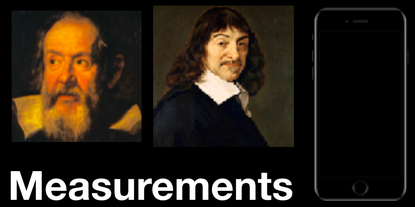
# Generalization

**Prepared by: Joseph Bakarji**

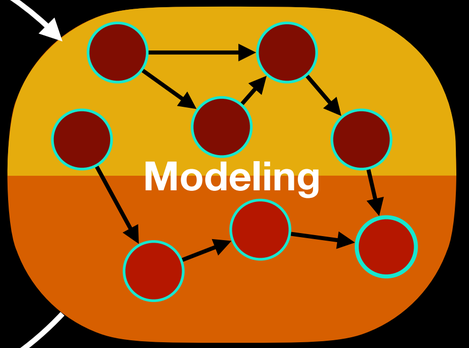
Compression



Measurements

Learning

Data



Modeling

Seen

Unseen

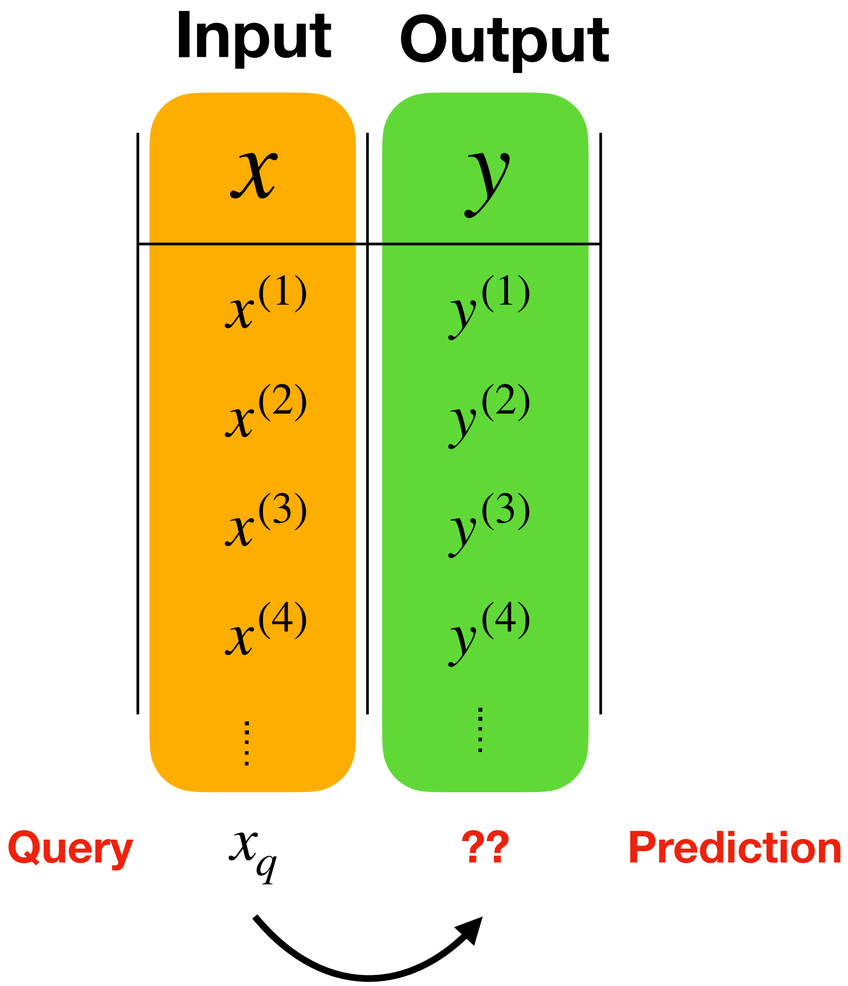
Inference

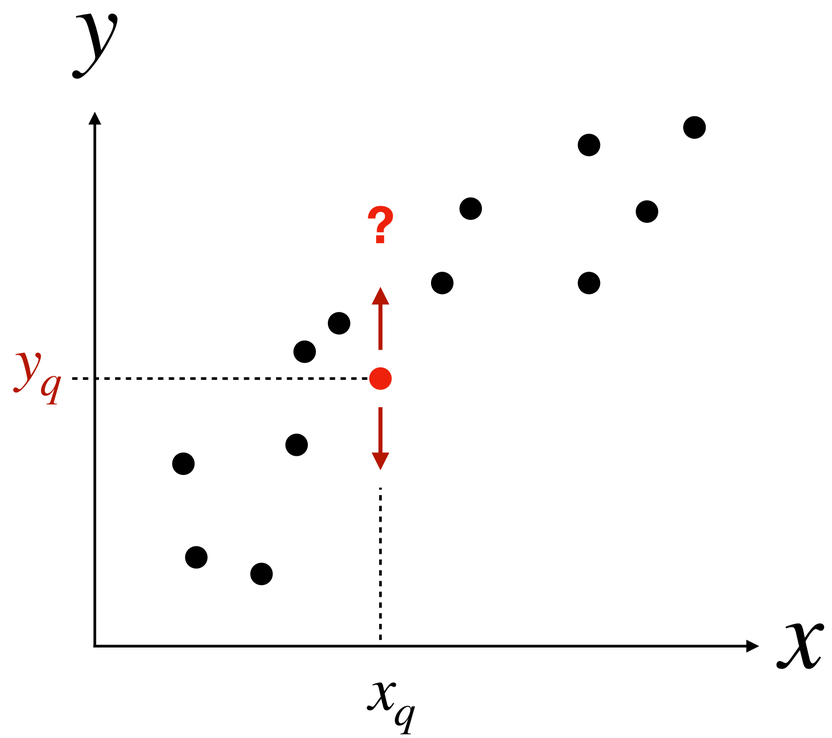
Projection

World

Reconstruction

# Given new input, what's the output?



# Linear Regression

**1. Assume a linear hypothesis**

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

**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**

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

**5. Predict unseen data**

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

**4. Optimal predictor**

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

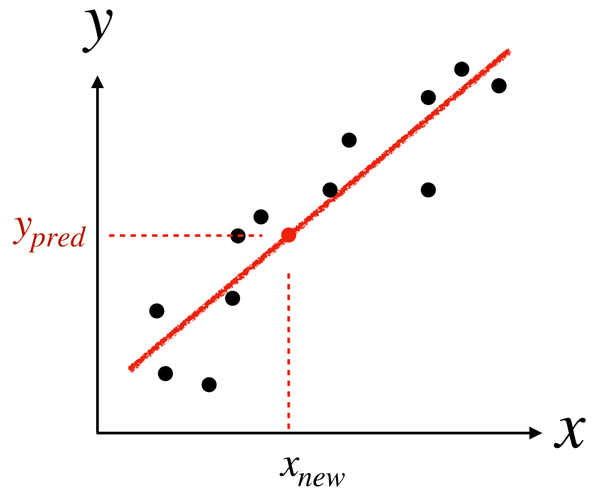
$\hat{\theta}$

**SGD**

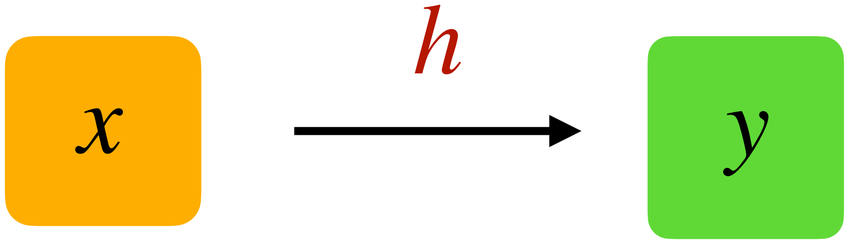
**for** t = 1...T:

  **for** $i$ = 1...n:

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

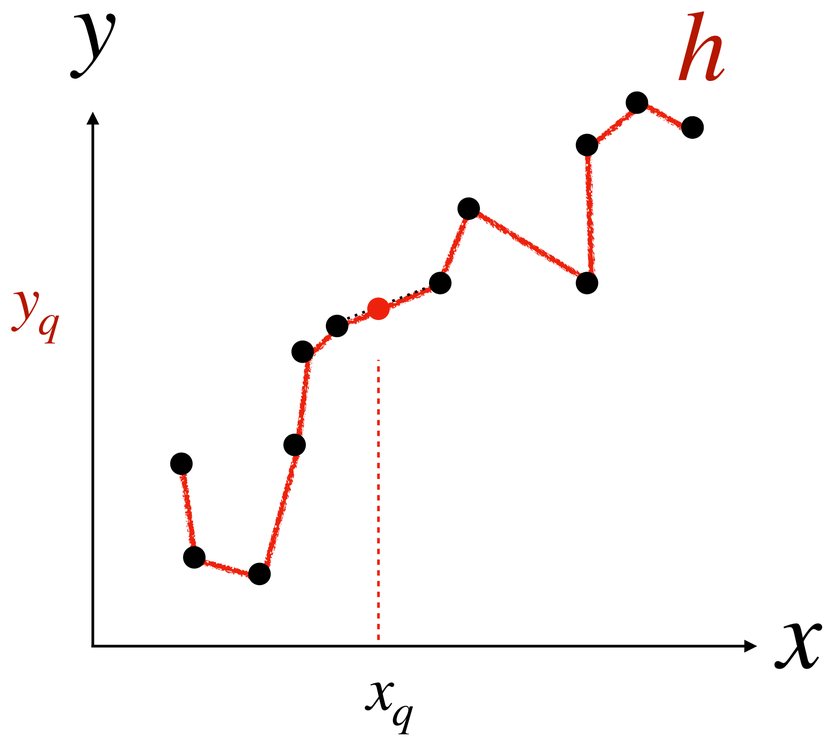


# Given new input, what's the output?

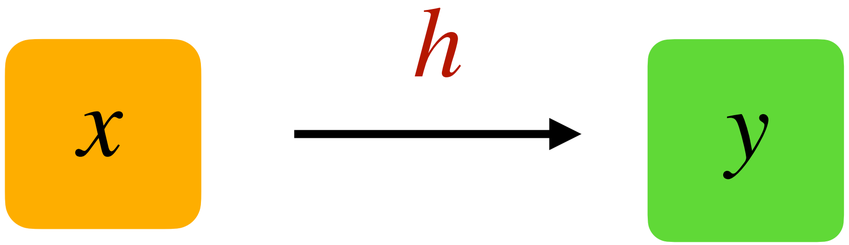



Given the data,
find a **function** $h$, also called a **hypothesis,**
that predicts an output, given an input

