)$ are scalar. η and y have the same dimensions.

Example 1: Bernoulli Distribution -> Logistic Regression

$$p(y; \eta) = b(y) \exp\left\{\eta^\top y - a(\eta)\right\}$$

- y → **Data**
- η → **Natural Parameters**

Bernoulli Distribution

$$p(y; \phi) = \phi^y (1-\phi)^{1-y} = \exp\left\{ y \log \frac{\phi}{1-\phi} + \log(1-\phi) \right\}$$

- $\log \frac{\phi}{1-\phi}$ → η
- $\log(1-\phi)$ → $a(\eta)$

Show that term is only a function of η

Example 2: Gaussian Distribution -> Linear Regression

Data

$$p(y;\eta) = b(y)\,\exp\{\eta^\top y - a(\eta)\}$$

Natural Parameters

Gaussian Distribution

$$p(y;\mu) = \frac{1}{\sqrt{2\pi}}\exp\left\{-\frac{1}{2}(y-\mu)^2\right\} = \frac{1}{\sqrt{2\pi}}e^{-y^2/2}\left\{\mu y - \frac{1}{2}\mu^2\right\}$$

$b(y)$ η $a(\eta)$

Why do we care?

Data

$$p(y;\eta) = b(y)\exp\left\{\eta^\top y - a(\eta)\right\}$$

Natural Parameters

$\theta^\top x$

Inference is Easy:

$$E[y;\eta] = \frac{da(\eta)}{d\eta} \qquad Var[y;\eta] = \frac{d^2a(\eta)}{d\eta^2}$$

Learning is Easy: **Maximum Likelihood Estimation** leads to **convex** problem in η

Generalized Linear Models

Assumption: $p(y \mid x; \theta)$ is an exponential family

Data Type → Probability Distribution

Binary → Bernoulli ⟶ **Logistic Regression**

Real → Gaussian ⟶ **Linear Regression**

Counts → Poisson

Positive Real → Gamma, Exponential

Distributions → Dirichlet

Generalized Linear Models

Assumption: $p(y \mid x; \theta)$ is an exponential family

The natural parameter is linear in the inputs

$$\eta = \theta^\top x$$

Predictor is a natural consequence

$$h_\theta(x) = E[y \mid x; \theta]$$

Generalized Linear Models

Assumption: $p(y \mid x; \theta)$ is an exponential family

Data Input: x → Linear Model: $\theta^\top x$ $\xrightarrow{\eta}$ Exponential Model: η, $a(\eta)$, $b(y)$, $\vdots$

Learning

$$\max_{\theta} \log(p(y \mid x; \theta))$$

Inference

$$E[y \mid x; \theta]$$

Update Rule:

$$\theta := \theta - \alpha \sum_{i=1}^{n} \left(h_\theta\left(x^{(i)}\right) - y^{(i)} \right) x^{(i)}$$

Terminology

Model parameter → Natural parameter → Canonical parameter

$\theta \xrightarrow{\theta^\top x} \eta \xrightarrow{g} \phi$ (Bernoulli)

