بسم الله الرحمن الرحیم

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Introduction to Learning, Linear regression

Iran University of Science and Technology

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Courtesy: slides are adopted partly from Dr. Soleymani, Sharif University

Outline

- Introduction to Learning
- Linear Regression
- Gradient Descent
- Generalized Linear Regression

A Definition of ML

- Tom Mitchell (1998):Well-posed learning problem
  - “A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E”.
- Using the observed data to make better decisions
  - Generalizing from the observed data

ML Definition: Example

- Consider an email program that learns how to filter spam according to emails you do or do not mark as spam.

  - T: Classifying emails as spam or not spam.
  - E: Watching you label emails as spam or not spam.
  - P: The number (or fraction) of emails correctly classified as spam/not spam.

The essence of machine learning

- A pattern exist
- We do not know it mathematically
- We have data on it

Example: Home Price

- Housing price prediction

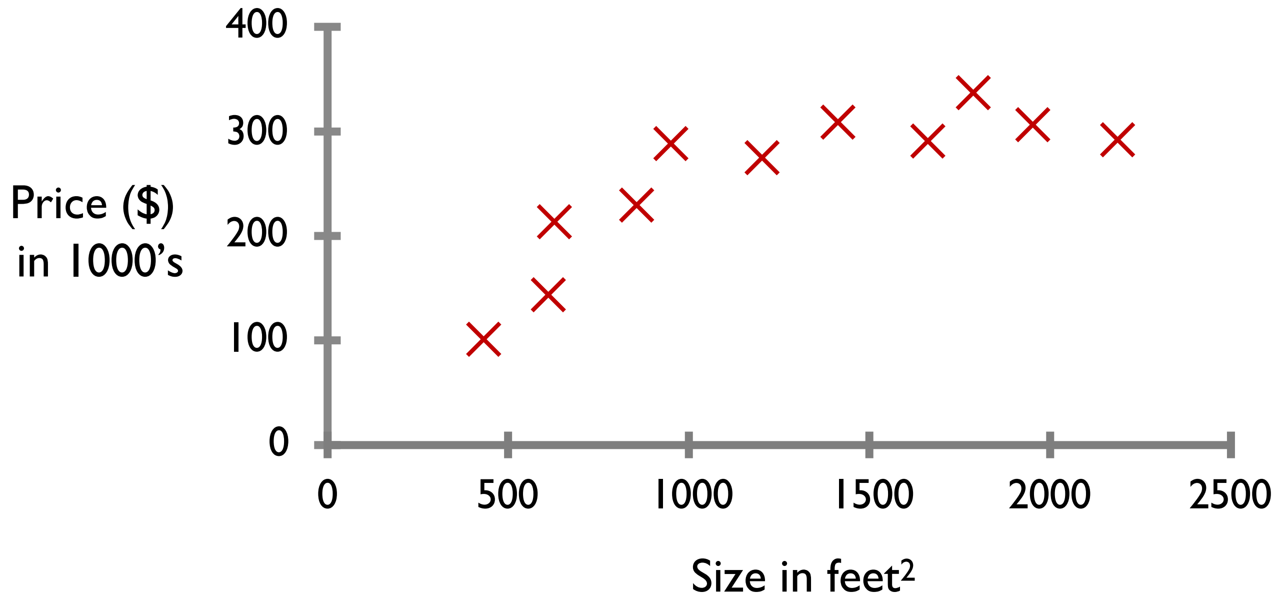
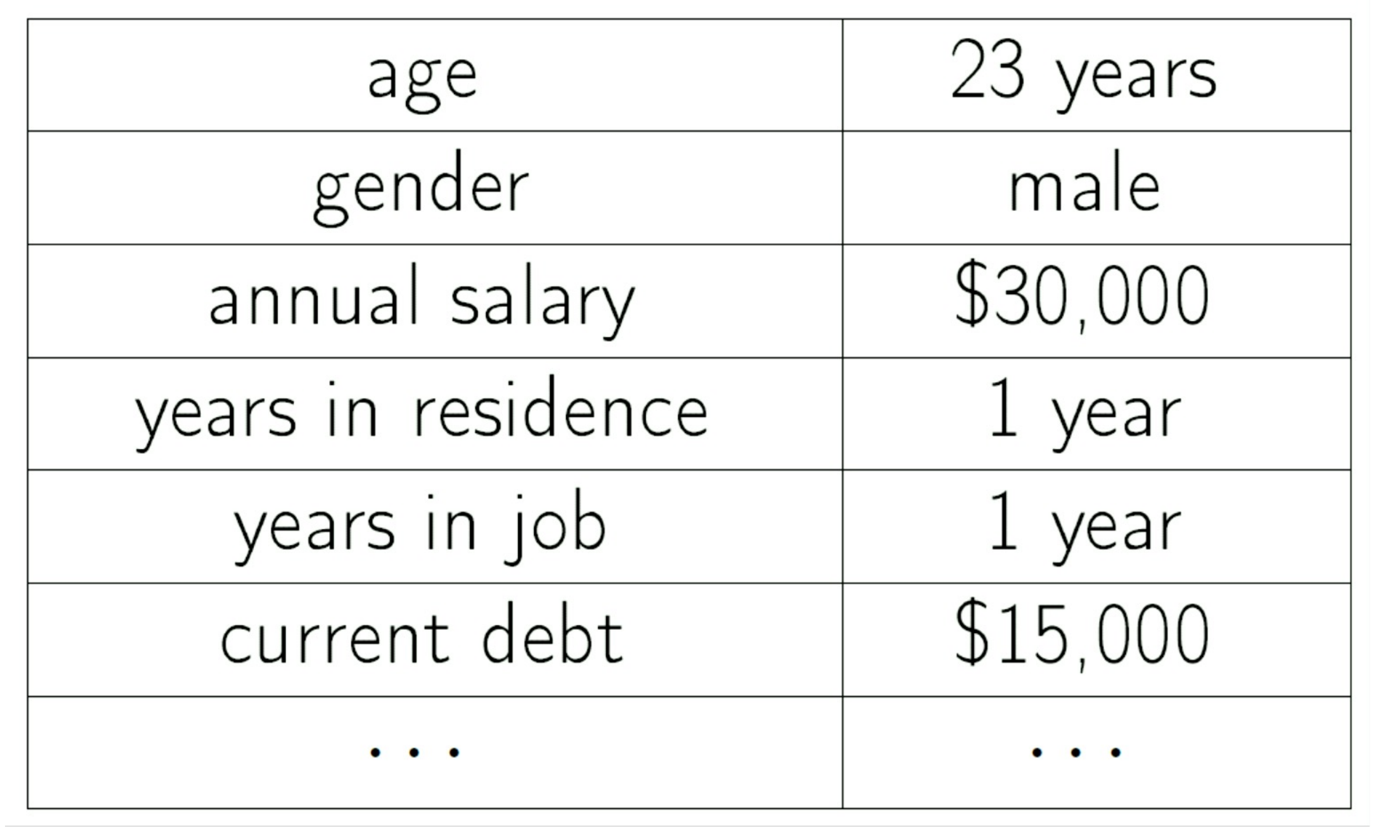


Figure adopted from slides of Andrew Ng,
Machine Learning course, Stanford.

Example: Bank loan

- Applicant form as the input:



age	23 years
gender	male
annual salary	$30,000
years in residence	1 year
years in job	1 year
current debt	$15,000
...	...

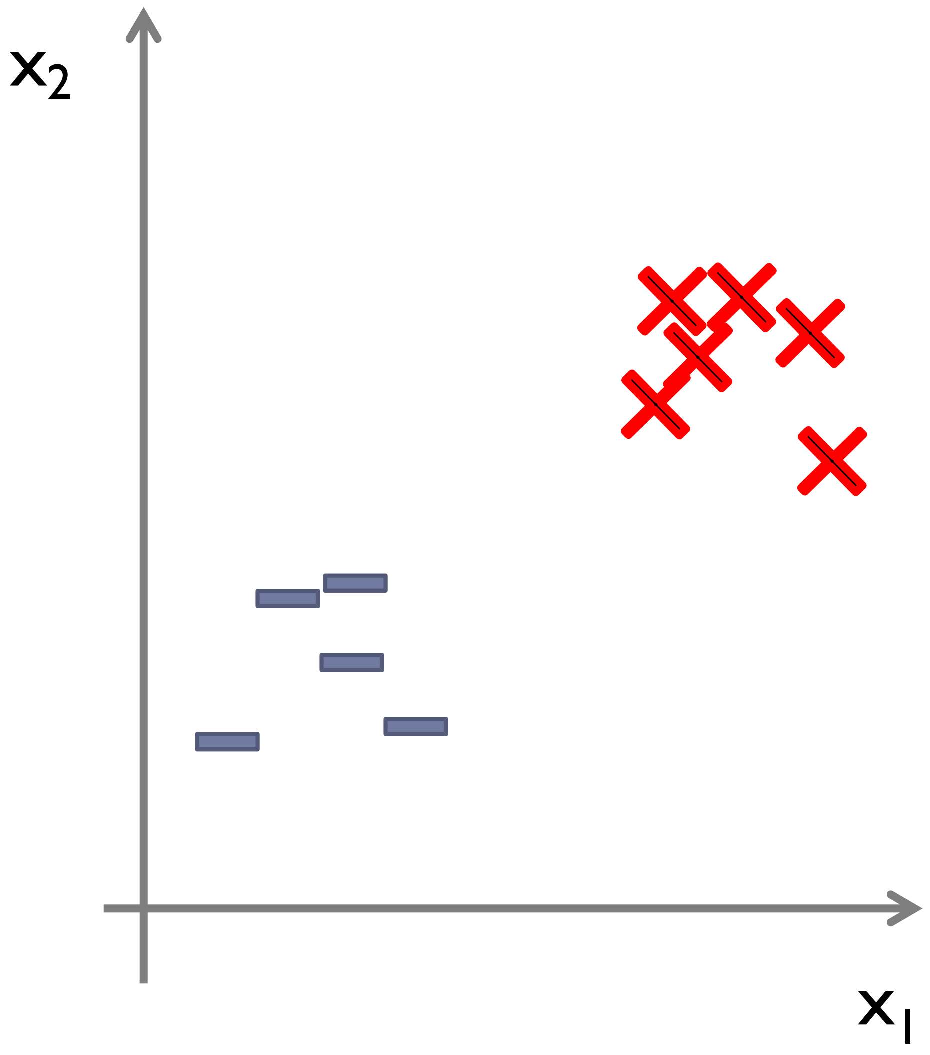
- Output: approving or denying the request

Components of (Supervised) Learning

- Unknown target function: $f: \mathcal{X} \to \mathcal{Y}$
  - Input space: $\mathcal{X}$
  - Output space: $\mathcal{Y}$
- Training data: $(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \ldots, (\boldsymbol{x}_N, y_N)$

- Picka formula $g: \mathcal{X} \to \mathcal{Y}$ that approximates the target function f
  - selected from a set of hypotheses $\mathcal{H}$