*Linear Interpolation*

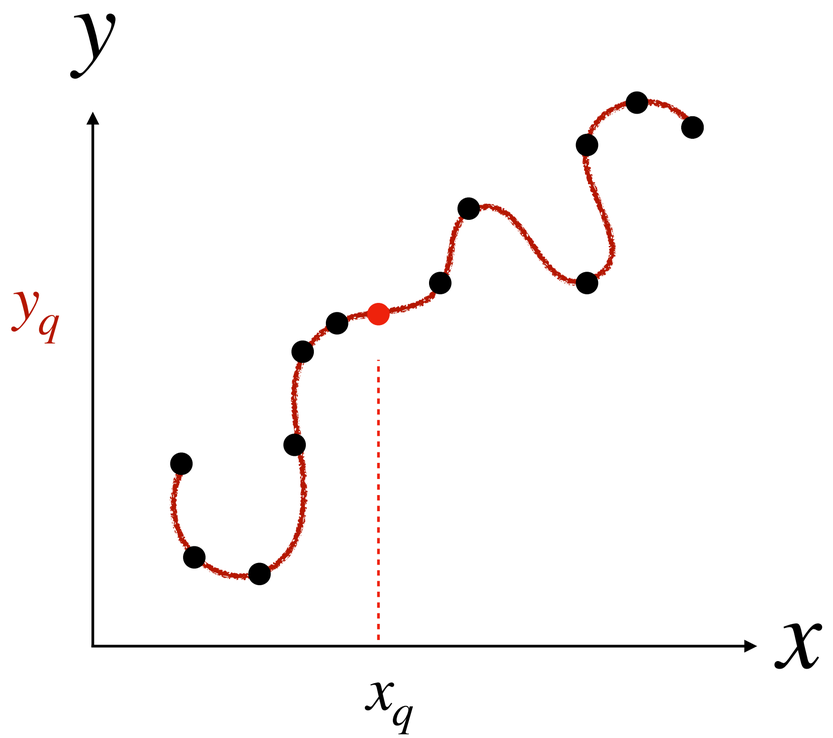


# Given new input, what's the output?

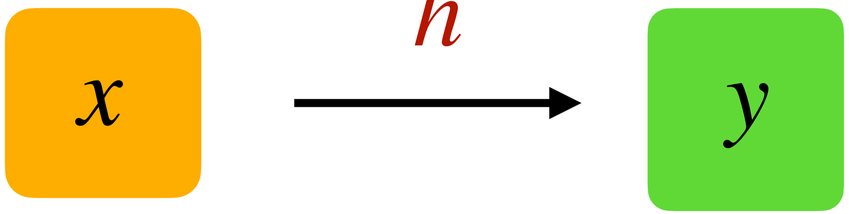



Given the data,
find a **function** $h$, also called a **hypothesis,**
that predicts an output, given an input

*Polynomial Interpolation*

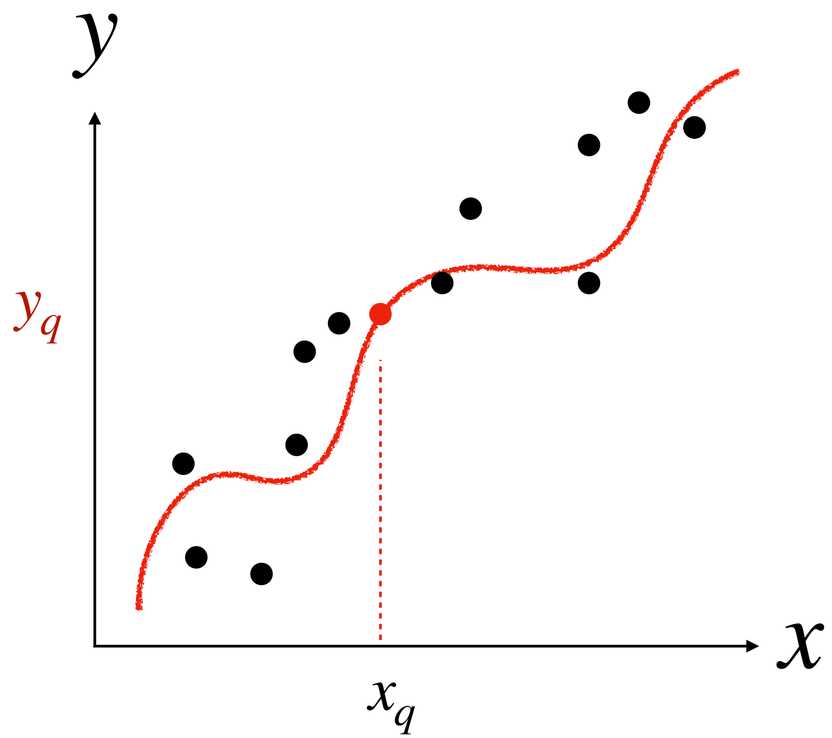


# Given new input, what's the output?

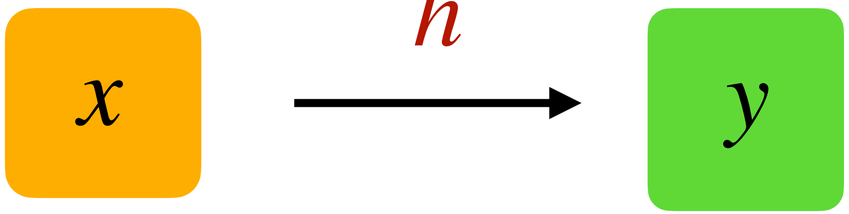



Given the data,
find a **function** $h$, also called a **hypothesis,**
that predicts an output, given an input

*Some other function?*



# How do you choose the hypothesis?

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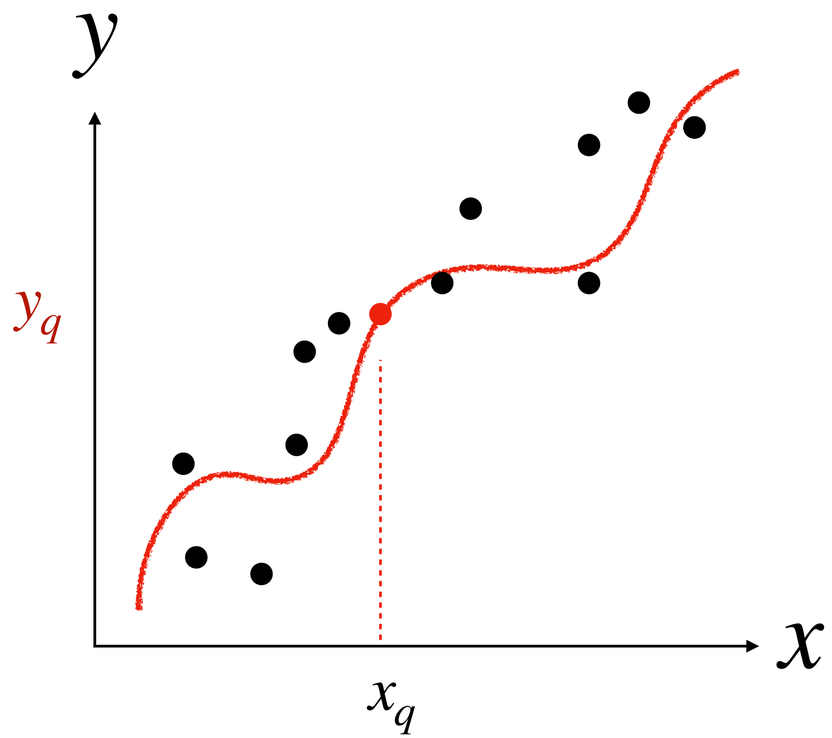
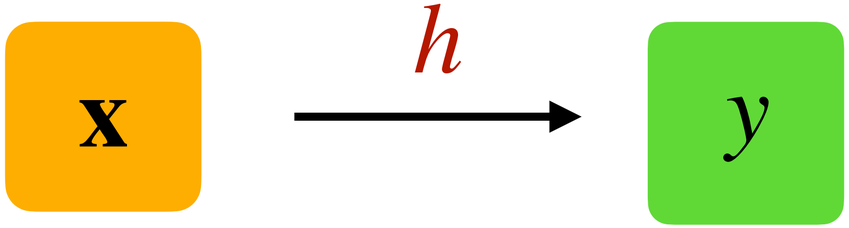
*Some other function?*



# What happens if we have more inputs?

**Assume a linear hypothesis**




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

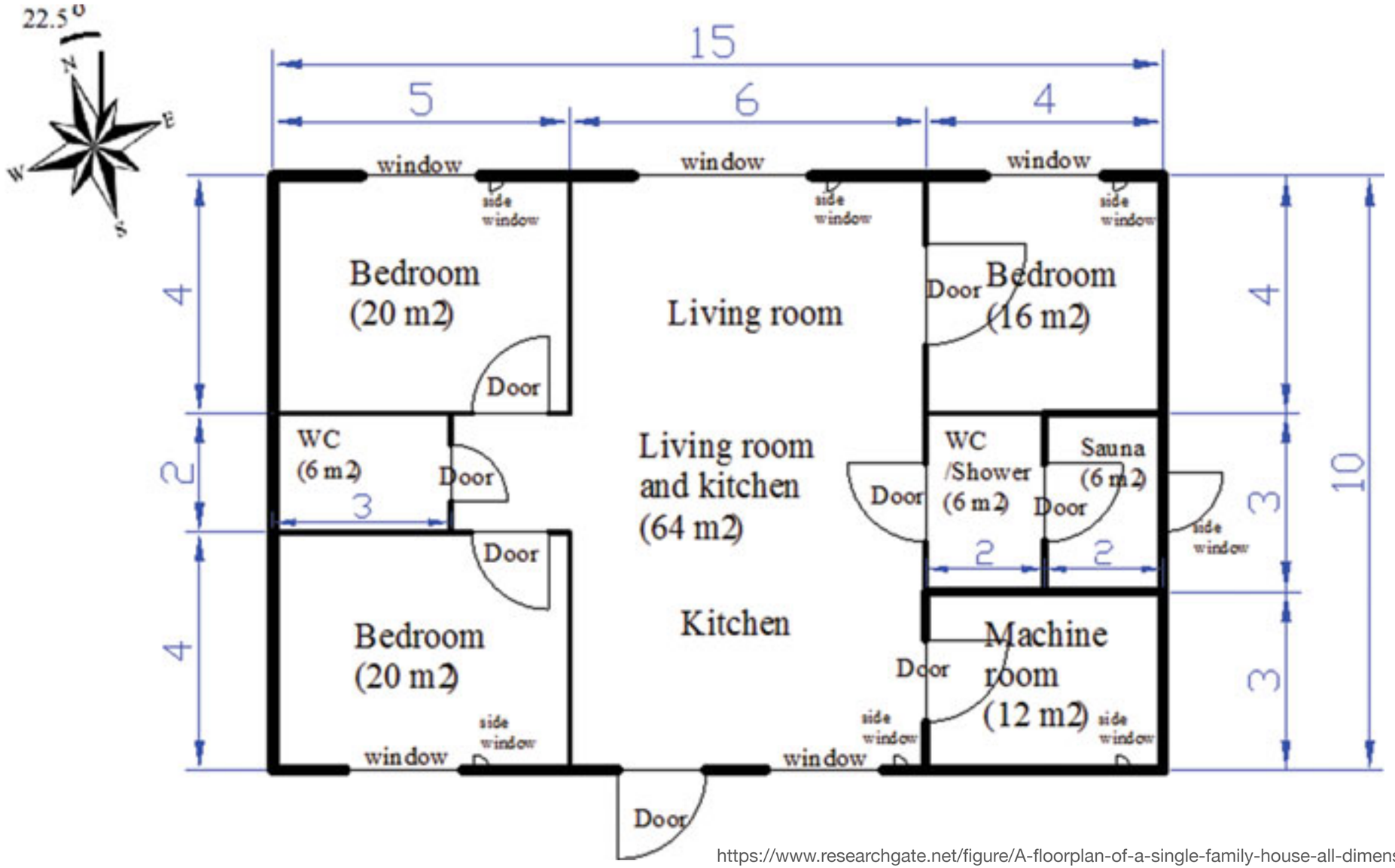
$$h_\theta(\mathbf{x}) = \underbrace{[\theta_0, \theta_1, \theta_2, \theta_3, \ldots]}_{\theta} \cdot \underbrace{[1, x_1, x_2, x_3, \ldots]}_{\mathbf{x}}$$