g: *Canonical response*

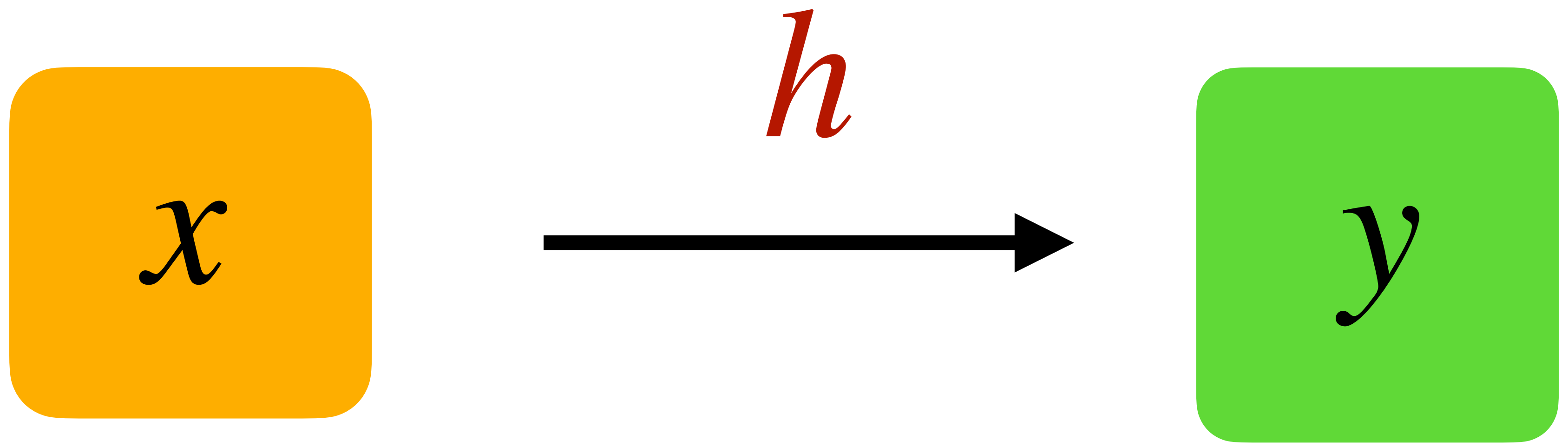
$h_\theta(x)$

Logistic Regression:

$$h_\theta(x) = E[y \mid x; \theta]$$

$$\phi = \frac{1}{1 + e^{-\eta}} = \frac{1}{1 + e^{-\theta^\top x}}$$

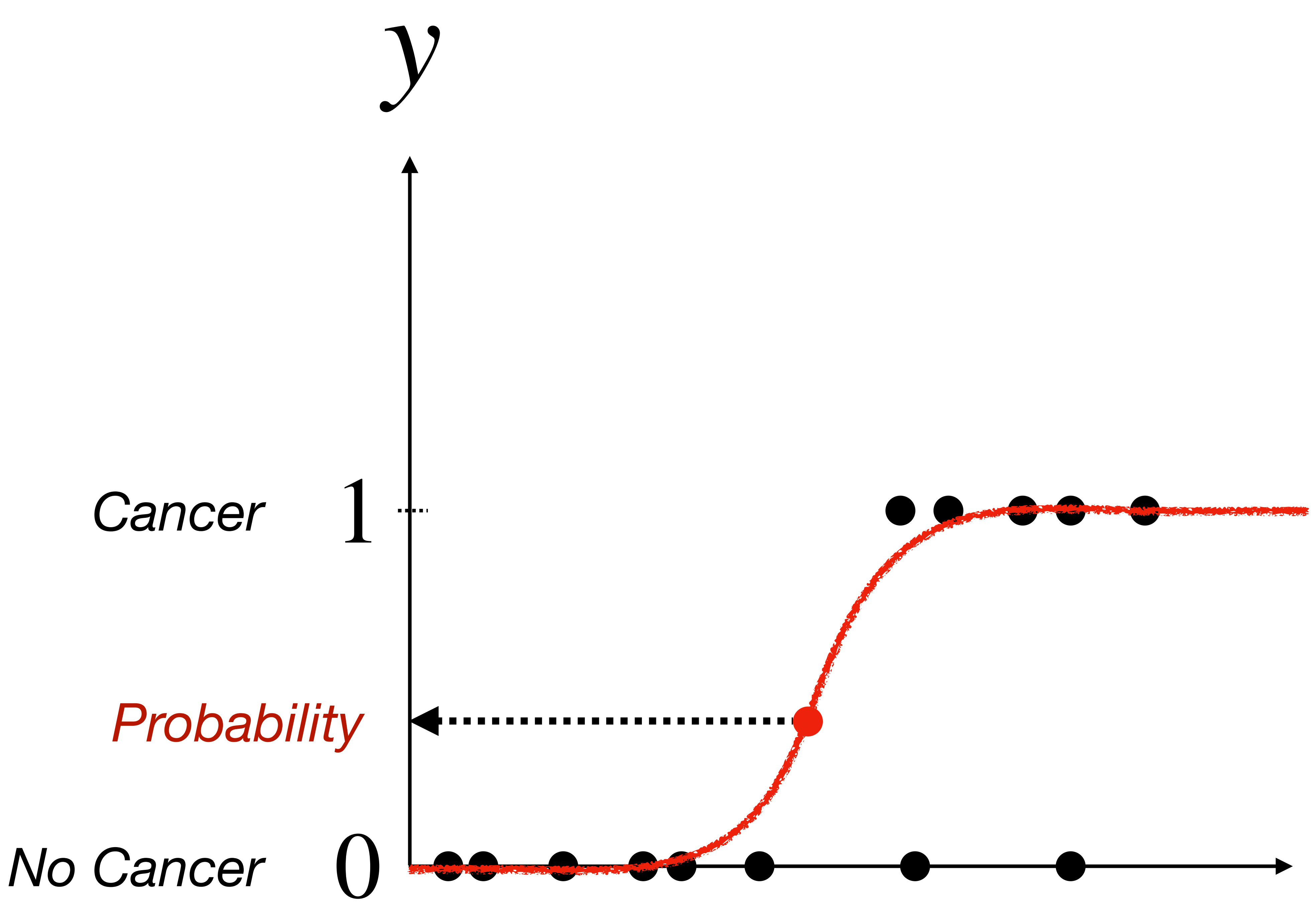
Back to classification



$$y = h_\theta(x)$$

$$y \in [0,1]$$

What if we have more outputs?