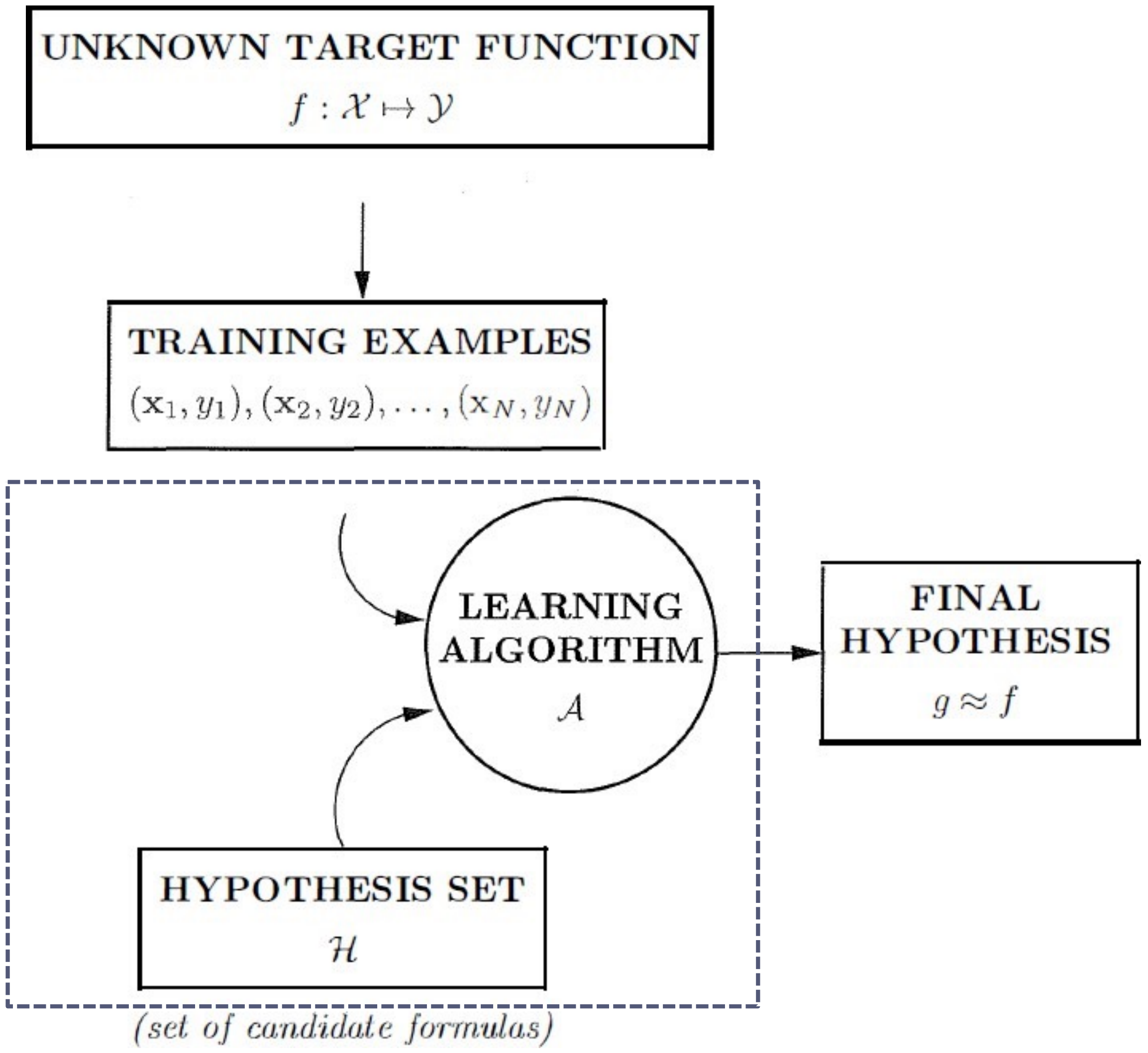
Training data: Example



Training data

x_1	x_2	y	
0.9	2.3	1	▬
3.5	2.6	1	▬
2.6	3.3	1	▬
2.7	4.1	1	▬
1.8	3.9	1	▬
6.5	6.8	-1	✖
7.2	7.5	-1	✖
7.9	8.3	-1	✖
6.9	8.3	-1	✖
8.8	7.9	-1	✖
9.1	6.2	-1	✖

Components of (Supervised) Learning



UNKNOWN TARGET FUNCTION
$f : \mathcal{X} \mapsto \mathcal{Y}$
TRAINING EXAMPLES
$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_N, y_N)$
LEARNING ALGORITHM
$\mathcal{A}$
FINAL HYPOTHESIS
$g \approx f$
HYPOTHESIS SET
$\mathcal{H}$
(set of candidate formulas)

Learning model

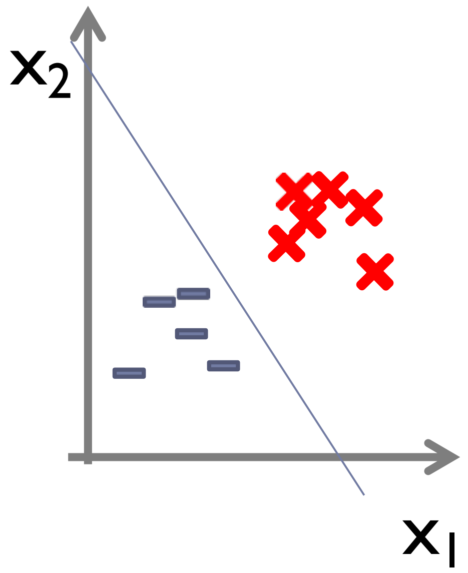
Solution Components

- Learning model composed of:
  - Learning algorithm
  - Hypothesis set

- Perceptron example

Perceptron classifier

- Input $\boldsymbol{x} = [x_1, \ldots, x_d]$
- Classifier:
  - If $\overset{d}{\underset{i=1}{}} w_i x_i > \text{threshold}$ then output 1
  - else output -1



- The linear formula $g \in \mathcal{H}$ can be written:

$$g(\boldsymbol{x}) = \text{sign}\left(\sum_{i=1}^{d} w_i x_i \quad + \quad w_0 \quad\right)$$

If we add a coordinate $x_0 = 1$ to the input:

$$g(\boldsymbol{x}) = \text{sign}\left(\sum_{i=0}^{d} w_i x_i \right)$$

Vector form

$$g(\boldsymbol{x}) = \text{sign}(\boldsymbol{w}^T \boldsymbol{x})$$

Perceptron learning algorithm: linearly separable data

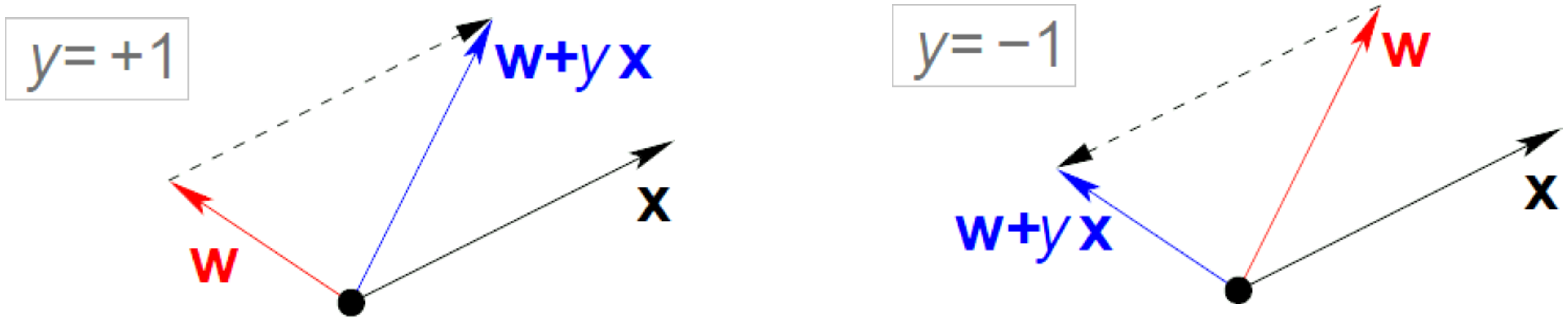
- Give the training data $\left(\boldsymbol{x}^{(1)}, y^{(1)}\right), \ldots, \left(\boldsymbol{x}^{(N)}, y^{(N)}\right)$

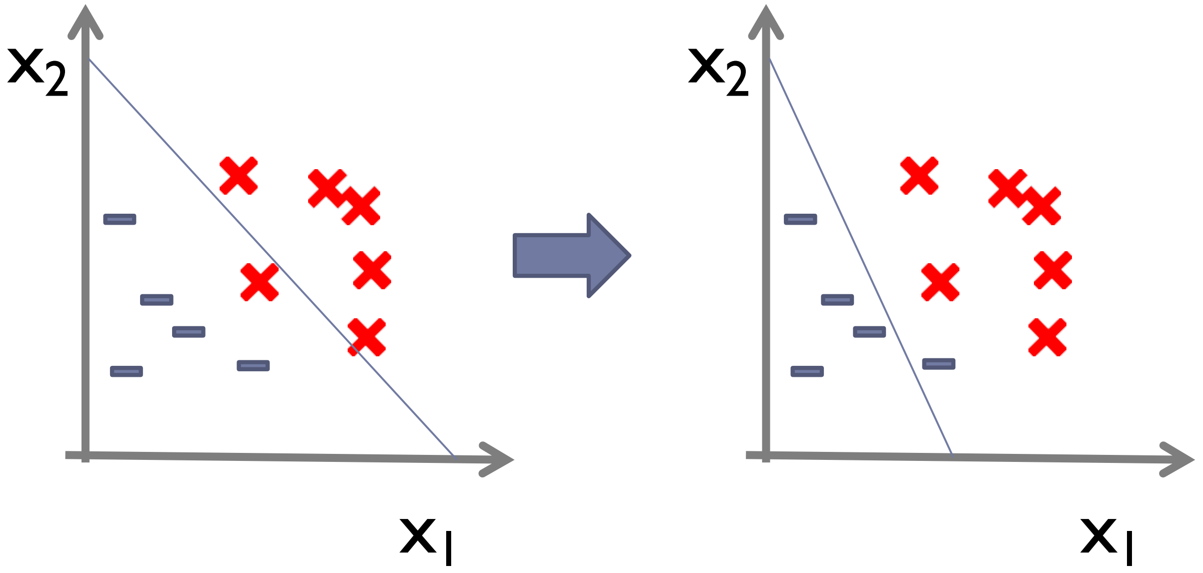
- Misclassified data $\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)$:

$$\operatorname{sign}(\boldsymbol{w}^T \boldsymbol{x}^{(n)}) \neq y^{(n)}$$

```
Repeat
    Pick a misclassified data $\left(\boldsymbol{x}^{(n)}, y^{(n)}\right)$ from training data and
    update $\boldsymbol{w}$:
        $\boldsymbol{w} = \boldsymbol{w} + y^{(n)} \boldsymbol{x}^{(n)}$
Until all training data points are correctly classified by $g$
```

Perceptron learning algorithm: Example of weight update





Experience (E) in ML

- Basic premise of learning:
  - “Using a set of observations to uncover an underlying process”

- We have different types of (getting) observations in different types or paradigms of ML methods

Paradigms of ML

- <u>Supervised learning</u> (regression, classification)
  - predicting a target variable for which we get to see examples.
- <u>Unsupervised learning</u>
  - revealing structure in the observed data
- <u>Reinforcement learning</u>
  - partial (indirect) feedback, no explicit guidance
  - Given rewards for a sequence of moves to learn a policy and utility functions

- Other paradigms: semi-supervised learning, active learning, online learning, etc.

Supervised Learning: Regression vs. Classification

- Supervised Learning
  - **Regression**: predict a continuous target variable
    - E.g., $y \in [0,1]$
  - **Classification**: predict a discrete target variable
    - E.g., $y \in \{1,2, \ldots, C\}$

Data in Supervised Learning

- Data are usually considered as vectors in a d dimensional space
  - Now, we make this assumption for illustrative purpose
    - We will see it is not necessary

Columns:
Features/attributes/dimensions

Rows:
Data/points/instances/examples/samples

Y column:
Target/outcome/response/label

	x_1	x_2	…	x_d	y (Target)
Sample1					
Sample 2					
…					
Sample n-1					
Sample n					