**weights** $\theta$ — $\mathbf{x}$ **inputs**

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

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

# You have the following map for each apartment. What is x?




https://www.researchgate.net/figure/A-floorplan-of-a-single-family-house-all-dimensions-in-meters_fig3_302981919

# 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

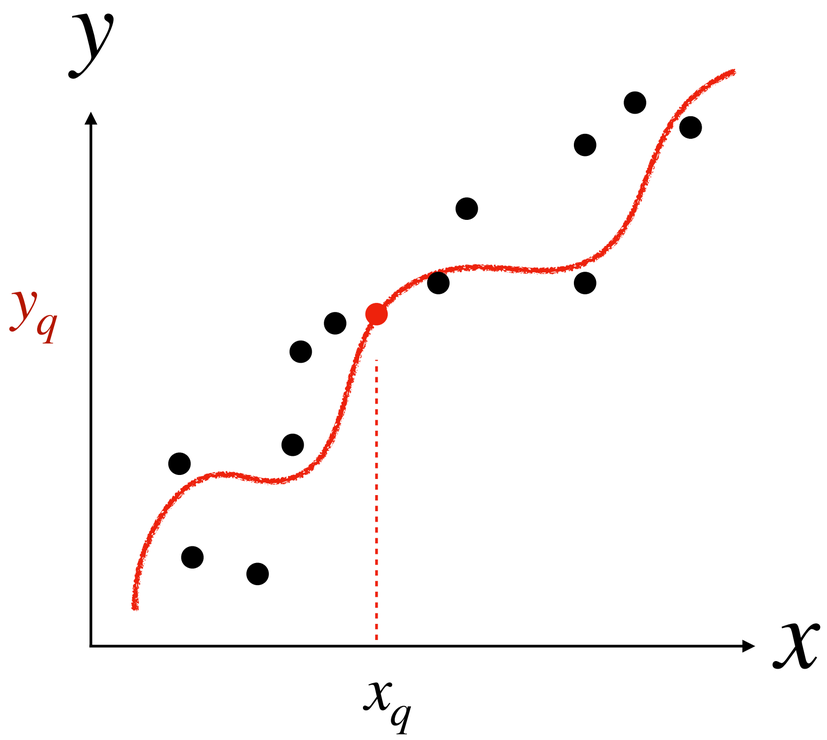
$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \ldots$$

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

*Feature map*

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

*Some other function?*



# Feature Engineering

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

| Input $x$ | Output $y$ |
|---|---|
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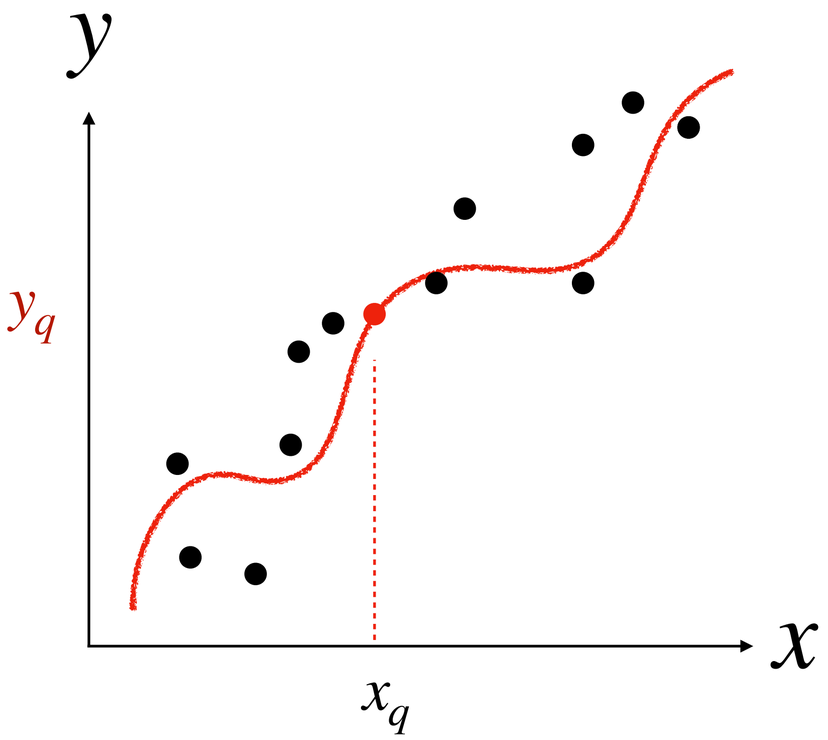
$$h_\theta(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \ldots$$

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

*Feature map*

*Some other function?*




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

# Feature Engineering

A feature map can also **drop features**

**Example:** construct a polynomial model

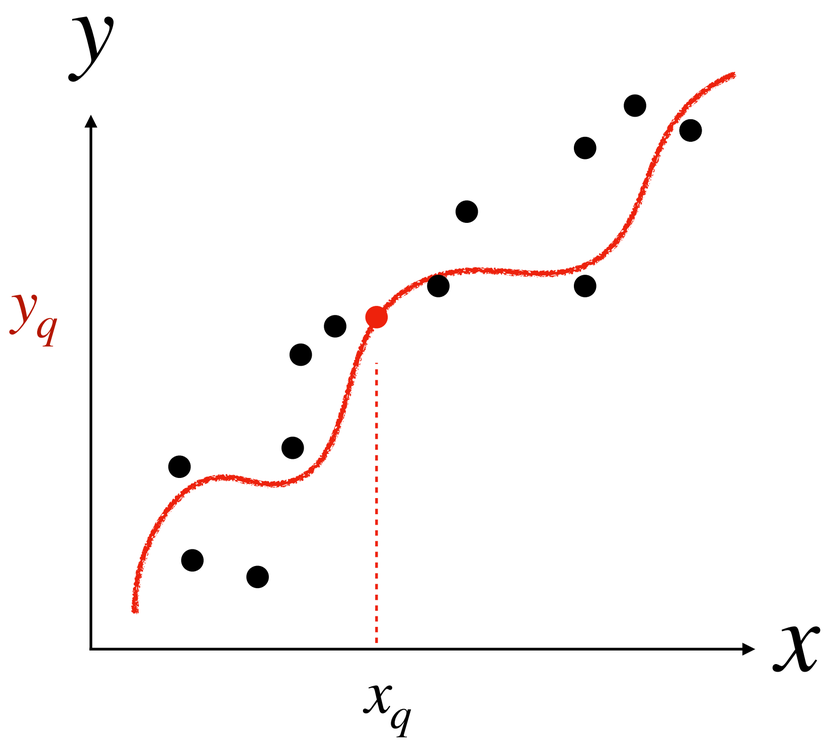
$$h_\theta(x) = \theta_1 x + \theta_3 x^3$$