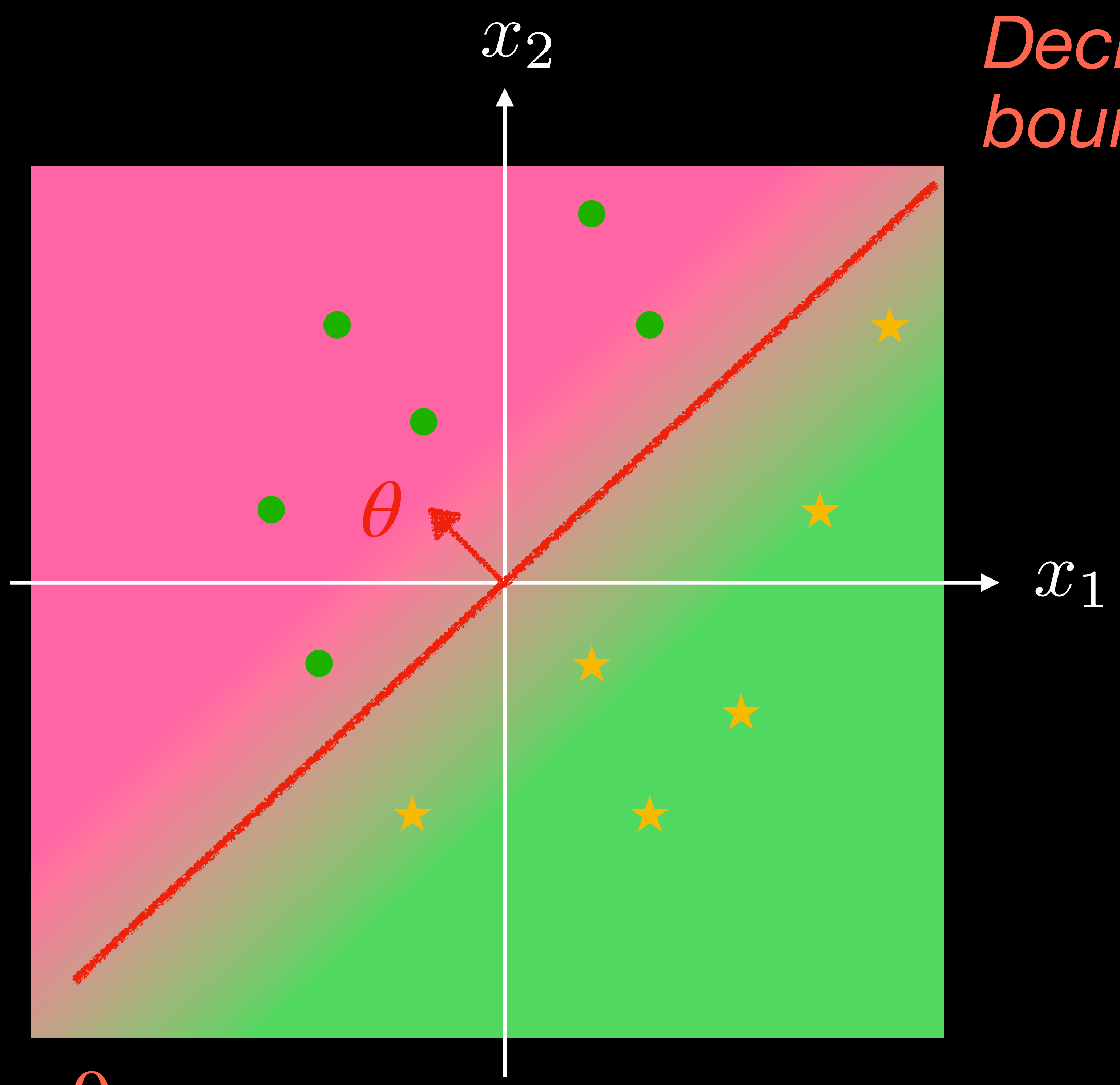
Classification

$x = [x_1, x_2]$

x_1	x_2	y
-2	-1	●
3	1	★
2	3	●
1	-1	★
	⋮	

★ 1

● 0



Decision boundary

$\theta^\top x = 0$

Logistic Regression

$h_\theta(x) = \sigma(\theta^\top x)$

how confident?