Regression: Example

- Housing price prediction

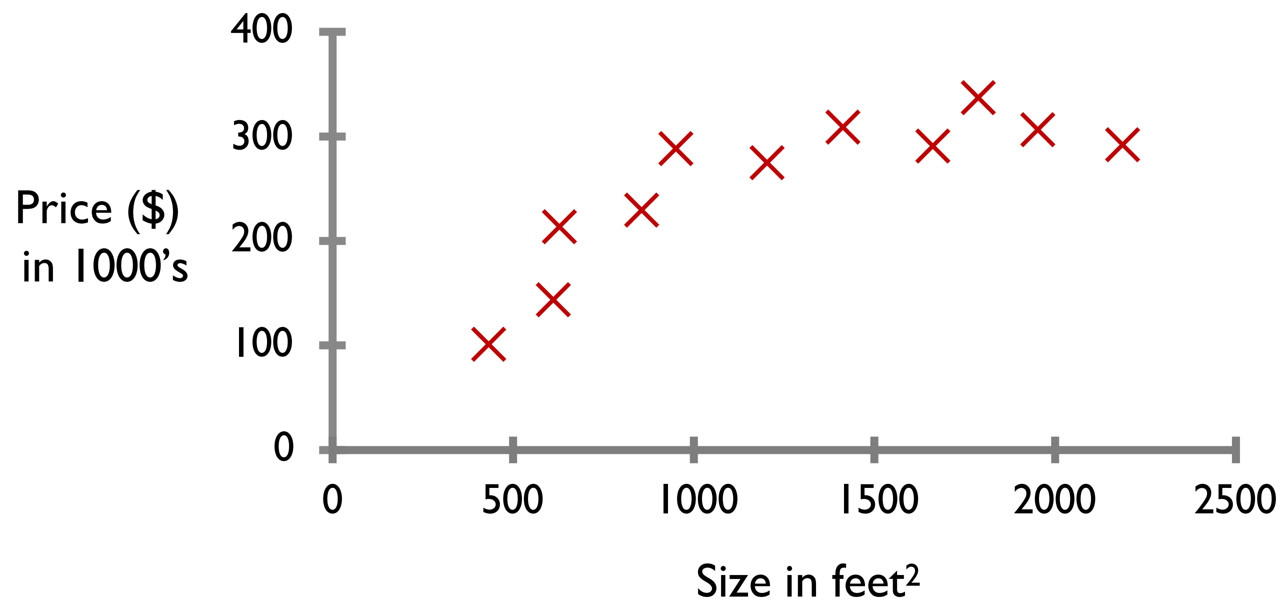
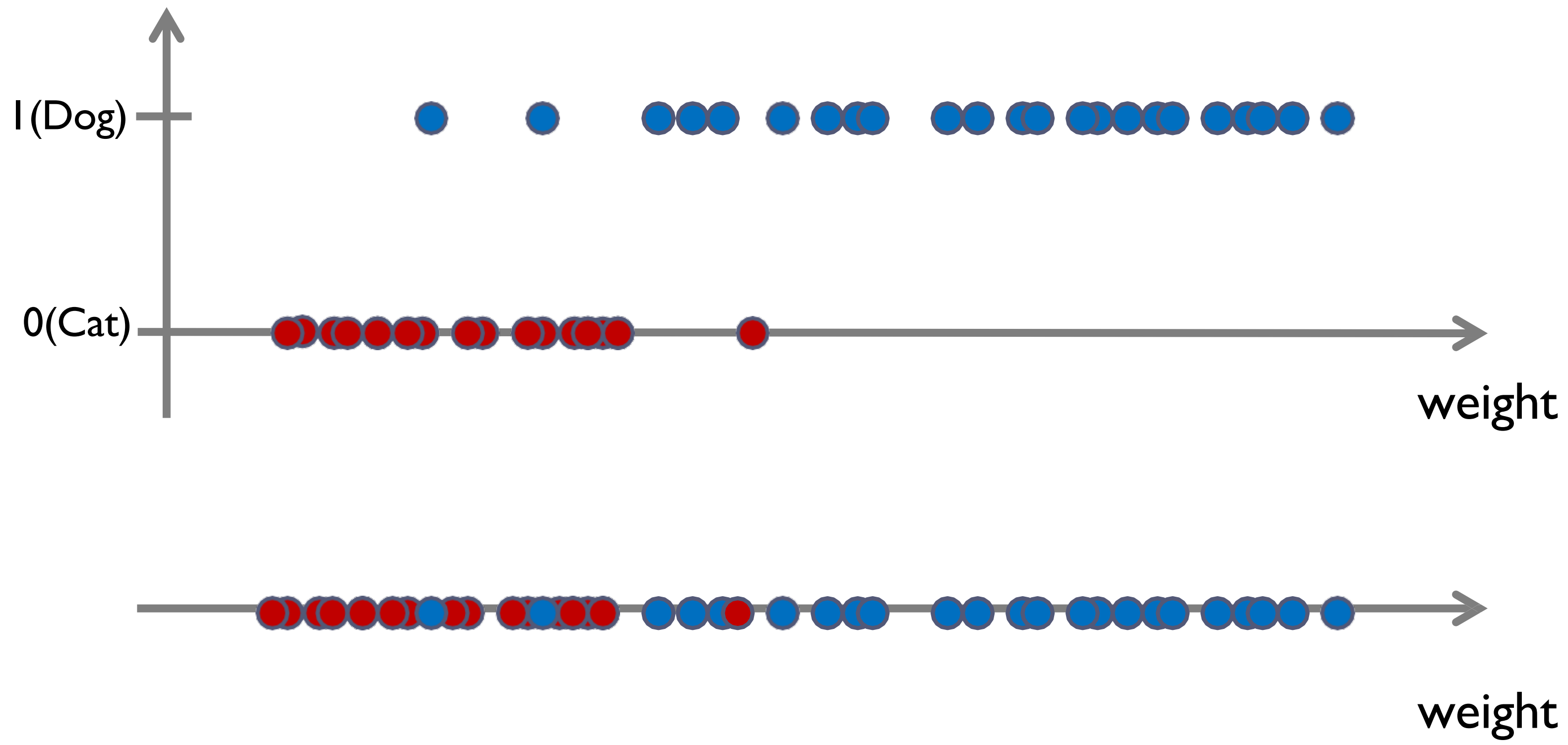


Figure adopted from slides of Andrew Ng

Classification: Example

- Weight (Cat, Dog)

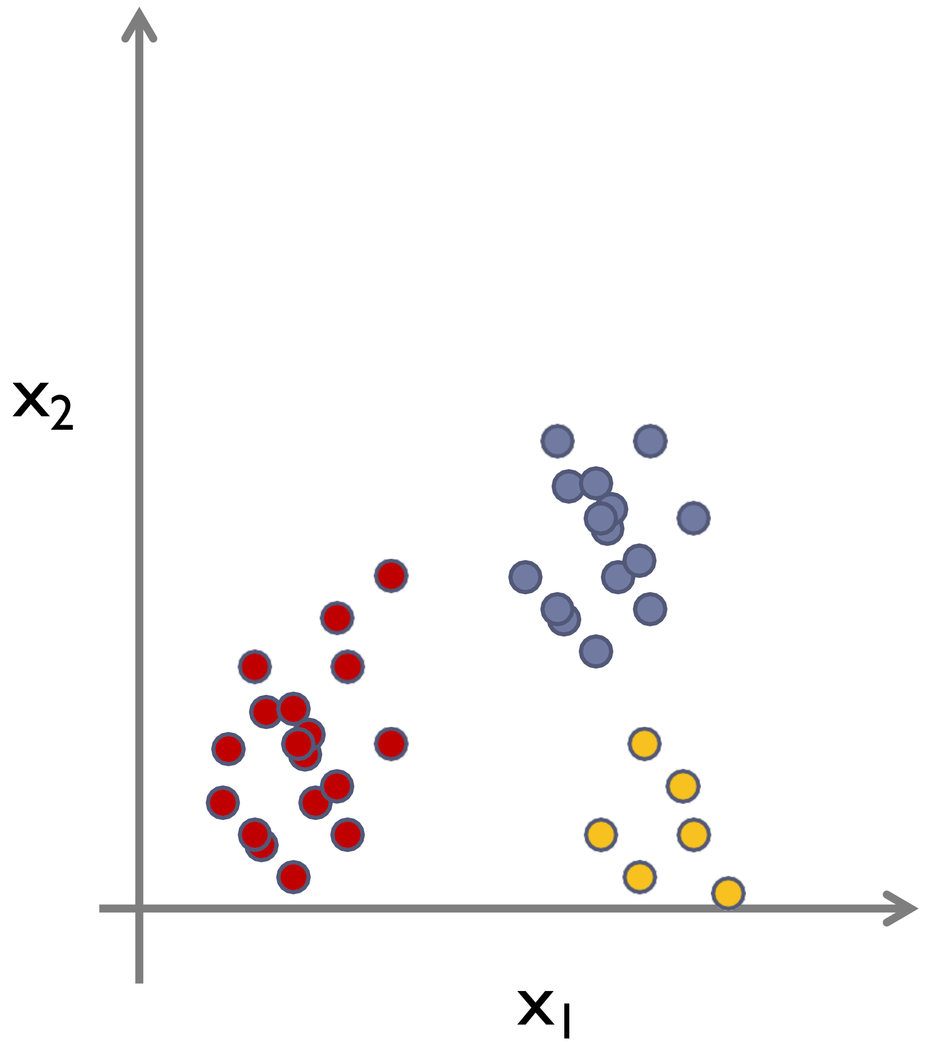


Supervised Learning vs. Unsupervised Learning

- Supervised learning
  - Given: Training set
    - labeled set of N input-output pairs $D = \{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{N}$
  - Goal: learning a mapping from $\boldsymbol{x}$ to y

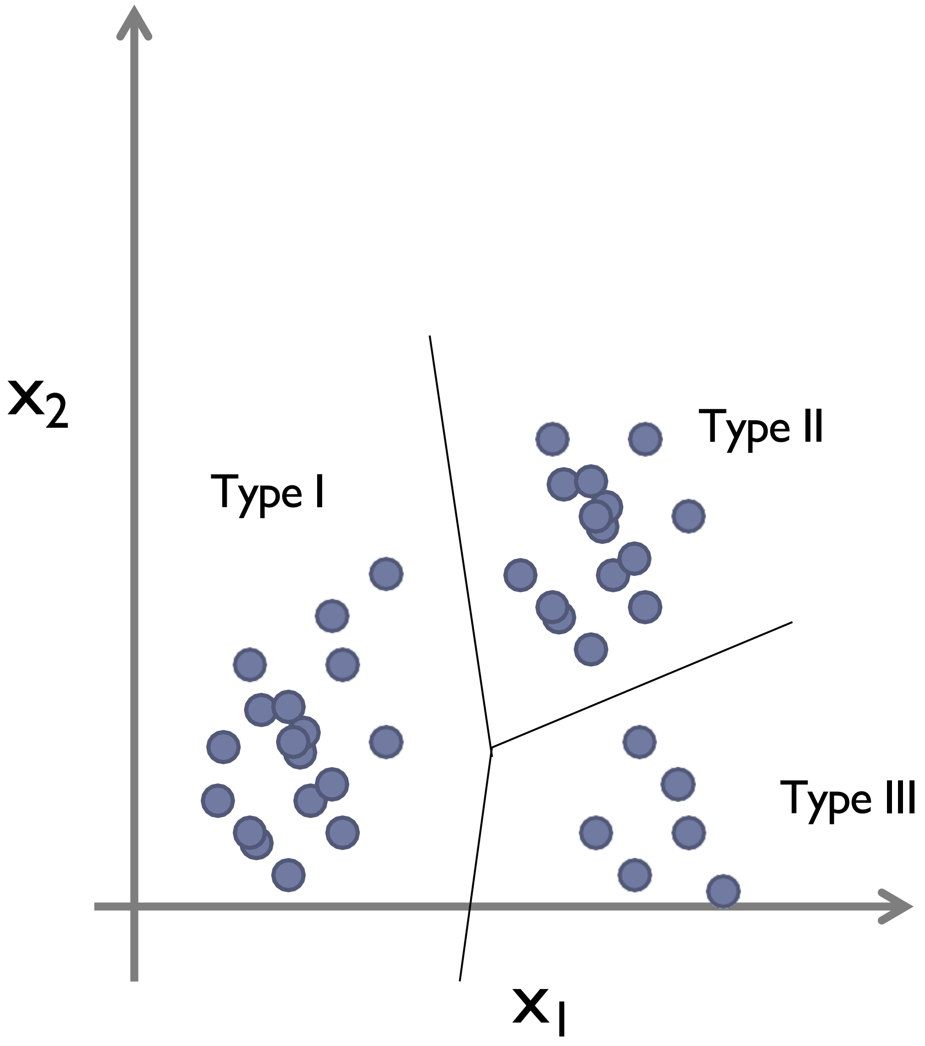
- Unsupervised learning
  - Given: Training set
    - $\{\boldsymbol{x}^{(i)}\}_{i=1}^{N}$
  - Goal: find groups or structures in the data
    - Discover the intrinsic structure in the data

Supervised Learning: Samples



Classification

Unsupervised Learning: Samples



Clustering

Sample Data in Unsupervised Learning

- Unsupervised Learning:

Columns:
Features/attributes/dimensions

Rows:
Data/points/instances/examples/s amples

	x_1	x_2	…	x_d
Sample1				
Sample 2				
…				
Sample n-1				
Sample n				

Unsupervised Learning: Example Applications

- Clustering docs based on their similarities
  - Grouping new stories in the Google news site
- Market segmentation:group customers into different market segments given a database of customer data.
- Social network analysis

Reinforcement Learning

Provides only an indication as to whether an action is correct or not

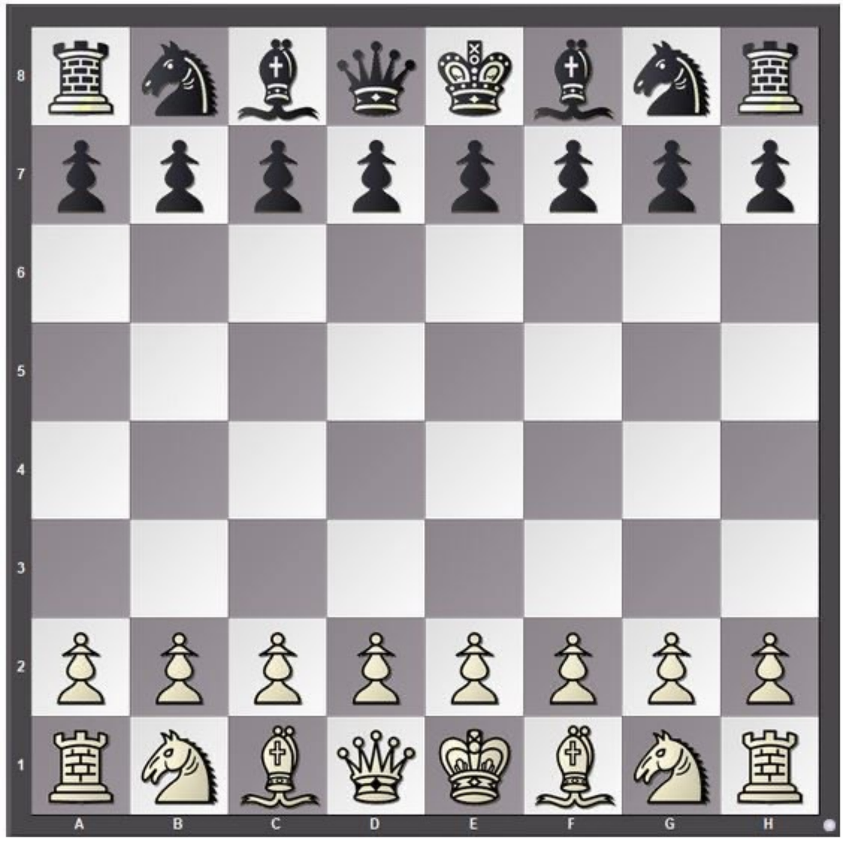
- Data in supervised learning:

  (input, correct output)
- Data in Reinforcement Learning:

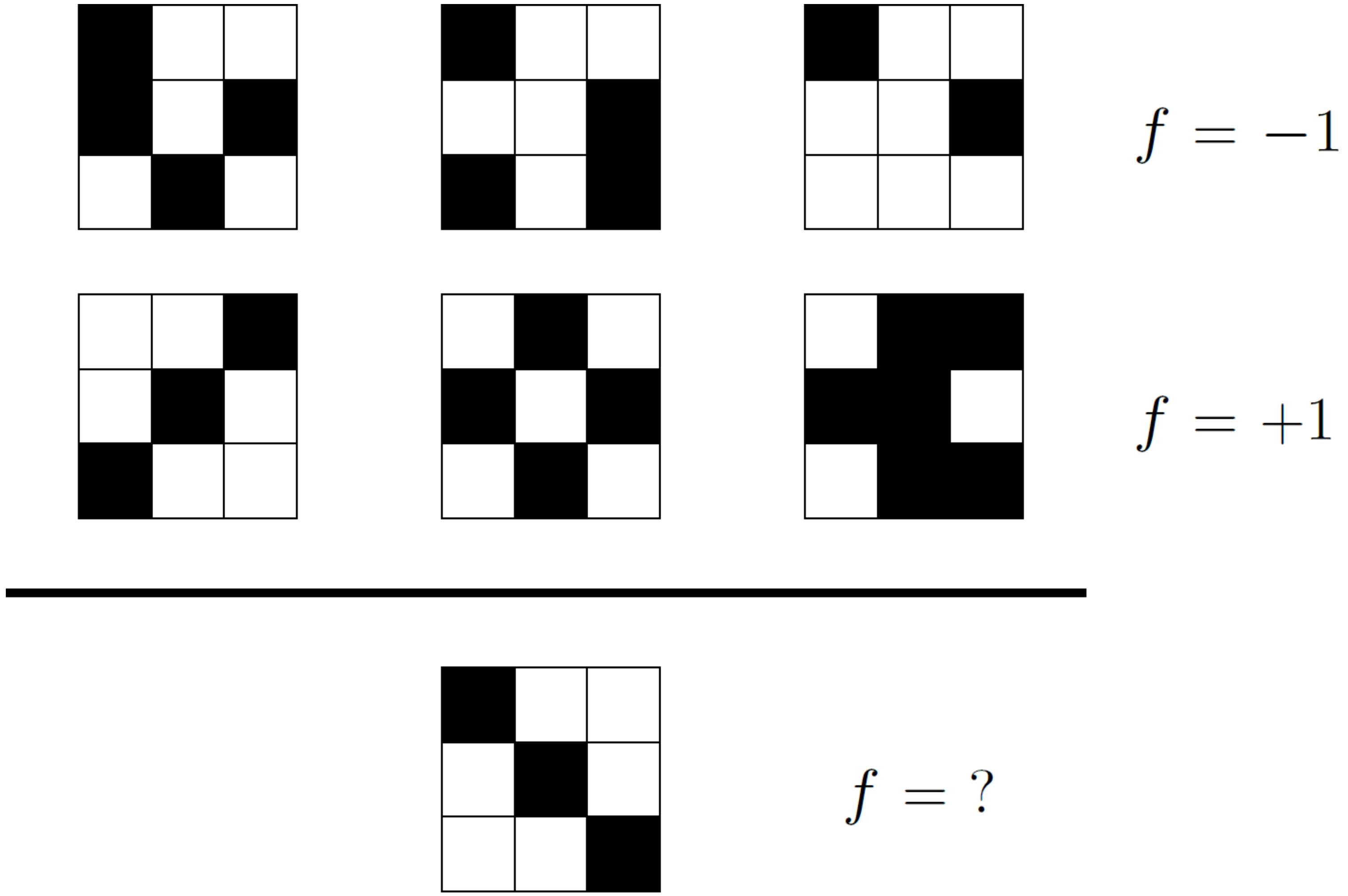
  (input, some output, a grade of reward for this output)

Reinforcement Learning

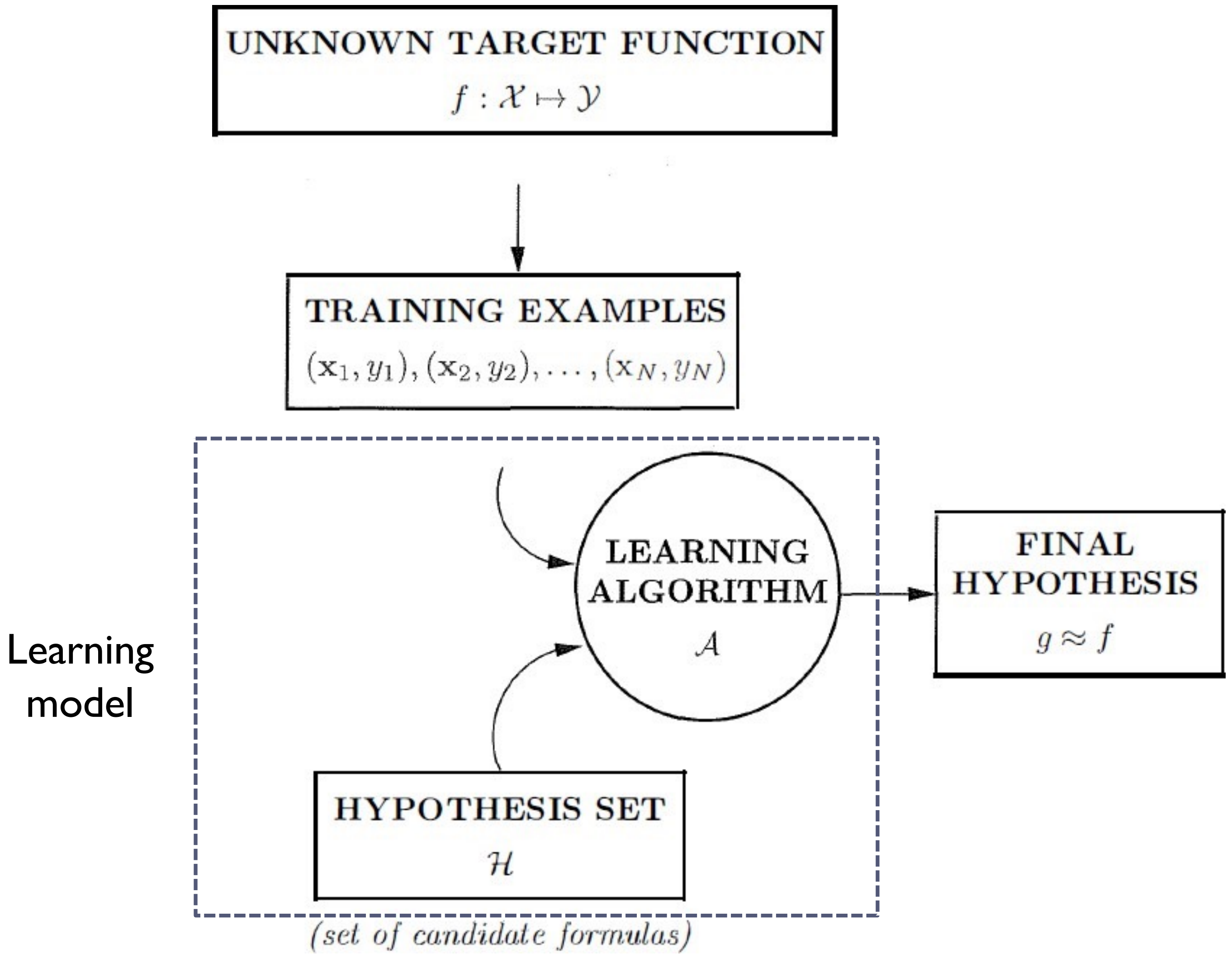
- Typically, we need to get a sequence of decisions
  - it is usually assumed that reward signals refer to the entire sequence



Example



Components of (Supervised) Learning

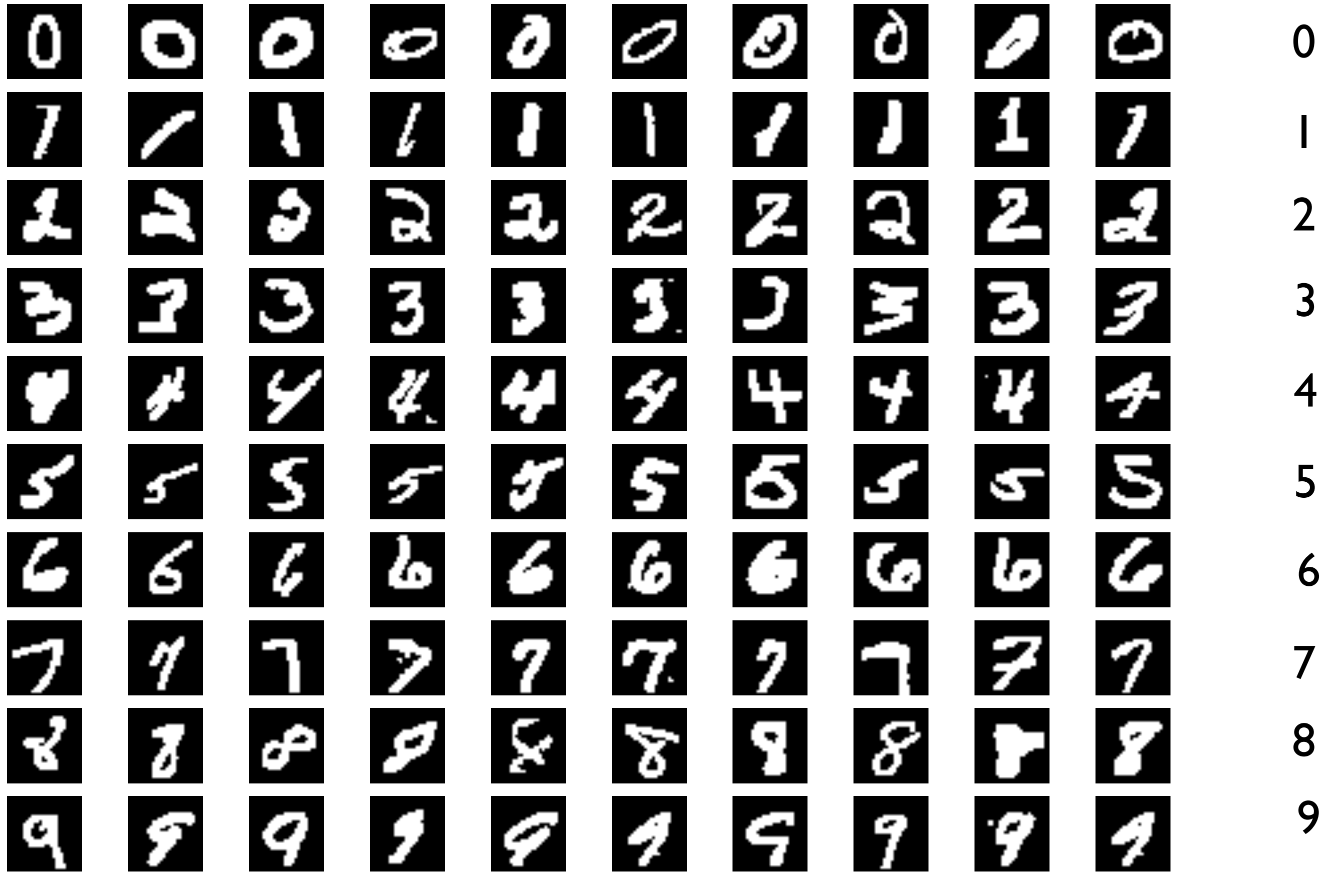


Main Steps of Learning Tasks

- Selection of hypothesis set (or model specification)
  - Which class of models (mappings) should we use for our data?
- Learning: find mapping f (from hypothesis set) based on the training data
  - Which notion of error should we use? (loss functions)
  - Optimization of loss function to find mapping f
- Evaluation: how well f generalizes to yet unseen examples
  - How do we ensure that the error on future data is minimized? (generalization)