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

$\phi(x)$ *Feature map*

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

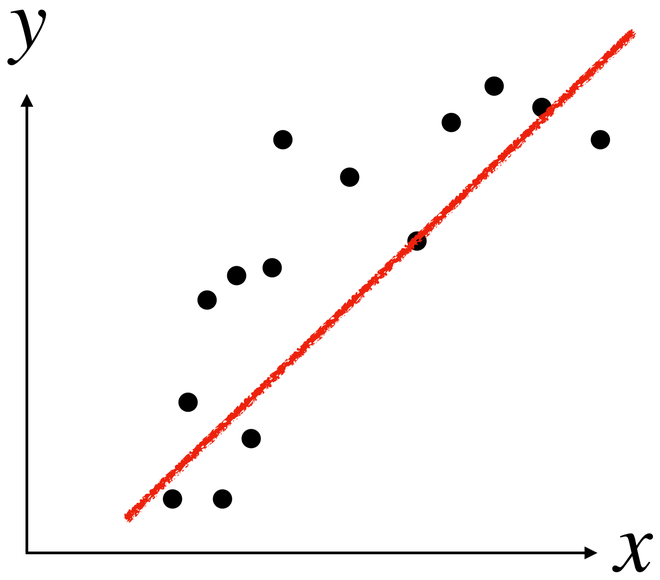
*Some other function?*



# How to choose $\phi(x)$?

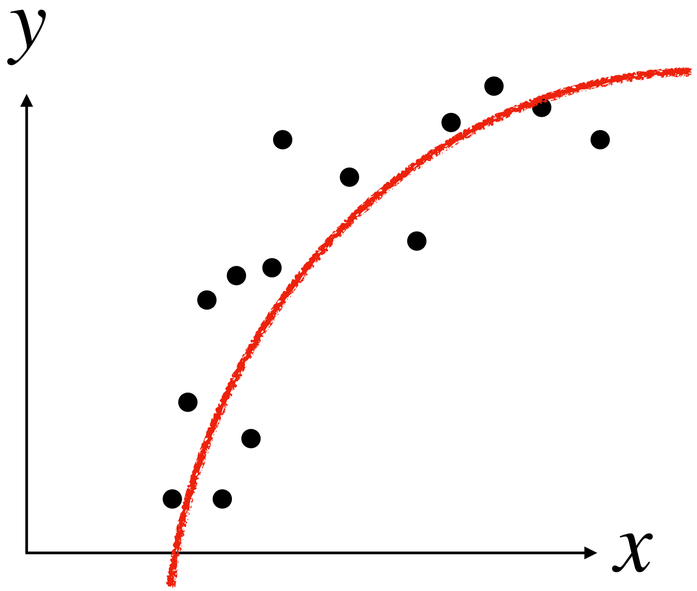
**How to optimize over $\phi(x)$**

**Underfitting**
**High Bias**



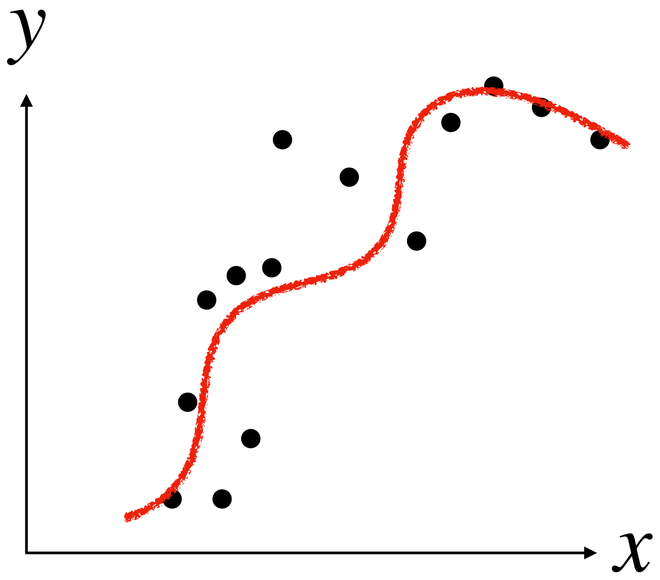

$\phi(x) = [1, x]$

**Just right**




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

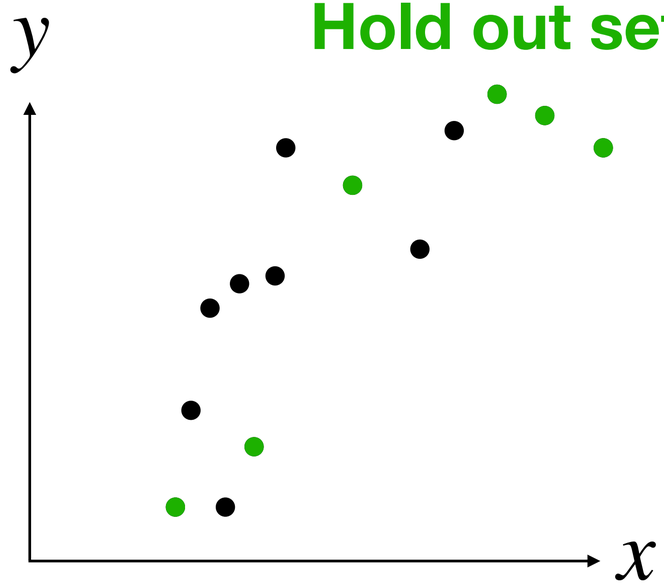
**Overfitting**
**High Variance**



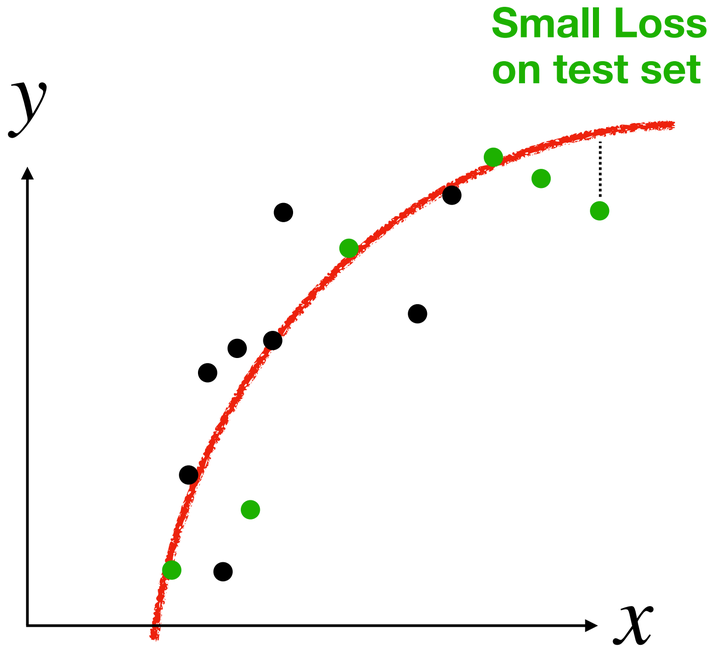

$\phi(x) = [1, x, x^2, x^3, \ldots]$

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

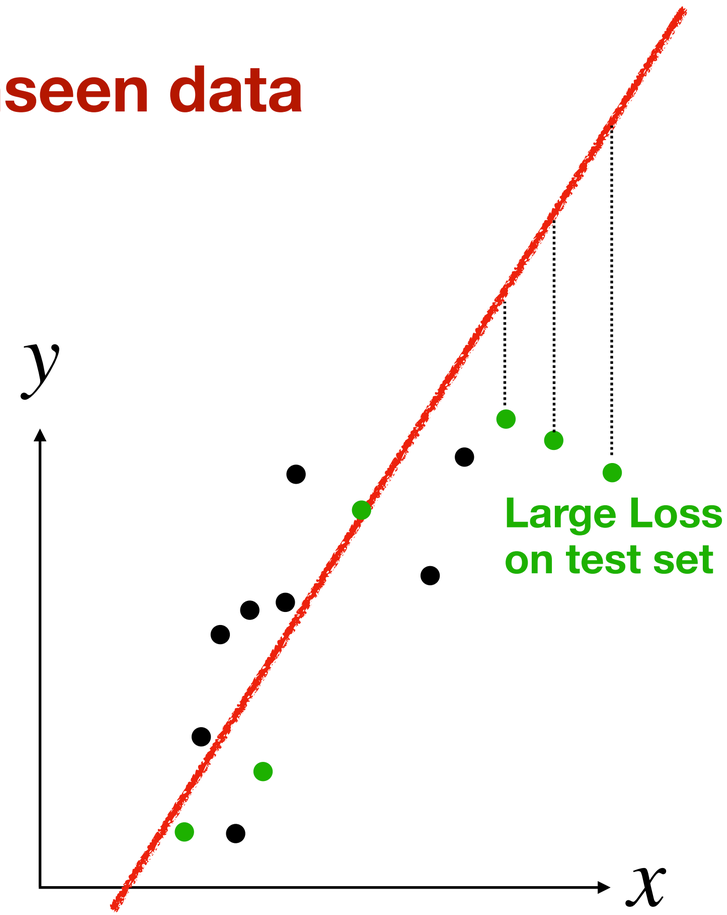
**The purpose of Machine Learning is to Generalize to unseen data**




**Create a test set to evaluate model**



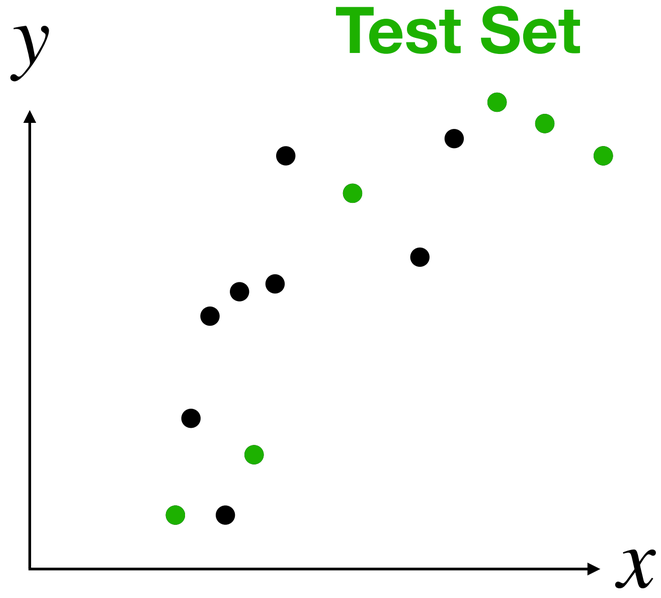

$$\phi(x) = [1, x, x^2]$$



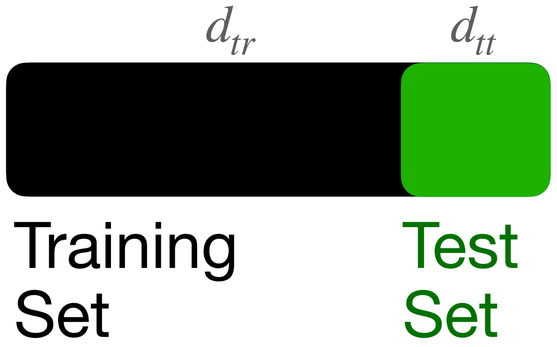

$$\phi(x) = [1, x]$$

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

**Define objective functions for each subset**




Split data:



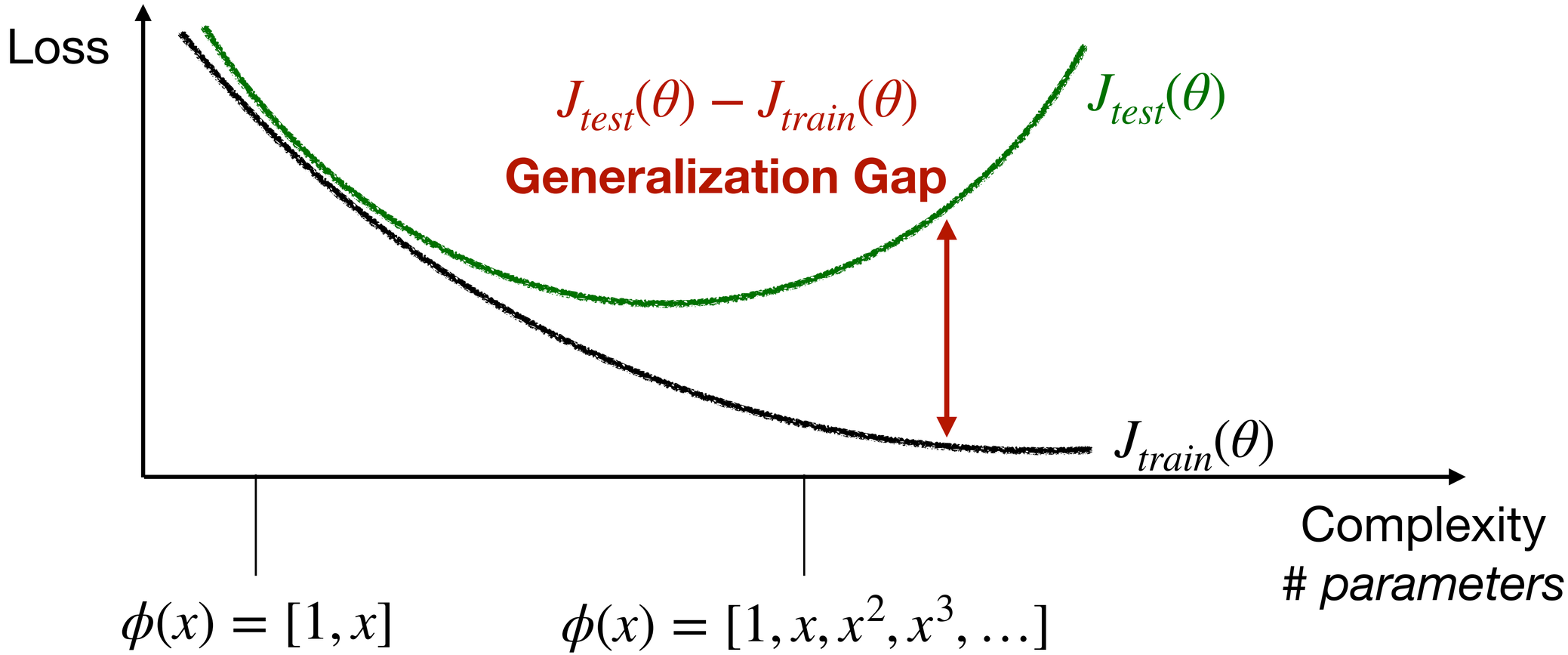

$$J_{train}(\theta) = \frac{1}{2d_{tr}} \sum_{i=1}^{d_{tr}} \left(\theta^\top \phi(x^{(i)}) - y^{(i)}\right)^2$$