score

$\theta^\top x$

how correct?

margin

$(\theta^\top x)y$

For $y \in [1, -1]$

Multiclass classification - Softmax

$$\mathbf{y} = h_\theta(\mathbf{x})$$

$$\mathbf{x} \longrightarrow \mathbf{y}$$

k discrete values for representing output

One-hot encoding

$$\begin{bmatrix}1\\0\\0\\0\end{bmatrix} \quad \begin{bmatrix}0\\1\\0\\0\end{bmatrix} \quad \begin{bmatrix}0\\0\\1\\0\end{bmatrix} \quad \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

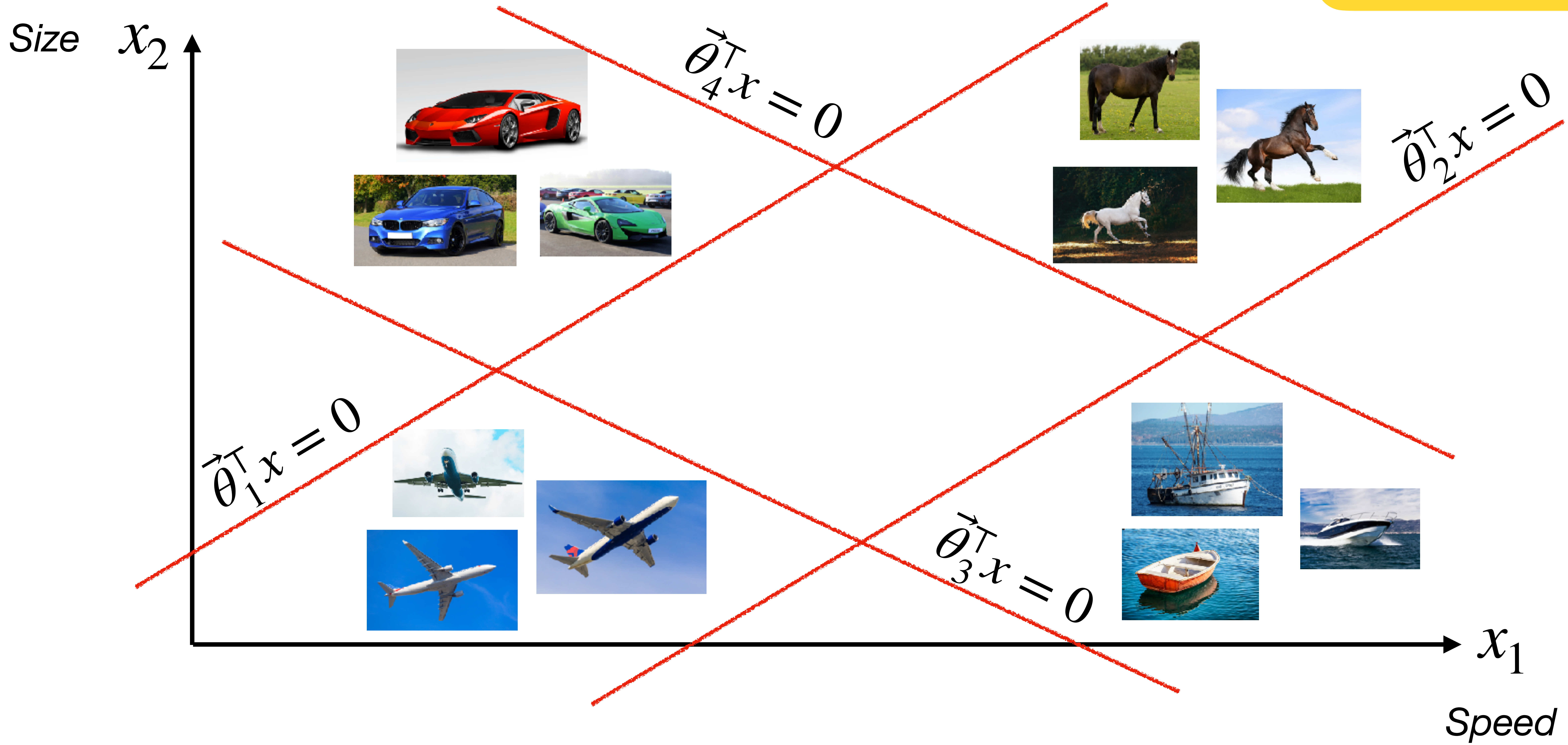
car plane boat horse

Multi-class classification - Softmax

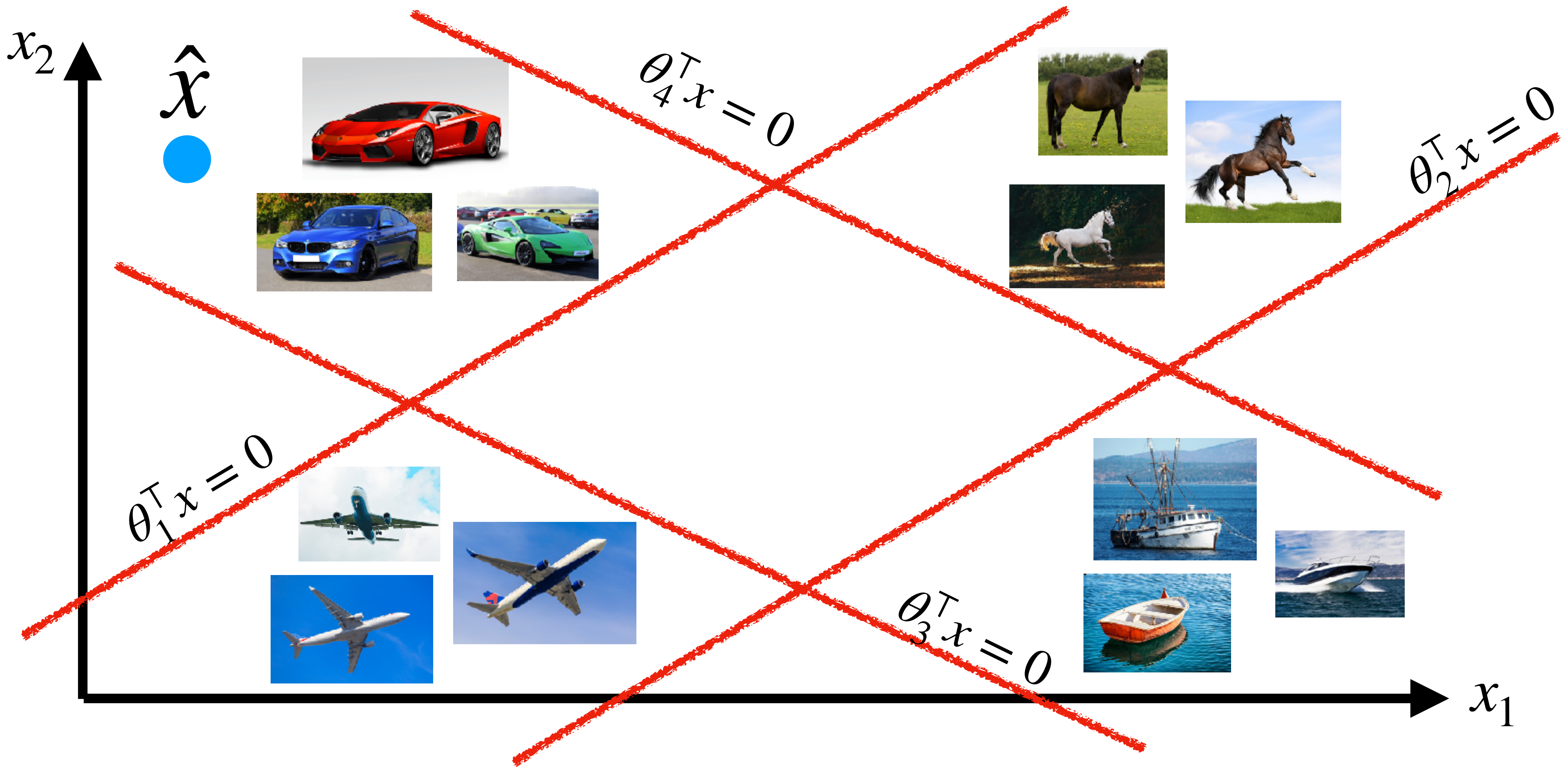
WARNING!!!