Handwritten Digit Recognition Example

- Data: labeled samples



Example: Input representation

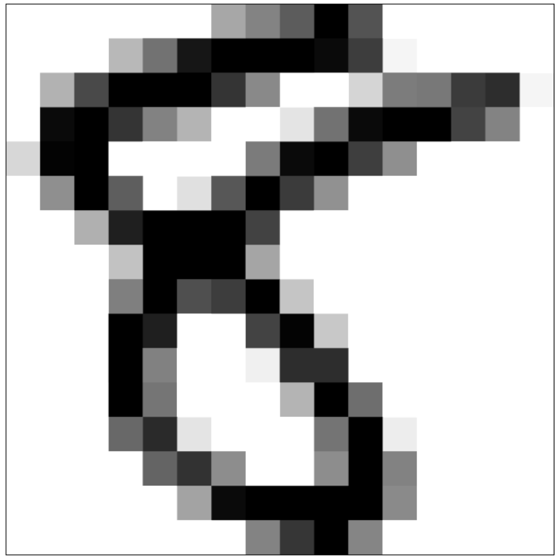
'raw' input $\mathbf{x} = (x_0, x_1, x_2, \cdots, x_{256})$

linear model: $(w_0, w_1, w_2, \cdots, w_{256})$

Features: Extract useful information, e.g.,

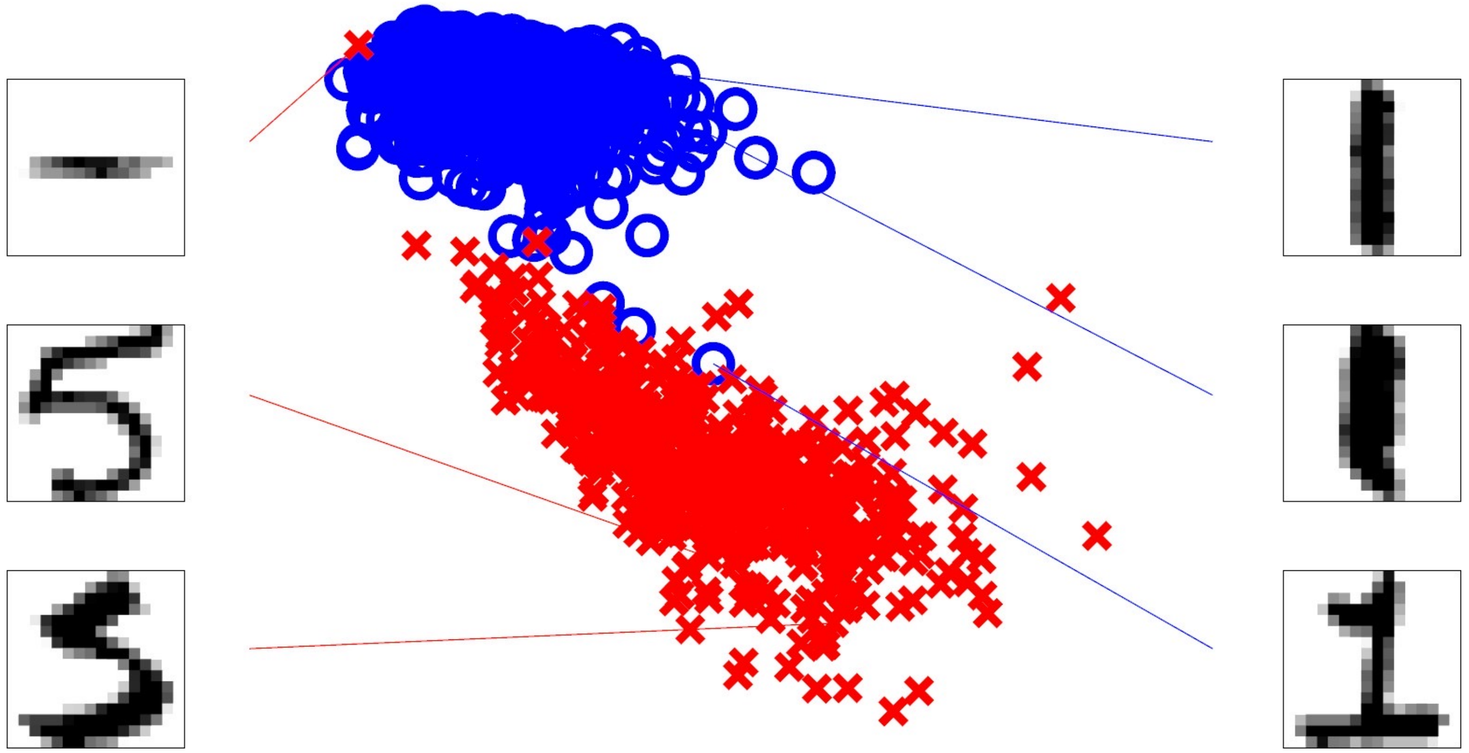
intensity and symmetry $\mathbf{x} = (x_0, x_1, x_2)$

linear model: (w_0, w_1, w_2)



Example: Illustration of features

$\mathbf{x} = (x_0, x_1, x_2)$ x_1: intensity x_2: symmetry



Linear regression, Cost Function and Generalization

Regression problem

- The goal is to make (real valued) predictions given features

- Example: predicting house price from 3 attributes

Size (m^2)	Age (year)	Region	Price (10^6T)
100	2	5	500
80	25	3	250
…	…	…	…

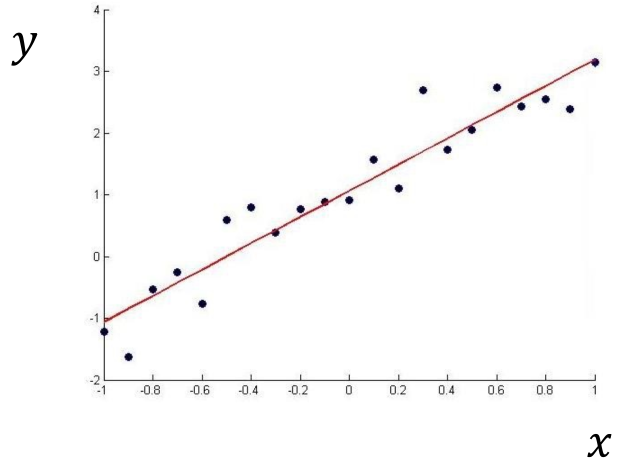
Learning problem

- Selecting a **hypothesis space**
  - Hypothesis space: a set of mappings from feature vector to target
- **Learning (estimation)**: optimization of a cost function
  - Based on the training set $D = \left\{\left(\boldsymbol{x}^{(i)}, y^{(i)}\right)\right\}_{i=1}^{n}$ and a cost function we find (an estimate) $f \in F$ of the target function
- **Evaluation**: we measure how well f generalizes to unseen examples

Linear regression: hypothesis space

- Univariate

$$f : \mathbb{R} \to \mathbb{R} \quad f(x; \boldsymbol{w}) = w_0 + w_1 x$$



- Multivariate

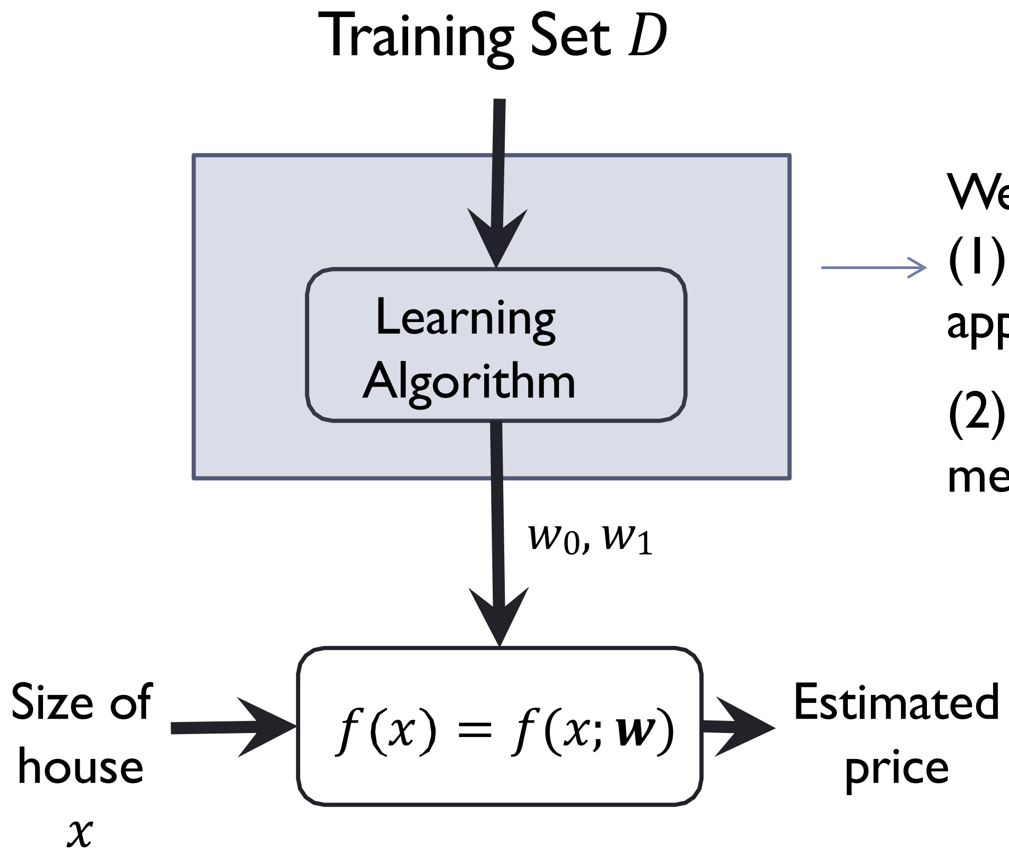
$$f : \mathbb{R}^d \to \mathbb{R} \quad f(\boldsymbol{x}; \boldsymbol{w}) = w_0 + w_1 x_1 + \ldots w_d x_d$$

$\boldsymbol{w} = [w_0, w_1, \ldots, w_d]^T$ are parameters we need to set.

Learning algorithm

- Select how to measure the error (i.e. prediction loss)
- Find the minimum of the resulting error or cost function

Learning algorithm

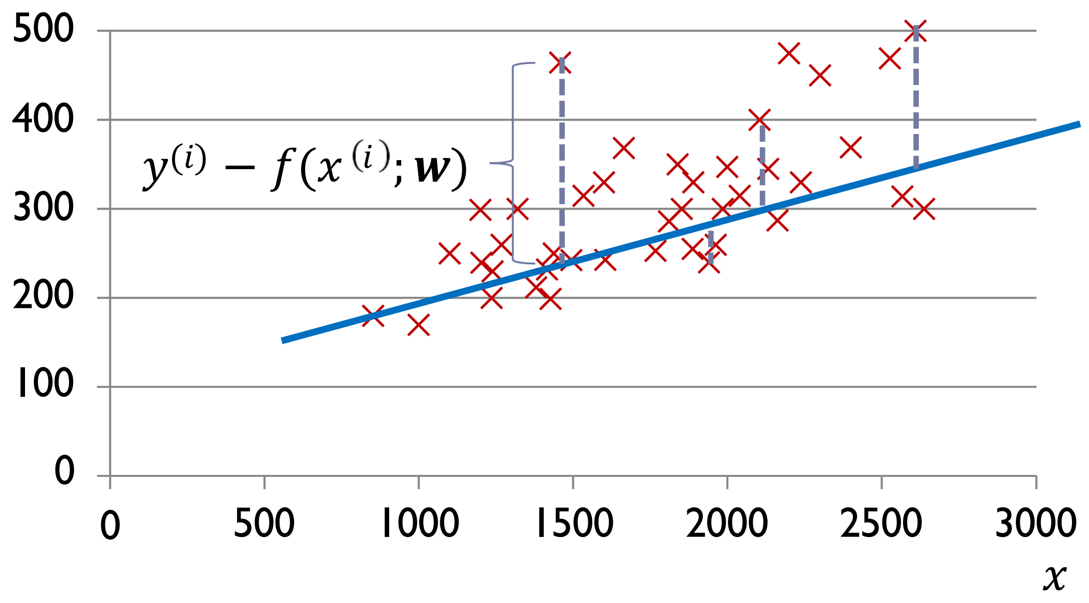


We need to

(1) measure how well $f(x; \boldsymbol{w})$ approximates the target

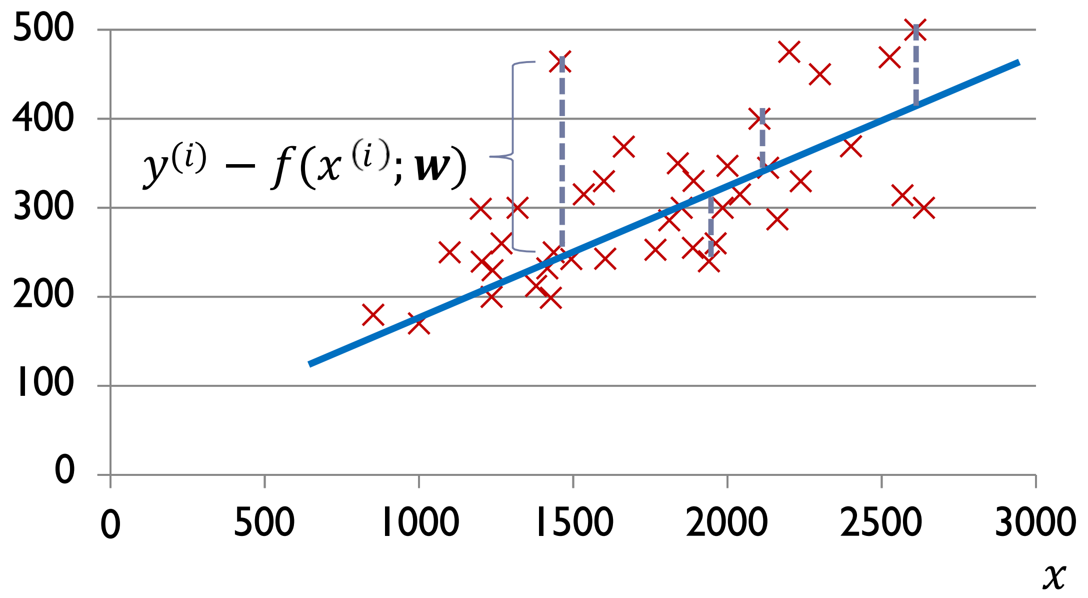
(2) choose $\boldsymbol{w}$ to minimize the error measure