**Create a Test set to evaluate model**

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

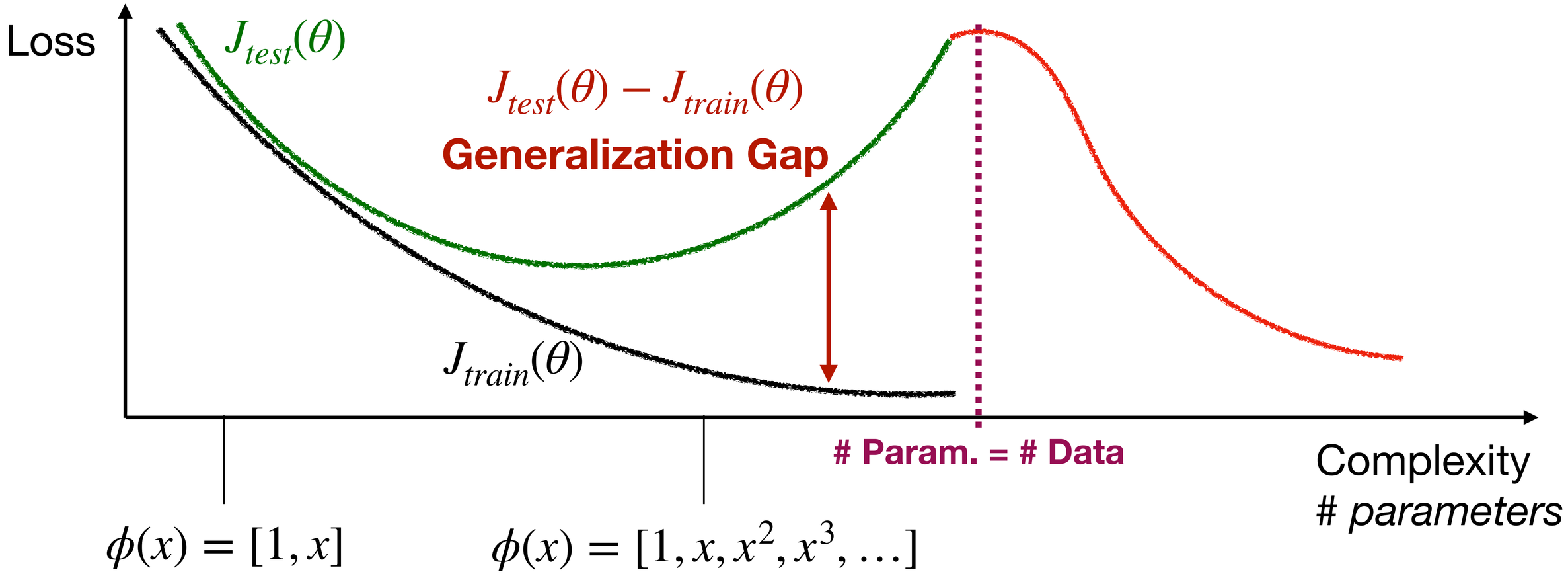
# Variance Bias Trade-off

## Error as a function of complexity



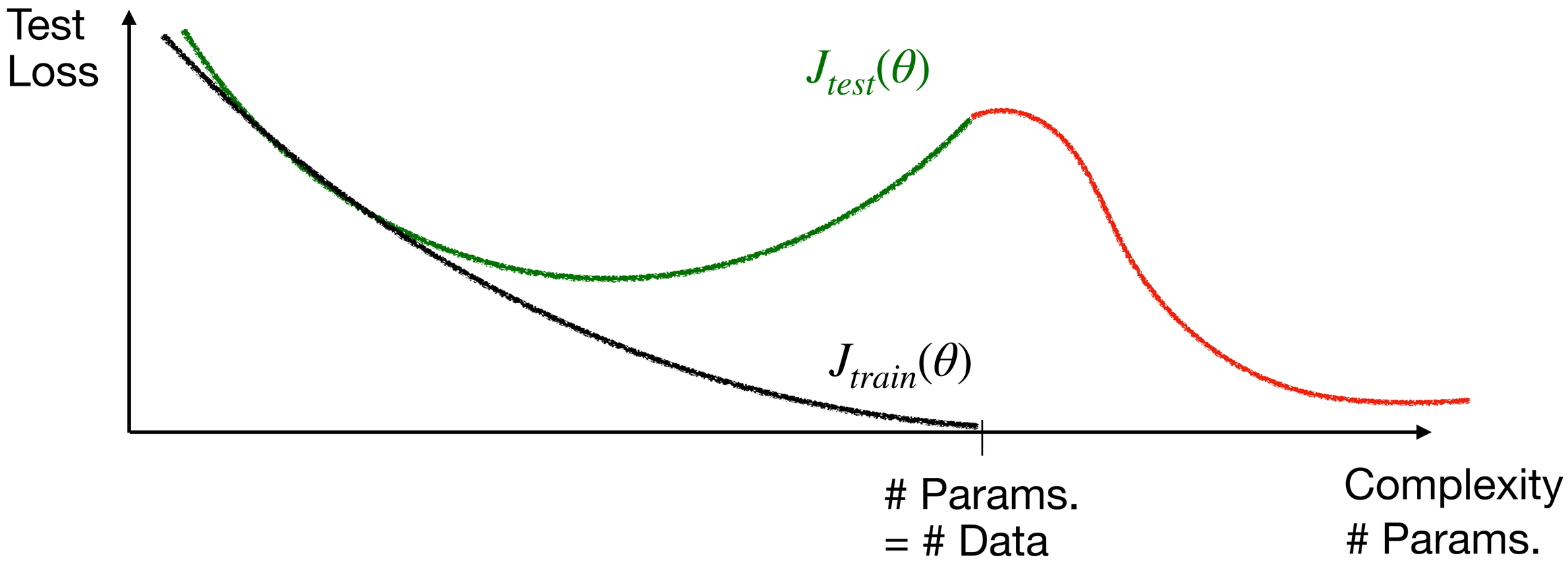
# Variance Bias Trade-off

## Error as a function of complexity



# Double Descent

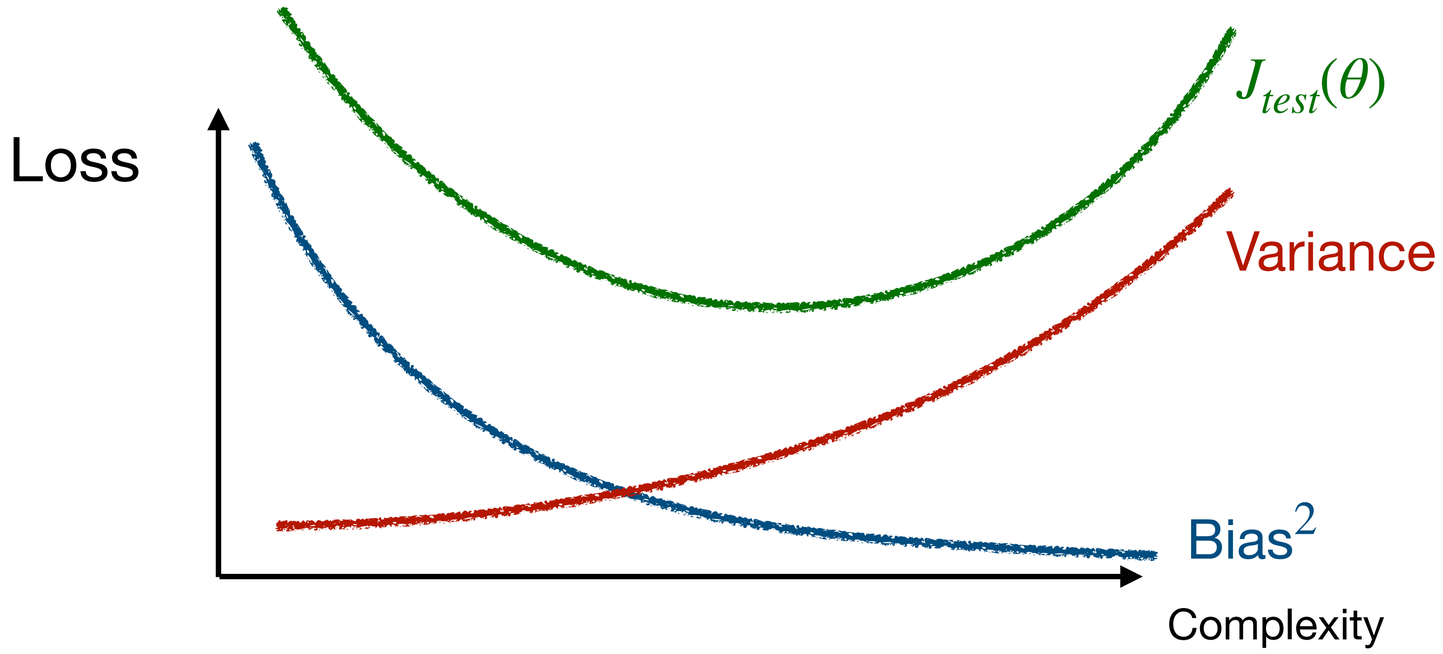
## Model-wise



# Decomposition of Test Error

- Test error can be written as

$$J_{test}(\theta) \sim Bias^2 + Variance$$



# Decomposition of Test Error

## See derivation in Section 8.1.1

- Draw a training dataset $S = \{x^{(i)}, y^{(i)}\}_{i=1}^{n}$ such that $y^{(i)} = h^*(x^{(i)}) + \xi^{(i)}$ where $\xi^{(i)} \sim \mathcal{N}(0, \sigma^2)$
- Train a model on the dataset, denoted by $\hat{h}_S$
- Take a test example $(x, y)$ such that $y = h^*(x) + \xi$ where $\xi \sim \mathcal{N}(0, \sigma^2)$ and measure the expected test error (averaged over the random draw of the training set $S$ and the randomness of $\xi$)