Notation Alert

$\vec{\theta}_i$ is a vector



How to turn scores into probabilities?



WARNING!!!

Notation Alert

$\vec{\theta}_i$ **is a vector**

Score

$\vec{\theta}_1^\top \hat{x} = 3$

$\vec{\theta}_2^\top \hat{x} = -0.3$

$\vec{\theta}_3^\top \hat{x} = -0.8$

$\vec{\theta}_4^\top \hat{x} = -22$

exp →

Positive Measure

$\exp(3) = 20.1$

$\exp(-0.3) = 0.75$

$\exp(-0.8) = 0.2$

$\exp(-22) = 0.00..1$

Normalize →

Softmax

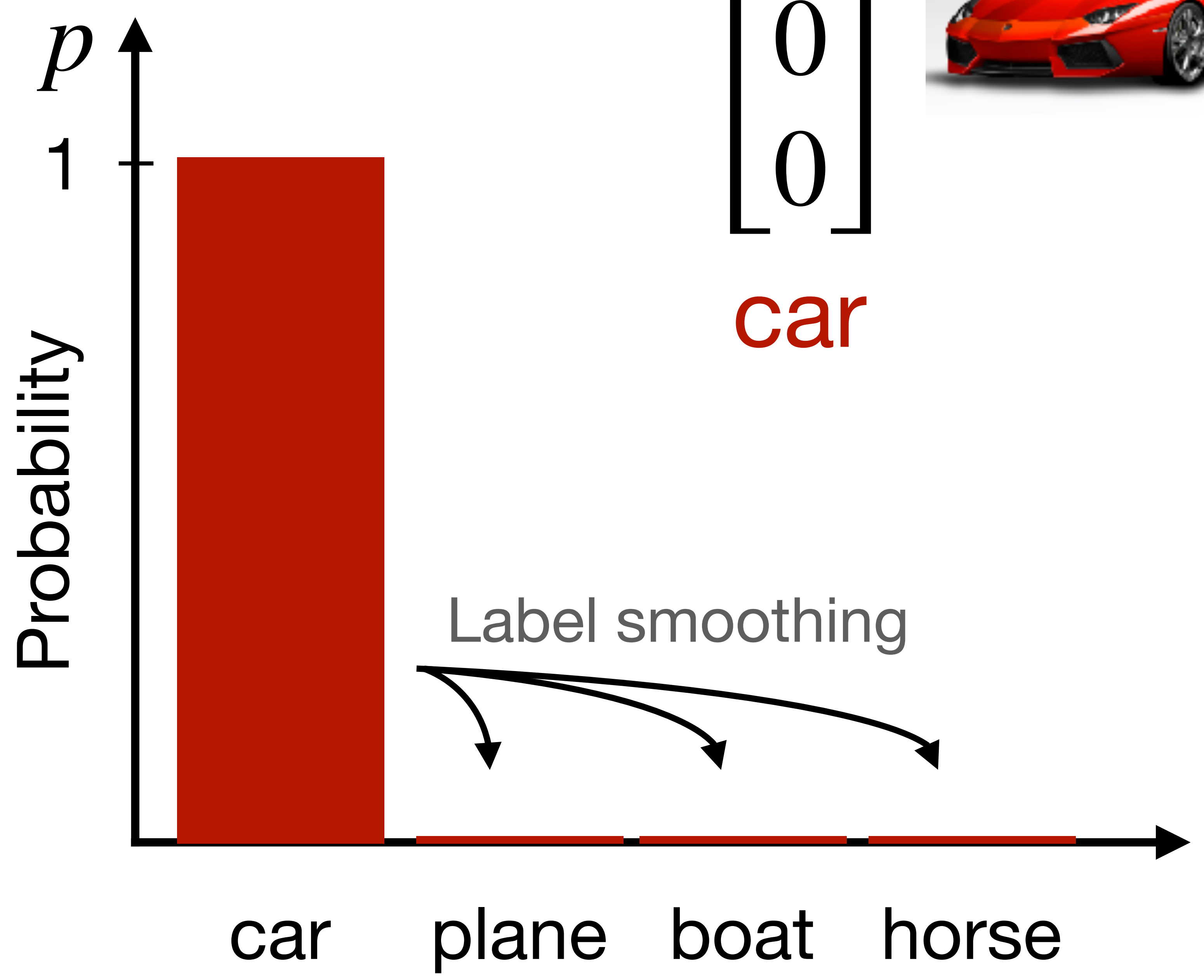
$$\hat{p}(y = i \mid x; \theta) = \frac{\exp\left(\vec{\theta}_i^\top x\right)}{\sum_{j=1}^{k} \exp\left(\vec{\theta}_j^\top x\right)}$$

How do you train?