How to measure the error



Squared error: $\left(y^{(i)} - f\left(x^{(i)}; \boldsymbol{w}\right)\right)^2$

Linear regression: univariate example



Cost function:

$$J(\boldsymbol{w}) = \sum_{i=1}^{n} \left(y^{(i)} - f(x; \boldsymbol{w})\right)^2$$

$$= \sum_{i=1}^{n} \left(y^{(i)} - w_0 - w_1 x^{(i)}\right)^2$$

Regression: squared loss

- In the SSE cost function, we used squared error as the prediction loss:

$$Loss(y, \hat{y}) = (y - \hat{y})^2 \qquad \hat{y} = f(\boldsymbol{x}; \boldsymbol{w})$$

- Cost function (based on the training set):

$$J(\boldsymbol{w}) = \sum_{i=1}^{n} Loss\left(y^{(i)}, f\left(\boldsymbol{x}^{(i)}; \boldsymbol{w}\right)\right)$$
$$= \sum_{i=1}^{n} \left(y^{(i)} - f\left(\boldsymbol{x}^{(i)}; \boldsymbol{w}\right)\right)^2$$

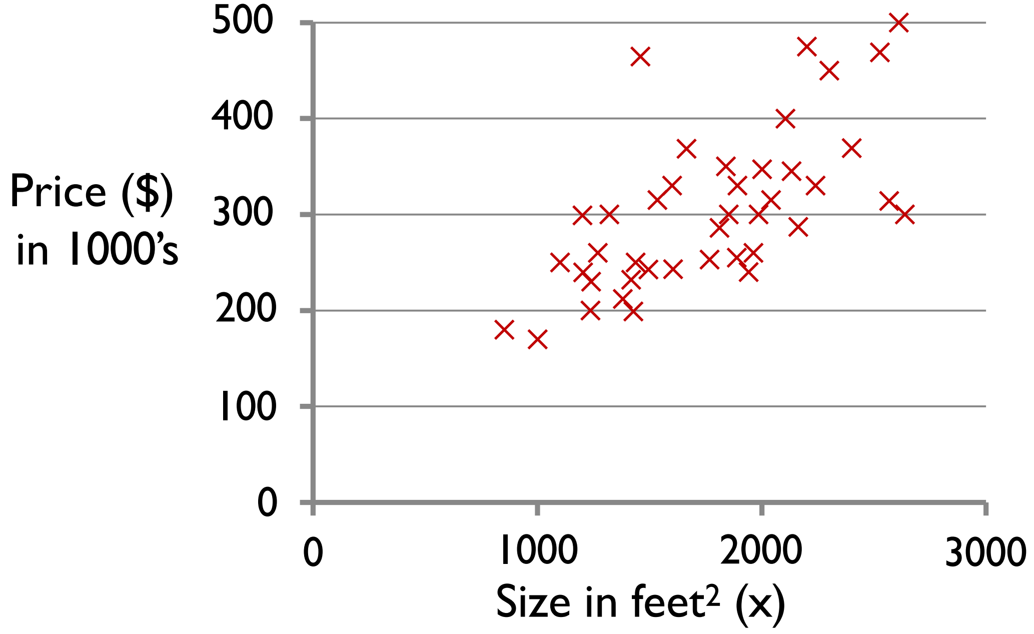
- Minimizing sum (or mean) of squared errors is a common approach in curve fitting, neural network, etc.

Sum of Squares Error (SSE) cost function

$$J(\boldsymbol{w}) = \sum_{1=i}^{n} \left(y^{(i)} - f(\boldsymbol{x}^{(i)}; \boldsymbol{w})\right)^2$$

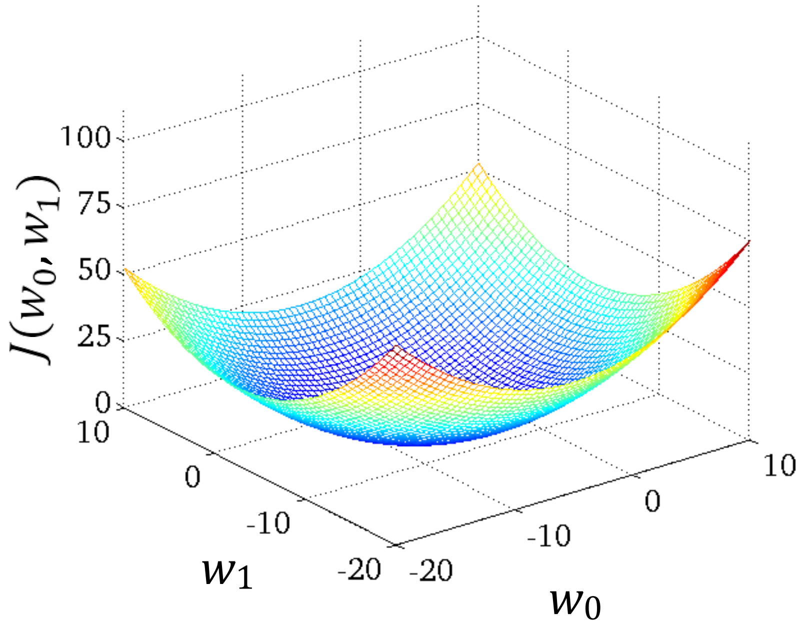
- $J(\boldsymbol{w})$: sum of the squares of the prediction errors on the training set
- We want to find the best regression function $f\left(\boldsymbol{x}^{(i)}; \boldsymbol{w}\right)$
  - equivalently, the best $\boldsymbol{w}$
- Minimize $J(\boldsymbol{w})$
  - Find optimal $f(\boldsymbol{x}) = f(\boldsymbol{x}; \boldsymbol{w})$ where $\boldsymbol{w} = \underset{\boldsymbol{w}}{\operatorname{argmin}} J(\boldsymbol{w})$

Cost function: univariate example



$J(\boldsymbol{w})$

(function of the parameters w_0, w_1)



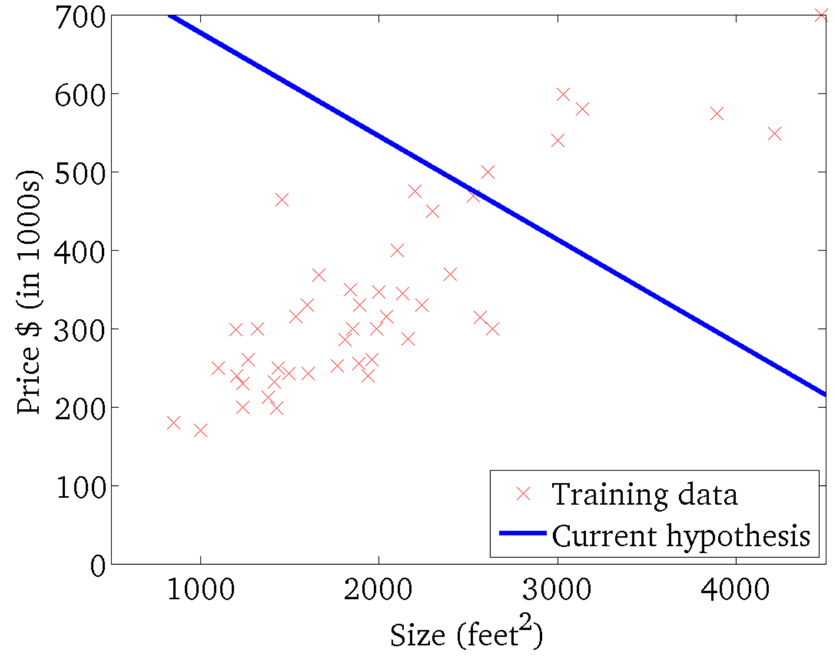
Cost function: univariate example

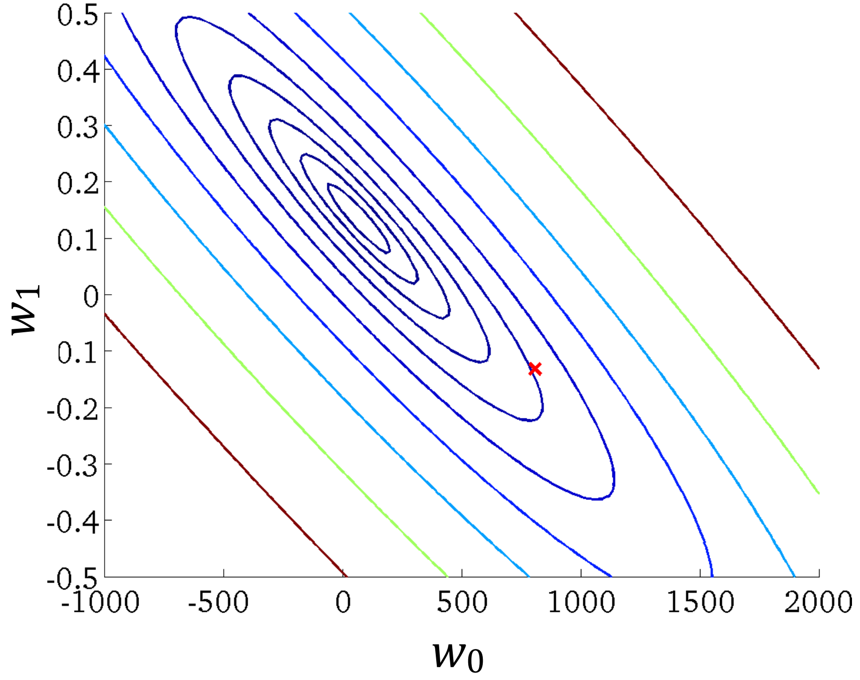
$$f(x; w_0, w_1) = w_0 + w_1 x$$

(for fixed w_0,w_1,this is a function of x)

$$J(w_0, w_1)$$

(function of the parameters w_0,w_1)





Cost function: univariate example

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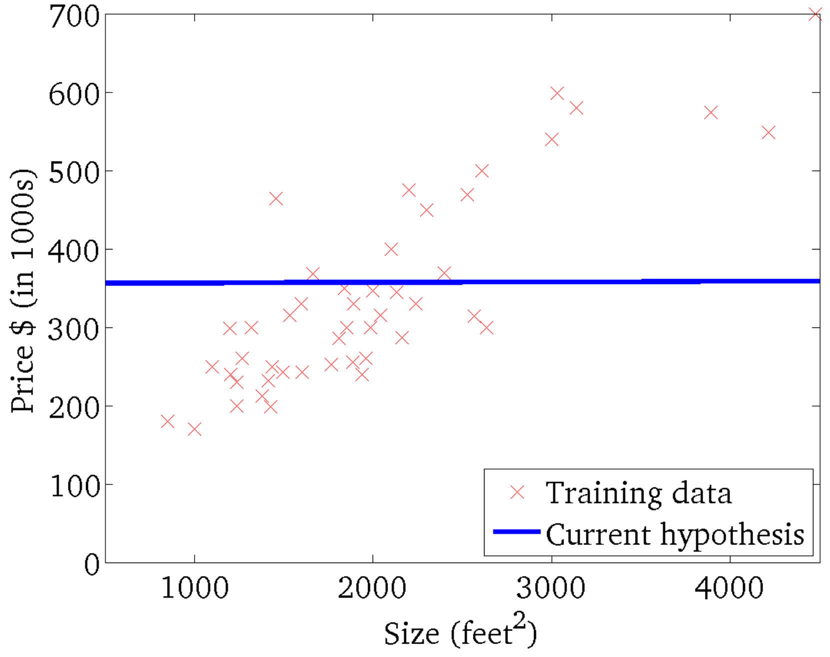
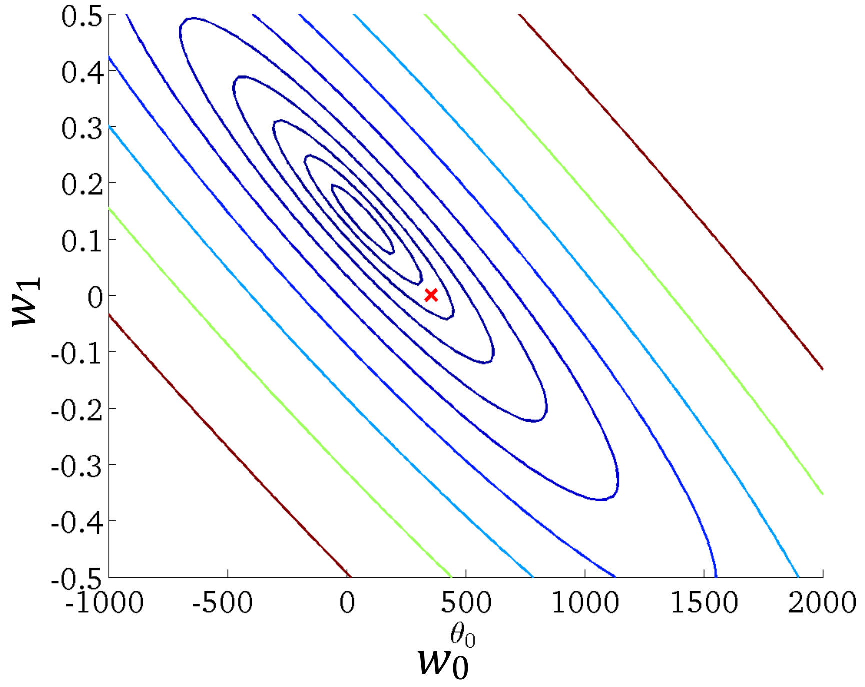