$$\text{MSE}(x) = \mathbb{E}_{S,\xi}\left[(y - \hat{h}_S(x))^2\right]$$

# **Decomposition of Test Error** for square loss

## See derivation in Section 8.1.1

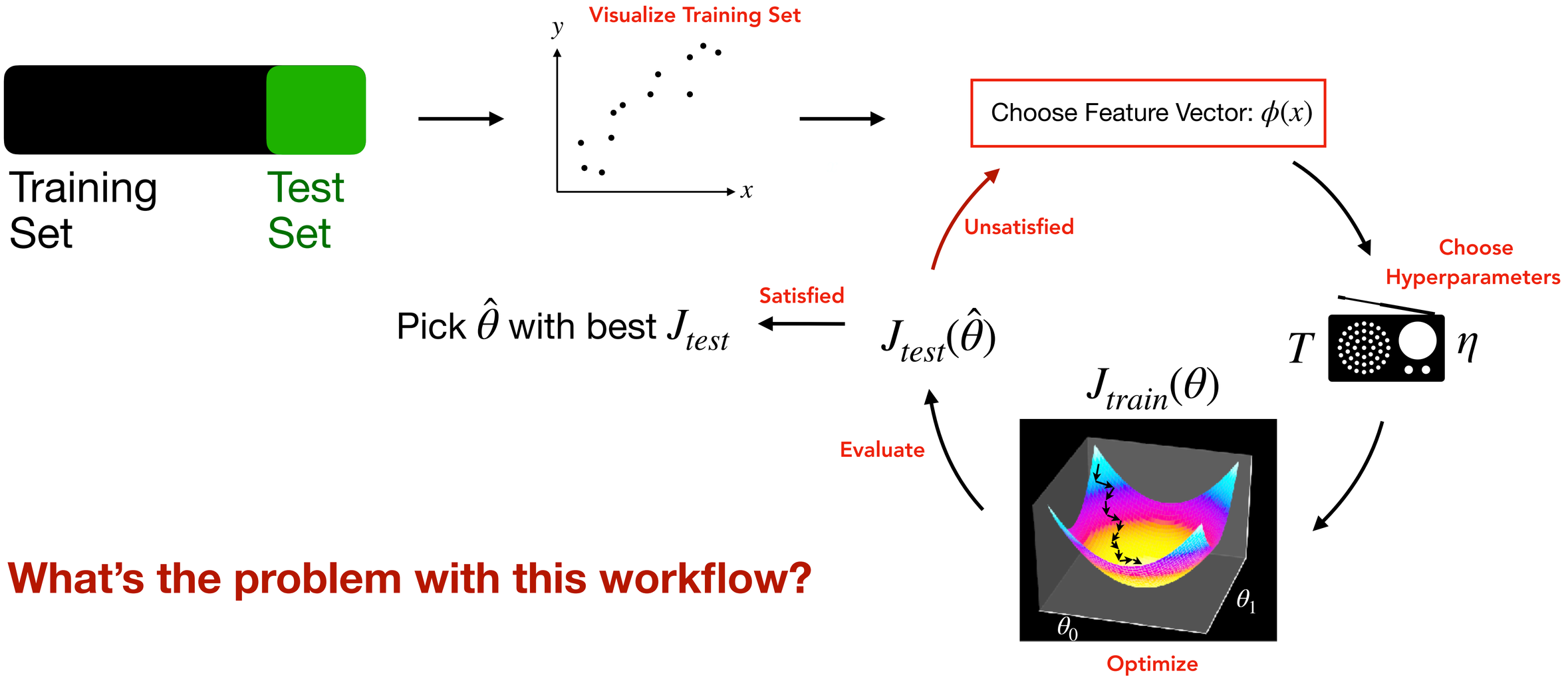
$$
\begin{aligned}
\mathrm{MSE}(x) &= \mathbb{E}\left[(y - \hat{h}_S(x))^2\right] \\
&= \mathbb{E}\left[(\xi + (h^*(x) - \hat{h}_S(x)))^2\right] \\
&= \mathbb{E}\left[\xi^2\right] + \mathbb{E}\left[(h^*(x) - \hat{h}_S(x))^2\right] \\
&= \sigma^2 + \mathbb{E}\left[(h^*(x) - \hat{h}_S(x))^2\right] \\
&= \sigma^2 + (h^*(x) - h_{\mathrm{avg}}(x))^2 + \mathbb{E}\left[(h_{\mathrm{avg}}(x) - \hat{h}_S(x))^2\right] \\
&= \underbrace{\sigma^2}_{\text{unavoidable}} + \underbrace{(h^*(x) - h_{\mathrm{avg}}(x))^2}_{\text{bias}^2} + \underbrace{\mathrm{var}(\hat{h}_S(x))}_{\text{variance}}
\end{aligned}
$$

# Other Hyperparameters

**$\phi$ is not the only unknown parameter over which we want to optimize**

- $T$: Number of Epochs
- $\eta$: Step size
- $\phi$: Feature vector

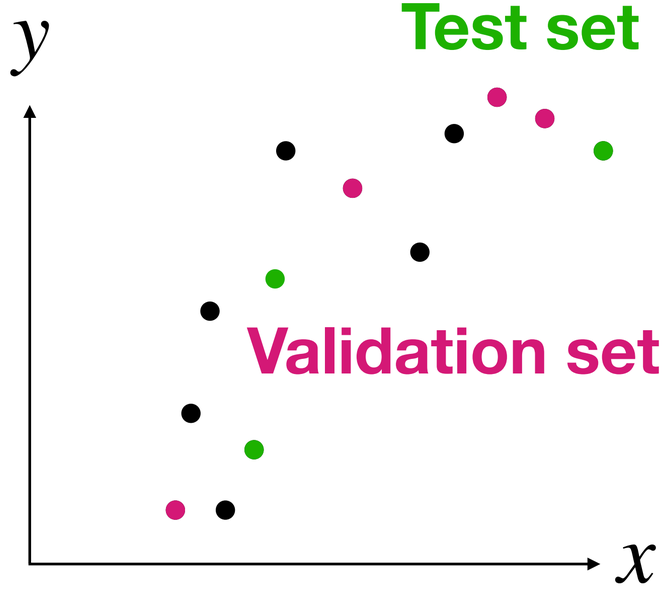
# Optimize over $\phi$ and other hyperparameters




**What's the problem with this workflow?**

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

## Define objective functions for each subset




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

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

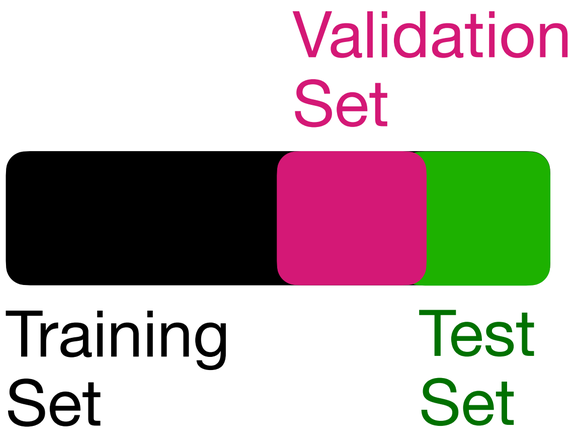
Split data:

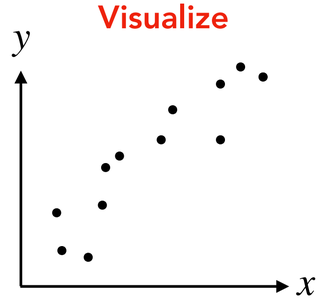

$$J_{train}(\theta) = \frac{1}{2d_{tr}} \sum_{i=1}^{d_{tr}} \left(\theta^\top \phi(x^{(i)}) - y^{(i)}\right)^2$$

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

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

# Machine Learning workflow - Cross Validation



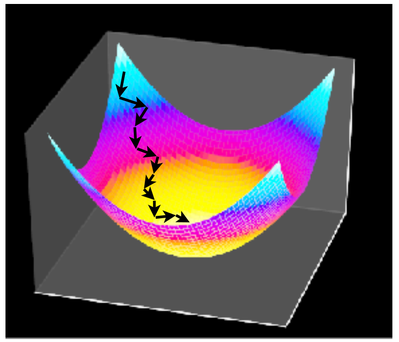

Can we automate feature extraction?

Choose Feature Vector: $\phi(x)$

Hyperparameter Tune

$T$ $\eta$

$J_{train}(\theta)$



Optimize

Evaluate

$J_{val}(\hat{\theta})$

not satisfied

satisfied

$J_{test}(\hat{\theta})$

**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

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

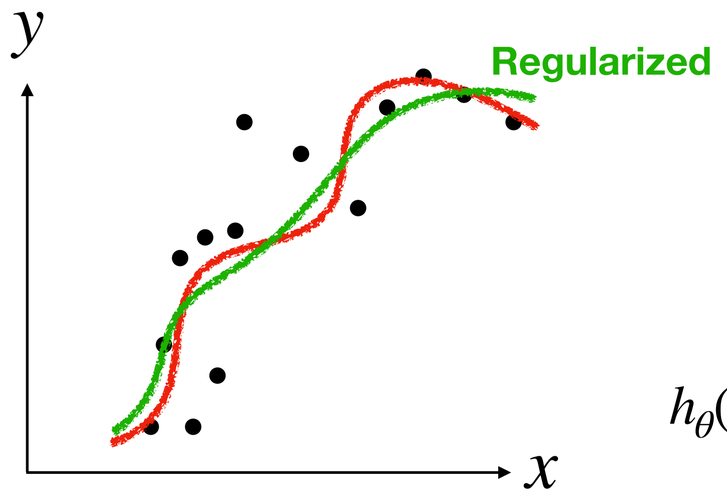
$$J_{reg}(\theta) = J(\theta) + \lambda\, R(\theta)$$