Given Label

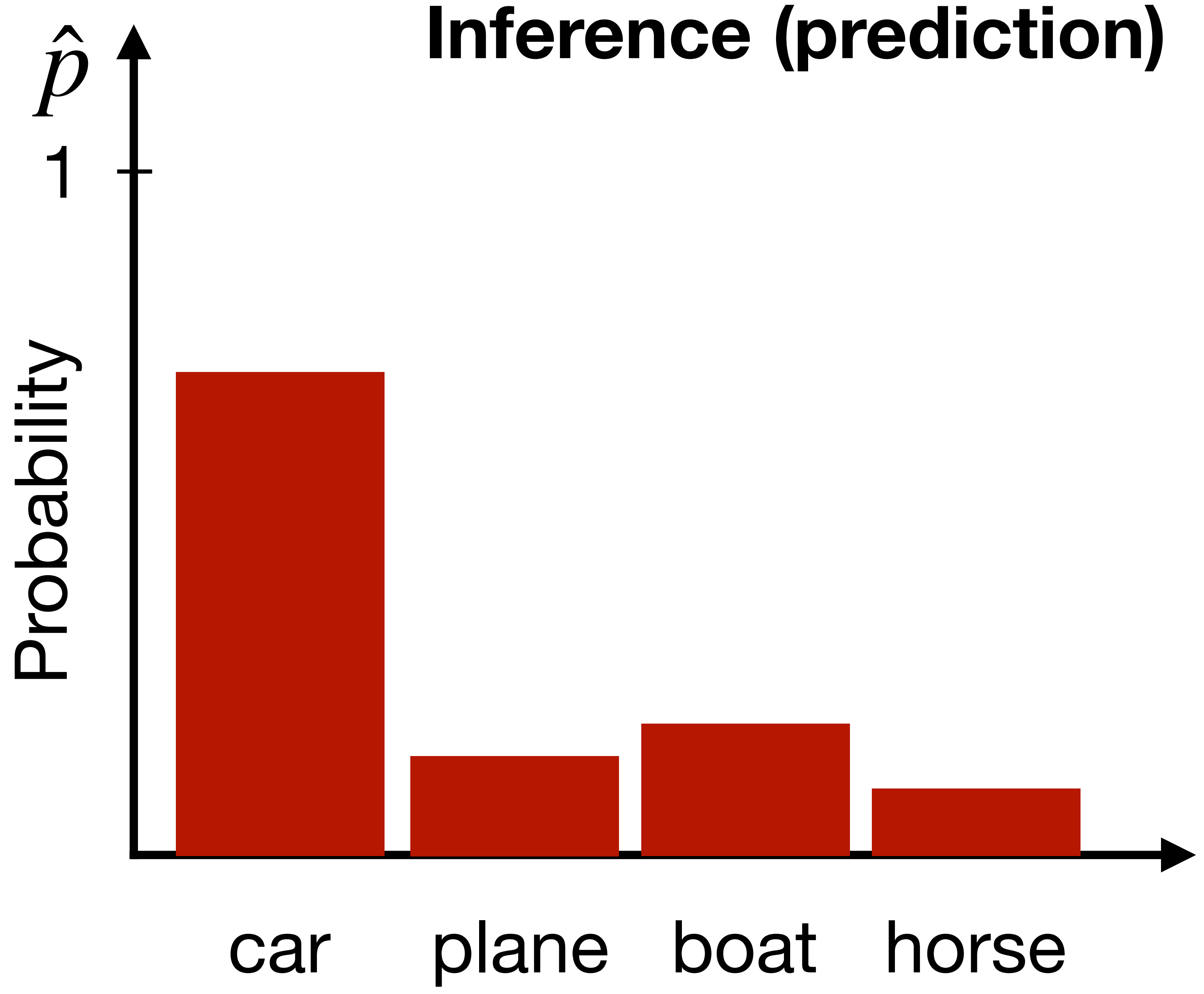
$$\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$$