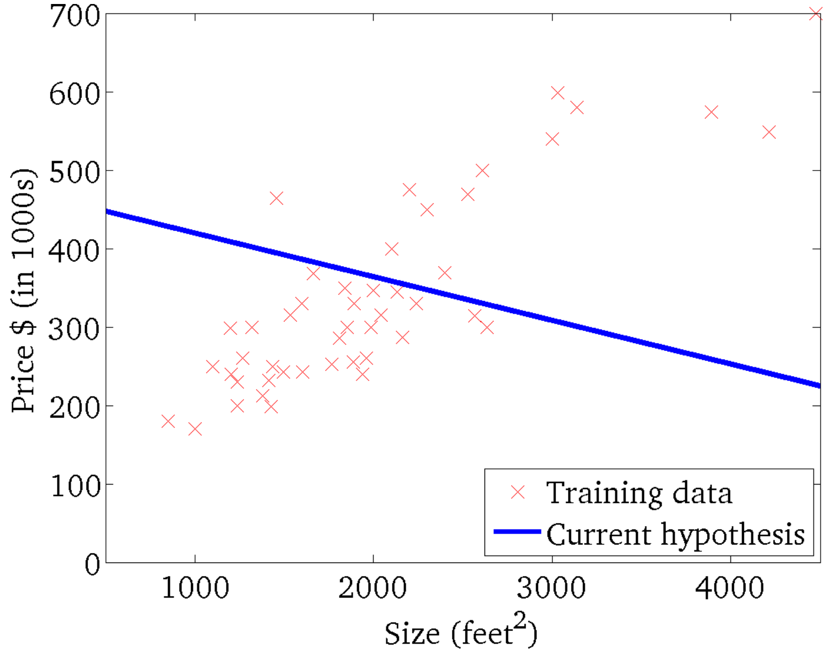
$J(w_0, w_1)$

(function of the parameters w_0,w_1)



Cost function: univariate example

$$f(x; w_0, w_1) = w_0 + w_1 x$$



$$J(w_0, w_1)$$

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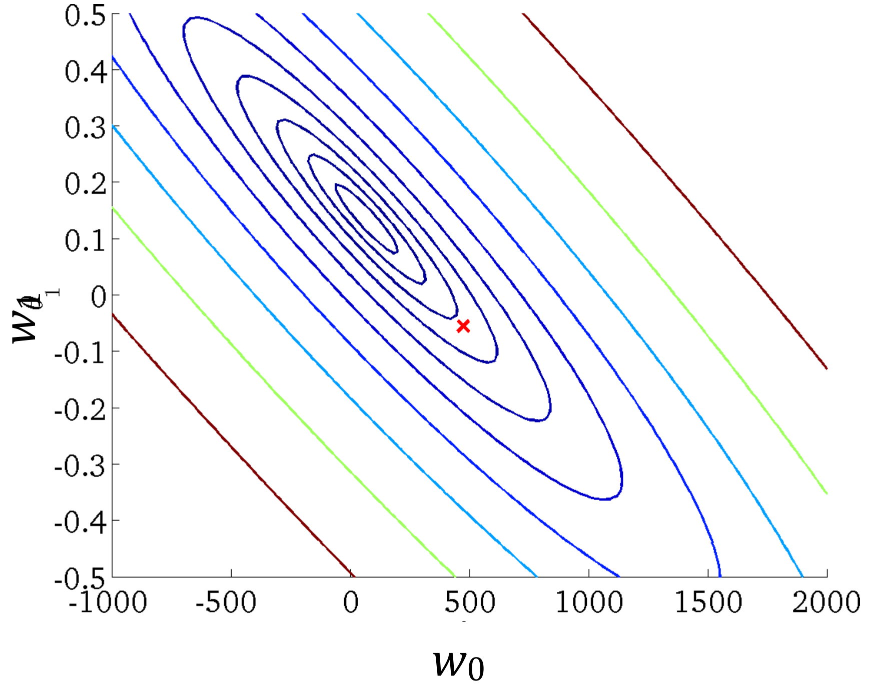

Cost function: univariate example

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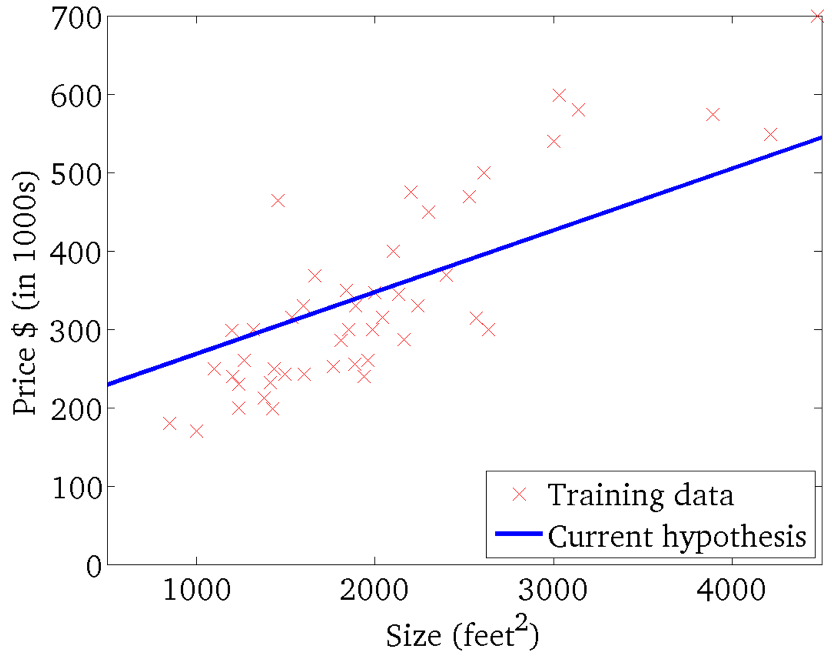

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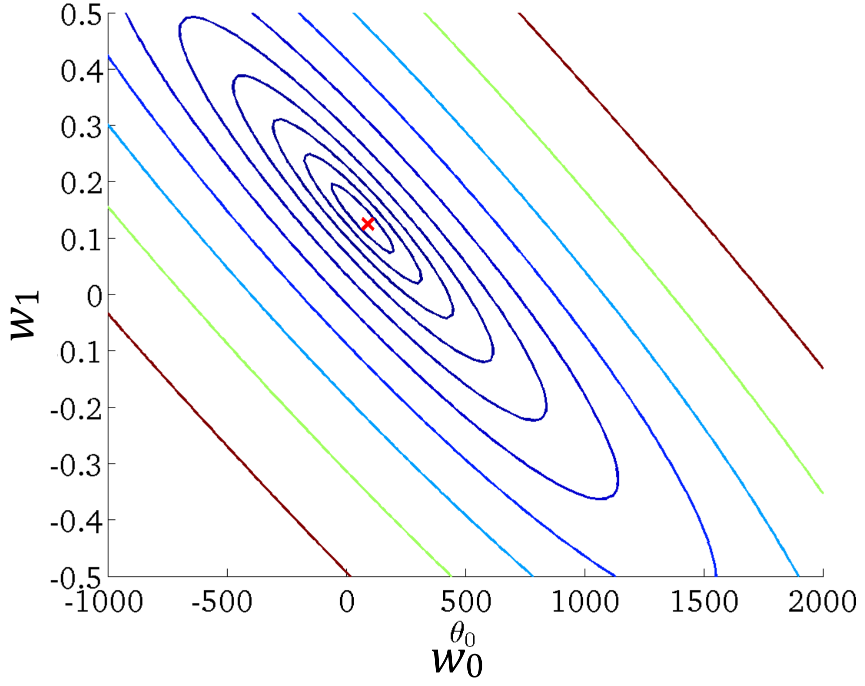


Cost function optimization: univariate

$$J(\boldsymbol{w}) = \frac{1}{2}\sum_{i=1}^{n}\left(y^{(i)} - w_0 - w_1 x^{(i)}\right)^2$$

- Necessary conditions for the"optimal" parameter values:

$$\frac{\partial J(\boldsymbol{w})}{\partial w_0} = 0$$

$$\frac{\partial J(\boldsymbol{w})}{\partial w_1} = 0$$

Optimality conditions: univariate

$$J(\boldsymbol{w}) = \frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - w_0 - w_1 x^{(i)}\right)^2$$

$$\frac{\partial J(\boldsymbol{w})}{\partial w_1} = \sum_{i=1}^{n} \left(y^{(i)} - w_0 - w_1 x^{(i)}\right)\left(-x^{(i)}\right) = 0$$

$$\frac{\partial J(\boldsymbol{w})}{\partial w_0} = \sum_{i=1}^{n} \left(y^{(i)} - w_0 - w_1 x^{(i)}\right)(-1) = 0$$

- A systems of 2 linear equations

Cost function: multivariate

- We have to minimize the empirical squared loss:

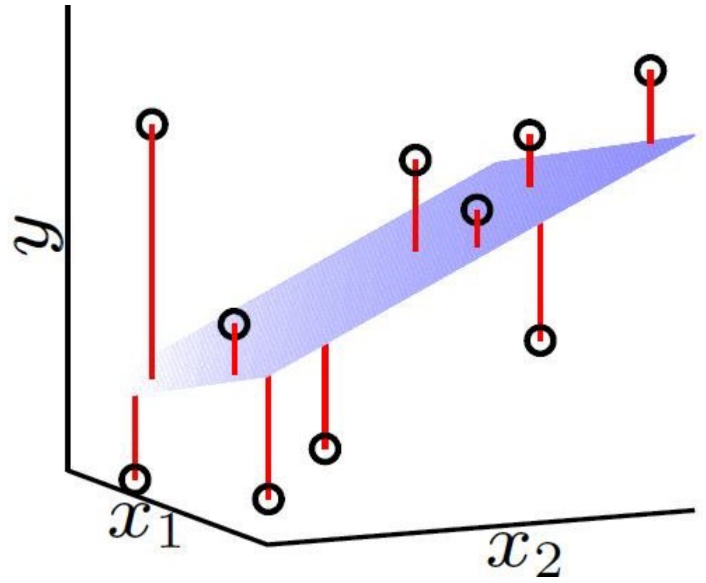
$$J(\boldsymbol{w}) = \sum_{1=i}^{n} \left(y^{(i)} - f(\boldsymbol{x}^{(i)};\boldsymbol{w})\right)^2$$

$$f(\boldsymbol{x};\boldsymbol{w}) = w_0 + w_1 x_1 + \ldots w_d x_d$$

$$\boldsymbol{w} = [w_0, w_1, \ldots, w_d]^T$$

$$\boldsymbol{w} = \underset{\boldsymbol{w} \in \mathbb{R}^{d+1}}{\operatorname{argmin}} J(\boldsymbol{w})$$

Cost function and optimal linear model



- Necessary conditions for the "optimal" parameter values:

$$\nabla_{\boldsymbol{w}} J(\boldsymbol{w}) = \mathbf{0}$$

- A system of $d + 1$ linear equations

Cost function: matrix notation

$$J(\boldsymbol{w}) = \sum_{i=1}^{n} \left(y^{(i)} - f(\boldsymbol{x}^{(i)}; \boldsymbol{w})\right)^2 =$$

$$= \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)}\right)^2$$

$$\boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix} \quad \boldsymbol{X} = \begin{bmatrix} 1 & x_1^{(1)} & \cdots & x_d^{(1)} \\ 1 & x_1^{(2)} & \cdots & x_d^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & \cdots & x_d^{(n)} \end{bmatrix} \quad \boldsymbol{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}$$

$$J(\boldsymbol{w}) = \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|^2$$

Minimizing cost function

Optimal linear weight vector (for SSE cost function):

$$J(\boldsymbol{w}) = \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|^2$$

$$\nabla_{\boldsymbol{w}} J(\boldsymbol{w}) = 2\boldsymbol{X}^T(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w})$$

$$\nabla_{\boldsymbol{w}} J(\boldsymbol{w}) = \boldsymbol{0} \Rightarrow \boldsymbol{X}^T\boldsymbol{X}\boldsymbol{w} = \boldsymbol{X}^T\boldsymbol{y}$$

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

Minimizing cost function

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

$$\boldsymbol{w} = \boldsymbol{X}^{\dagger}\boldsymbol{y}$$

$$\boldsymbol{X}^{\dagger} = (\boldsymbol{X}^T\boldsymbol{X})^{-\mathbf{1}}\boldsymbol{X}^T$$

$\boldsymbol{X}^{\dagger}$ is pseudo inverse of $\boldsymbol{X}$

Another approach for optimizing the sum squared error

- Iterative approach for solving the following optimization problem:

$$J(\boldsymbol{w}) = \sum_{i=1}^{n} \left(y^{(i)} - f(\boldsymbol{x}^{(i)}; \boldsymbol{w})\right)^2$$