### L1 Regularization

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

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

Less coefficients



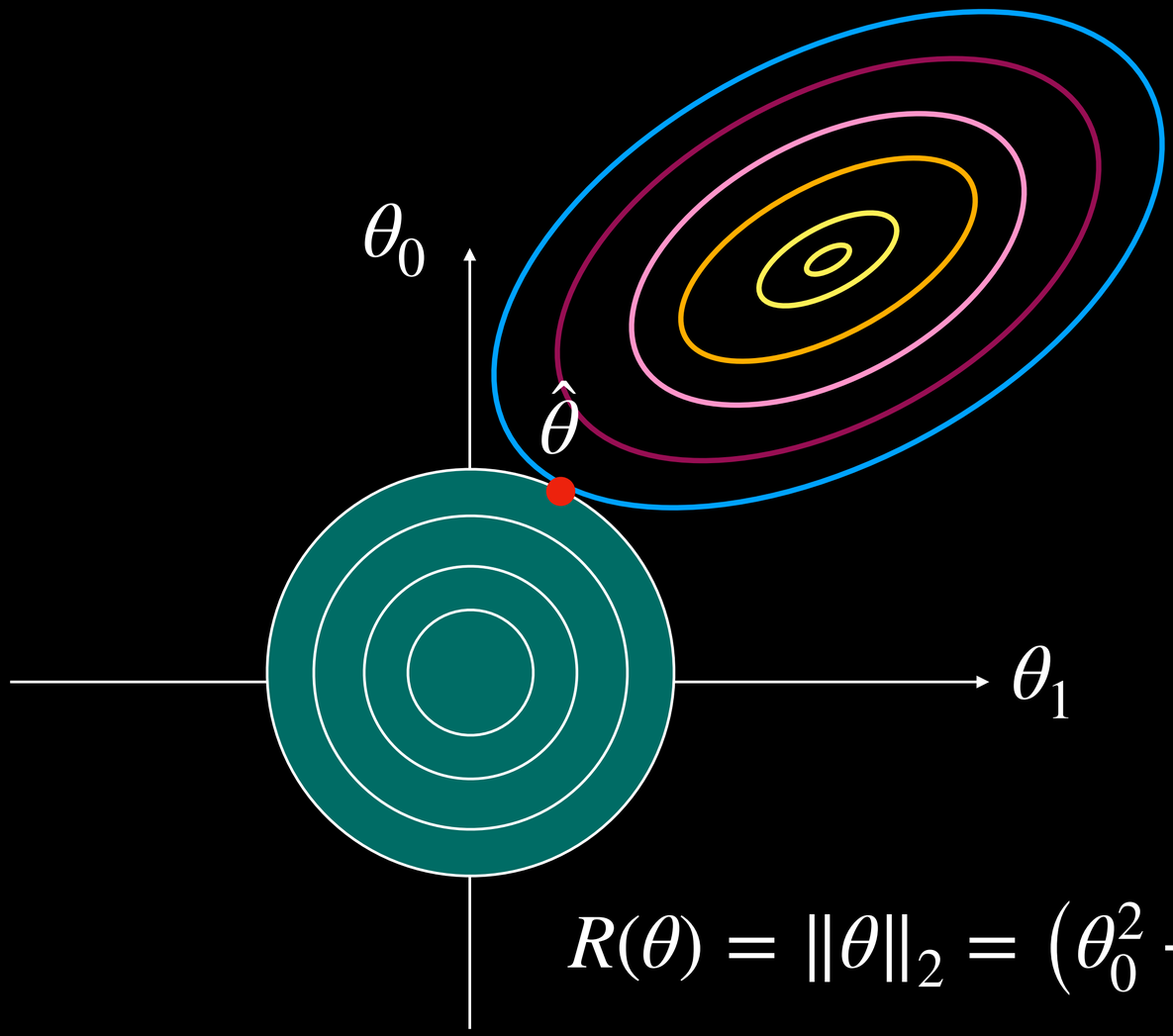

### L2 Regularization

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

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

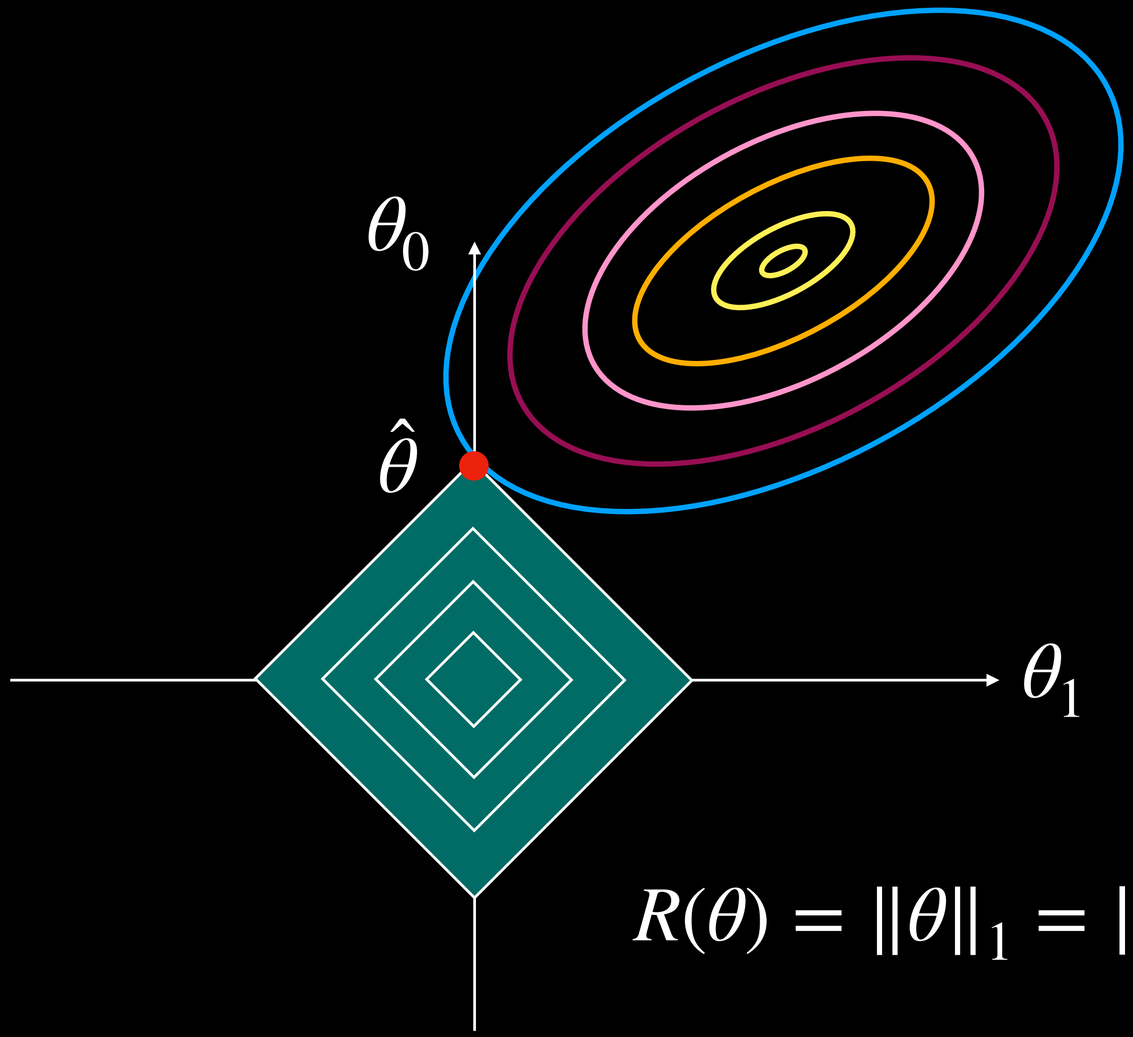
Smaller coefficients

# L2 Regularization



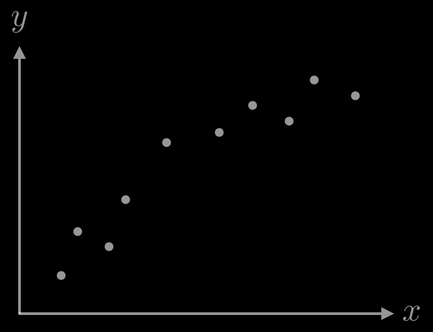

$$R(\theta) = \|\theta\|_2 = \left(\theta_0^2 + \theta_1^2 + \ldots\right)^{\frac{1}{2}}$$

# L1 Regularization




$$R(\theta) = \|\theta\|_1 = |\theta_0| + |\theta_1| + \ldots$$

# The ML workflow


How do I choose the feature vector?

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

not satisfied

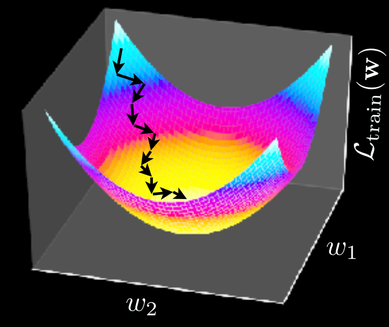
$\eta$

$T$ $\lambda$

$\mathcal{L}_{\text{val}}$

satisfied

$\mathcal{L}_{\text{test}}$



# How do I choose the feature vector?

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

$$f_{\mathbf{w}}(x) = \mathbf{w} \cdot \boxed{\phi(x)}$$

$\mathbf{x}$

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

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

$\phi(x) = [1,\ \ x,\ \sin(3x)]$

??????????????

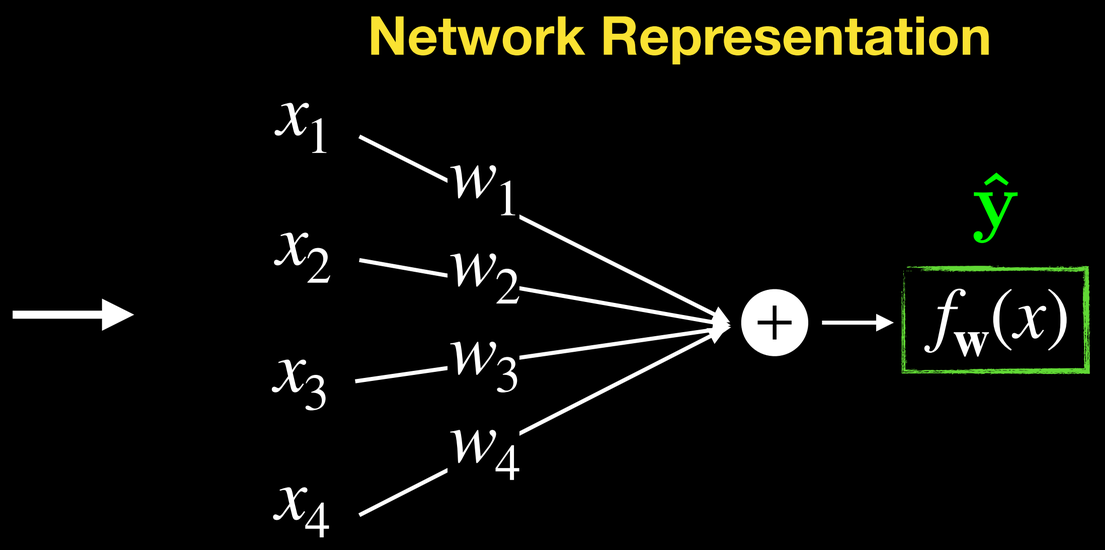
# Linear Predictor

$$f_{\mathbf{w}}(x) = \mathbf{w}^\top \mathbf{x}$$

$$\mathbf{w} = [w_1, w_2, w_3, w_4, \ldots]$$

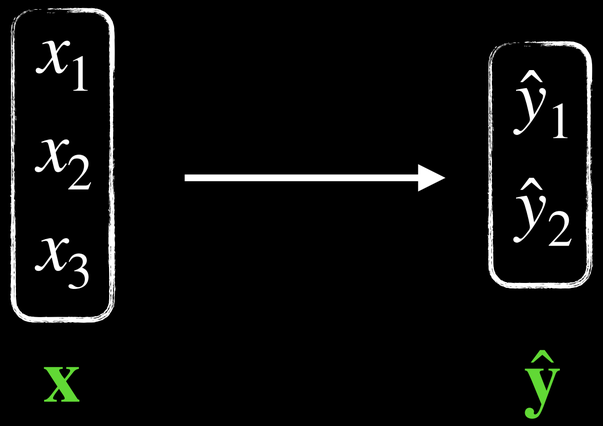
$$\mathbf{x} = [x_1, x_2, x_3, x_4, \ldots]$$

$$f_{\mathbf{w}}(\mathbf{x}) = w_1 x_1 + w_2 x_2 + w_3 x_3 + w_4 x_4$$



# Linear Predictor

2 outputs?




3 * 2 fitting parameters

$$\hat{y}_1 = \mathbf{w}_1 \cdot \mathbf{x} = w_{11}x_1 + w_{12}x_2 + w_{13}x_3$$

$$\hat{y}_2 = \mathbf{w}_2 \cdot \mathbf{x} = w_{21}x_1 + w_{22}x_2 + w_{23}x_3$$

Matrix form

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\hat{\mathbf{y}} = \mathbf{W}\mathbf{x}$$