car



x

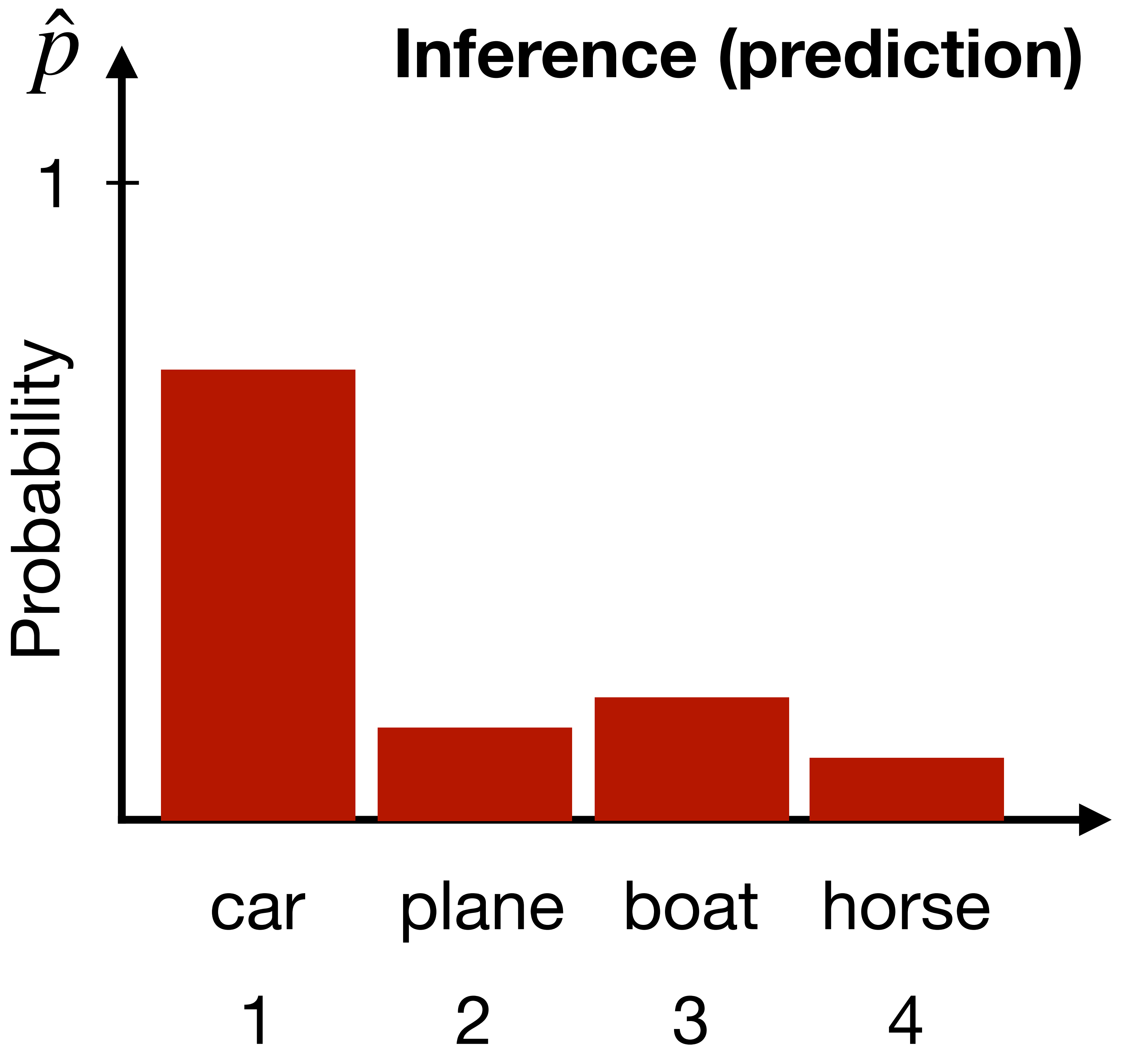
Inference (prediction)



$$\textbf{min} \quad \text{CrossEntropy}(p, \hat{p}) = -\sum_{i=1}^{k} p(y=i)\, \log\left(\hat{p}(y=i)\right)$$

$$= -\log\left(\hat{p}(y=1)\right)$$

How do you train?



$$\text{CrossEntropy}(p, \hat{p}) = -\sum_{i=1}^{k} p(y=i) \log\left(\hat{p}(y=i)\right)$$

Ground Truth

$$\textit{Logit} \quad = -\log\left(\hat{p}(y=1)\right)$$

$$= -\log\left(\frac{\exp\left(\vec{\theta}_i^\top x\right)}{\sum_{j=1}^{k} \exp\left(\vec{\theta}_j^\top x\right)}\right)$$

Train with Gradient Descent!