# From Matrix to Network

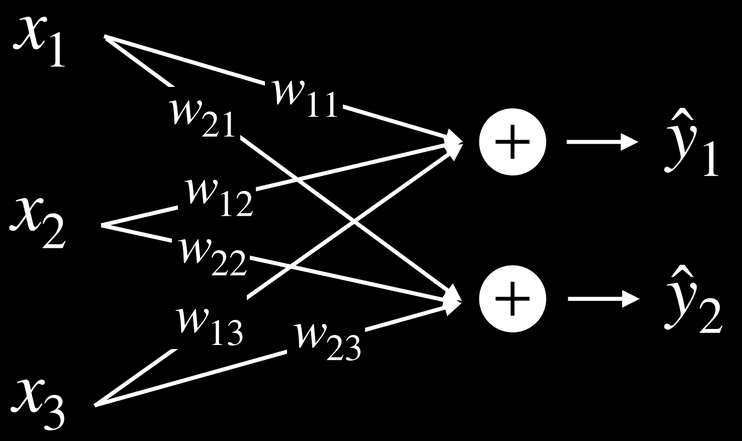
## Matrix Representation

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & w_{13} \\ w_{21} & w_{22} & w_{23} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$$

$$\hat{\mathbf{y}} = \mathbf{W} \mathbf{x}$$

## Network Representation

Account for Bias: 1 =




### Index notation

$$\hat{y}_i = \sum_{j=1}^{n} w_{ij} x_j$$

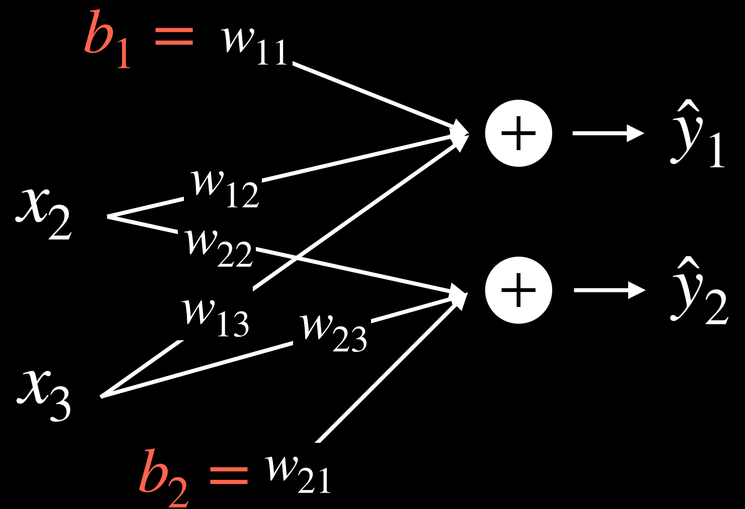
# Linear Predictor - Explicit Bias

**Matrix Representation**

$$\begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \end{bmatrix} = \begin{bmatrix} w_{12} & w_{13} \\ w_{22} & w_{23} \end{bmatrix} \begin{bmatrix} x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} w_{11} \\ w_{21} \end{bmatrix}$$

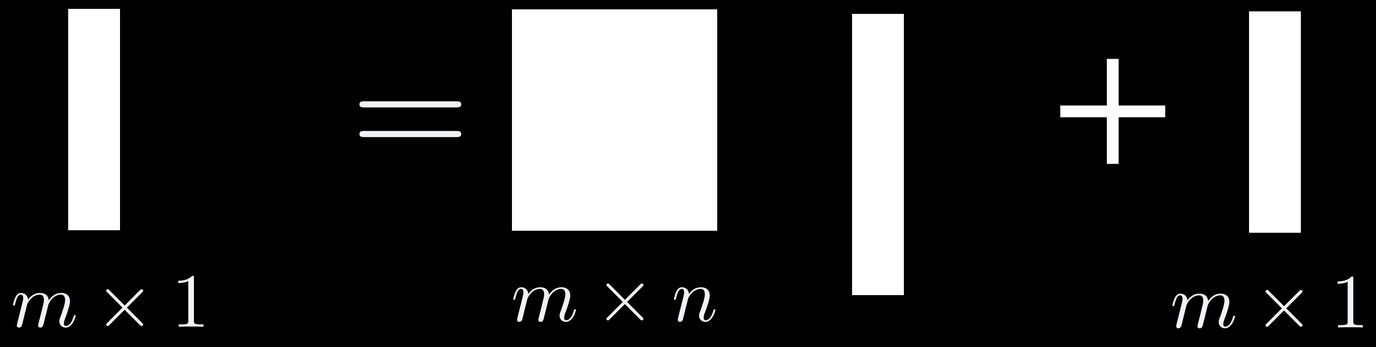
$$\hat{\mathbf{y}} = \mathbf{W}\ \mathbf{x}\ \mathbf{b}$$

**Network Representation**



# Linear Predictor

$$\hat{\mathbf{y}} = \mathbf{W}\ \mathbf{x} + \mathbf{b}$$



$m \times 1$

Number of outputs

$m \times n$

$n \times 1$

Number of inputs

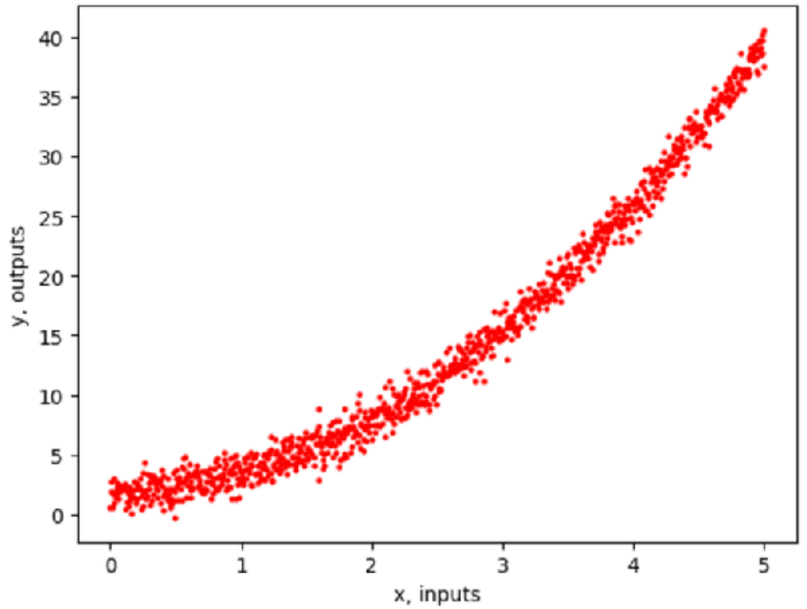
$m \times 1$

Some formulations explicitly account for $\mathbf{b}$, while others include the bias as part of $\mathbf{x}$ for simplicity of representation

# Create synthetic data

https://colab.research.google.com/drive/1tmEpFvxScWT0-2zzbkJtYxBrcDp2x5aH?usp=sharing

```
# 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)

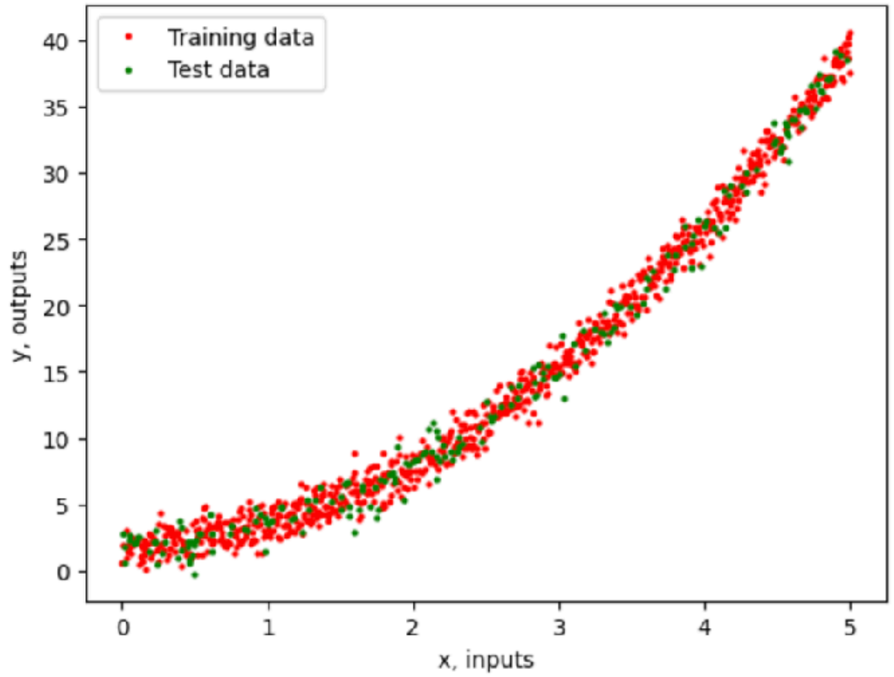
```python
# Create features

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

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

Gradient Descent Function

```python
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
```

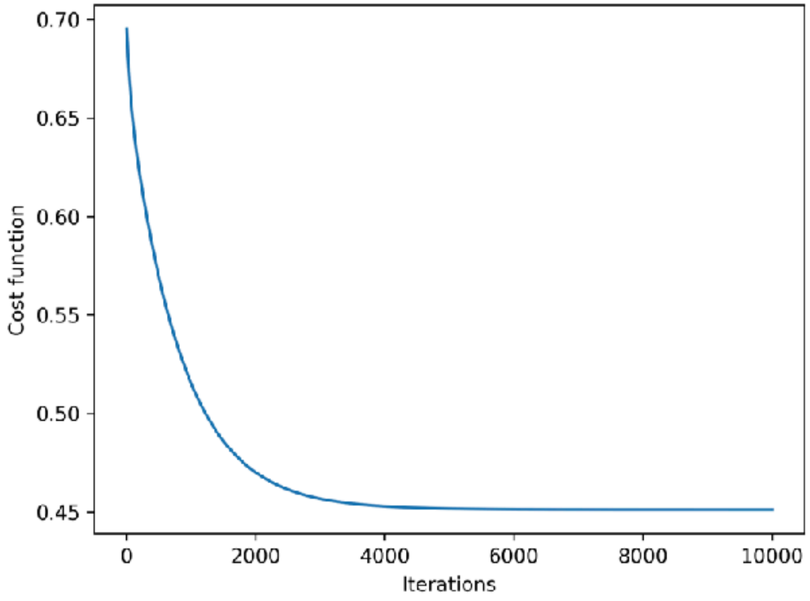
Gradient Descent Update

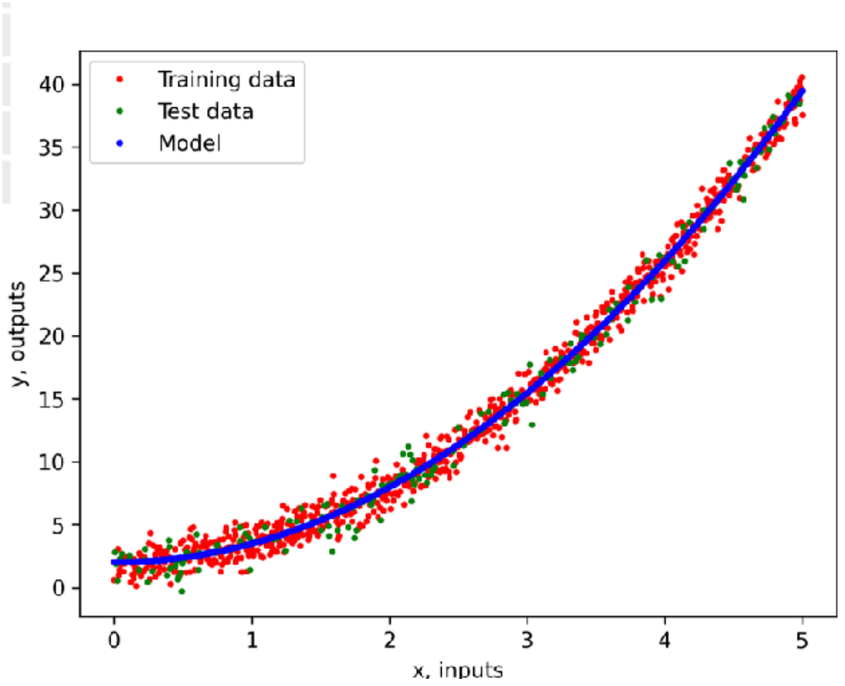
```python
theta = np.random.randn(degree+1, 1)
learning_rate = 0.01
num_iters = 10000
theta, J_history = gradient_descent(X_train, y_train, theta, learning_rate, num_iters)
```

```
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

```python
# 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

```python
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
```