Gradient descent

- Cost function: $J(\boldsymbol{w})$
- Optimization problem: $\boldsymbol{w} = \underset{\boldsymbol{w}}{\operatorname{argm}in}\, J(\boldsymbol{w})$
- Steps:
  - Start from $\boldsymbol{w}^0$
  - Repeat
    - Update $\boldsymbol{w}^t$ to $\boldsymbol{w}^{t+1}$ in order to reduce J
    - $t \leftarrow t + 1$
  - until we hopefully end up at a minimum

Gradient descent

- First-order optimization algorithm to find $\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}}\, J(\boldsymbol{w})$
  - Also known as "**steepest descent**"
- In each step, takes steps proportional to the negative of the gradient vector of the function at the current point $\boldsymbol{w}^t$:

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \gamma_t \nabla J(\boldsymbol{w}^t)$$

  - $J(\boldsymbol{w})$ <u>decreases fastest</u> if one goes from $\boldsymbol{w}^t$ in the direction of $-\nabla J(\boldsymbol{w}^t)$
  - Assumption: $J(\boldsymbol{w})$ is defined and differentiable in a neighborhood of a point $\boldsymbol{w}^t$

Gradient ascent takes steps proportional to (the positive of) the gradient to find a local maximum of the function

Gradient descent

- Minimize $J(\boldsymbol{w})$

Step size
(Learning rate parameter)

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \eta \nabla_{\boldsymbol{w}} J(\boldsymbol{w}^{t})$$

$$\nabla_{\boldsymbol{w}} J(\boldsymbol{w}) = [\frac{\partial J(\boldsymbol{w})}{\partial w_1}, \frac{\partial J(\boldsymbol{w})}{\partial w_2}, \dots, \frac{\partial J(\boldsymbol{w})}{\partial w_d}]$$

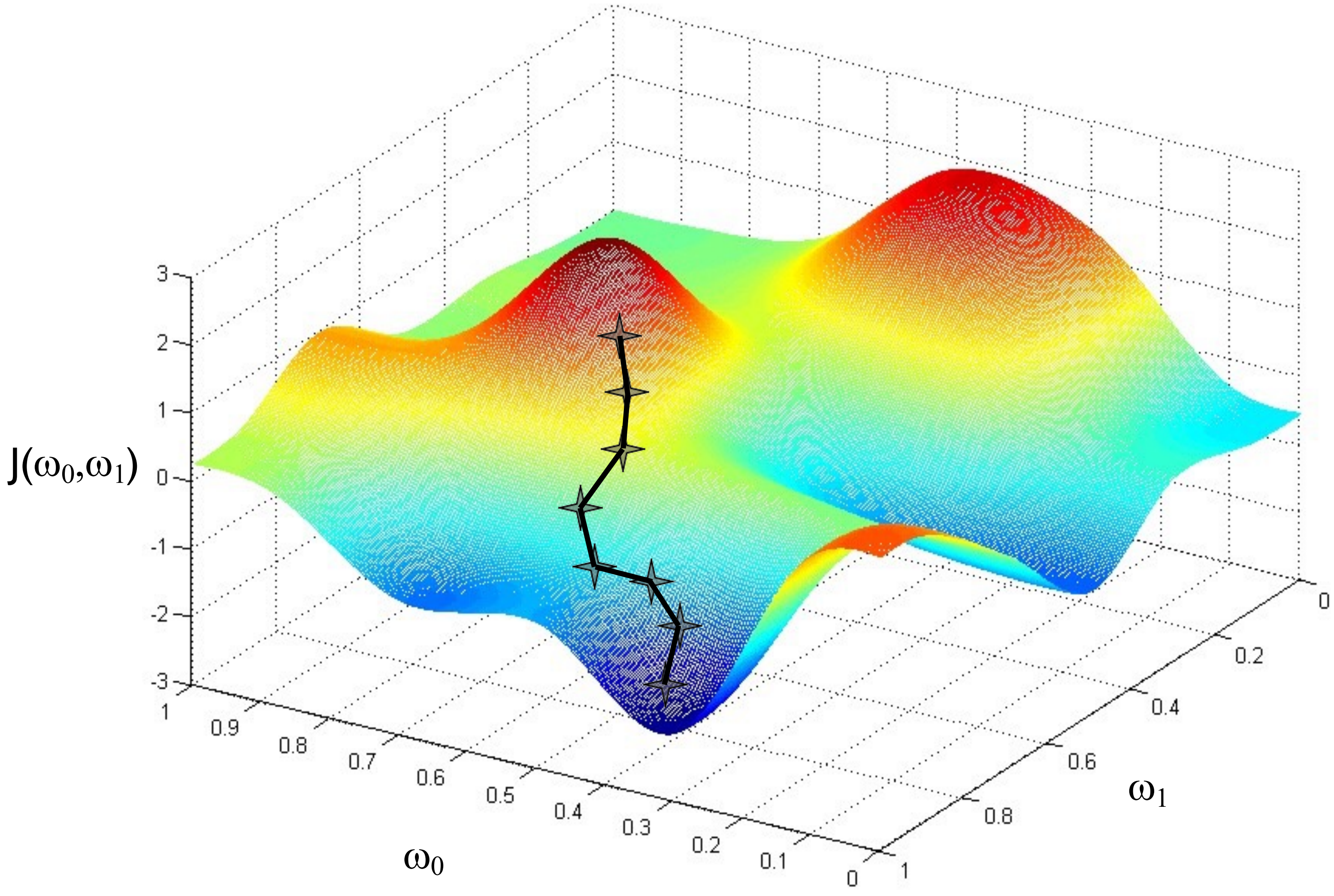
- If η is small enough, then $J\,(\boldsymbol{w}^{t+1}) \leq J(\boldsymbol{w}^{t})$.
- η can be allowed to change at every iteration as η_t.

Gradient descent

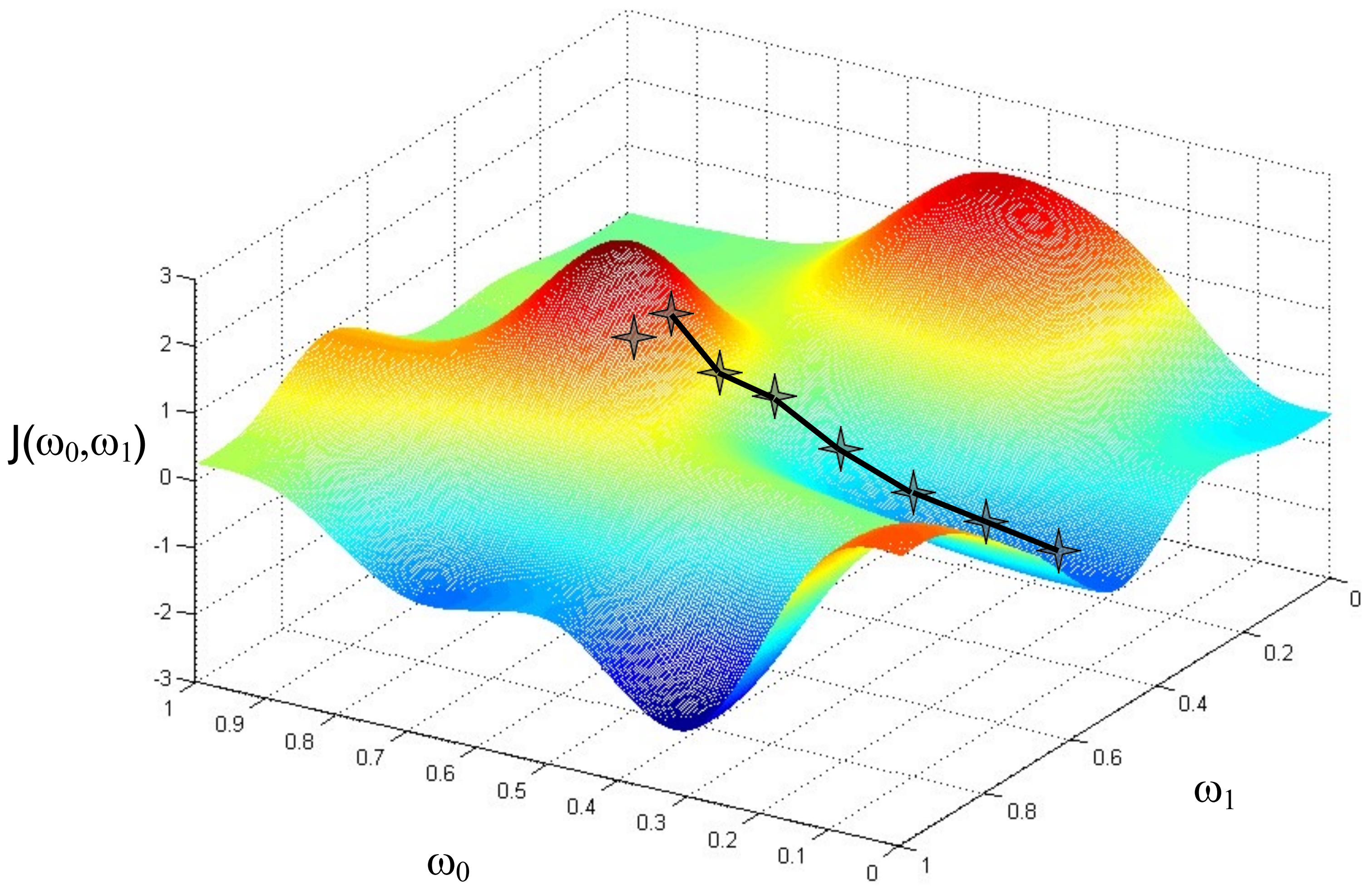
- Local minima problem

- However, when J is convex, all local minima are also global minima $\Rightarrow$ gradient descent can converge to the global solution.

Problem of gradient descent with non-convex cost functions



Problem of gradient descent with non-convex cost functions



Gradient descent for SSE cost function

- Minimize $J(\boldsymbol{w})$

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} - \eta \nabla_{\boldsymbol{w}} J(\boldsymbol{w}^{t})$$

- $J(\boldsymbol{w})$: Sum of squares error

$$J(\boldsymbol{w}) = \frac{1}{2} \sum_{i=1}^{n} \left(y^{(i)} - f\left(\boldsymbol{x}^{(i)}; \boldsymbol{w}\right) \right)^{2}$$

- Weight update rule for $f(\boldsymbol{x}; \boldsymbol{w}) = \boldsymbol{w}^{T}\boldsymbol{x}$:

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^{t} + \eta \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{w}^{t^{T}} \boldsymbol{x}^{(i)} \right) \boldsymbol{x}^{(i)}$$

Gradient descent for SSE cost function

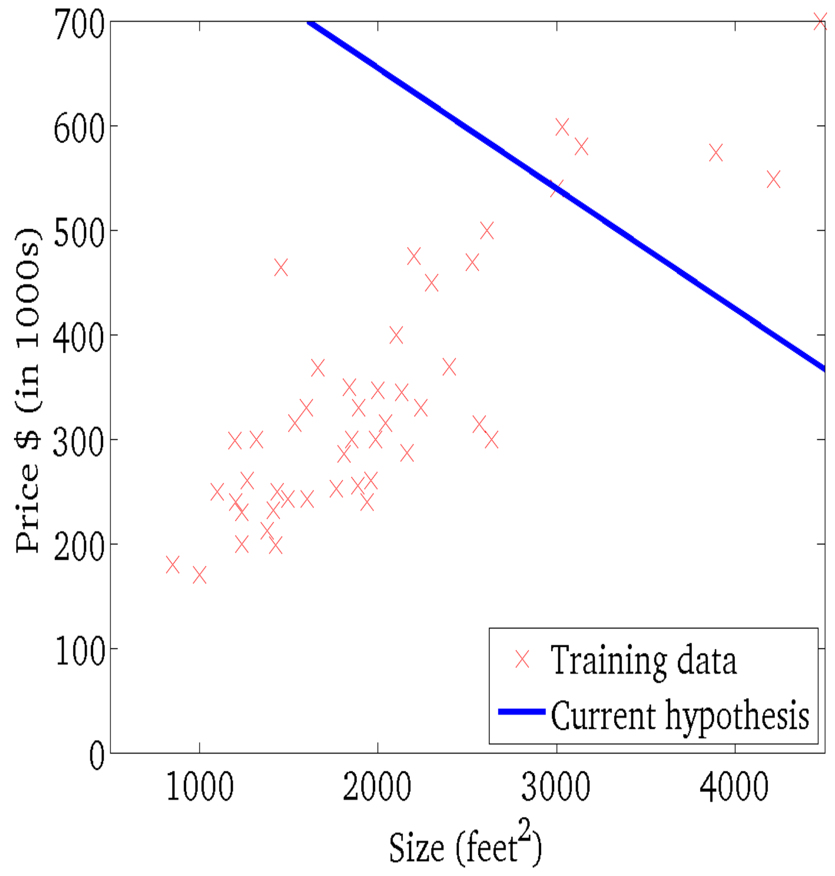
- Weight update rule: $f\ (\boldsymbol{x}; \boldsymbol{w}) = \boldsymbol{w}^T \boldsymbol{x}$

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t + \eta \sum_{1=i}^{n} \left(y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)} \right) \boldsymbol{x}^{(i)}$$

Batch mode: each step considers all training data

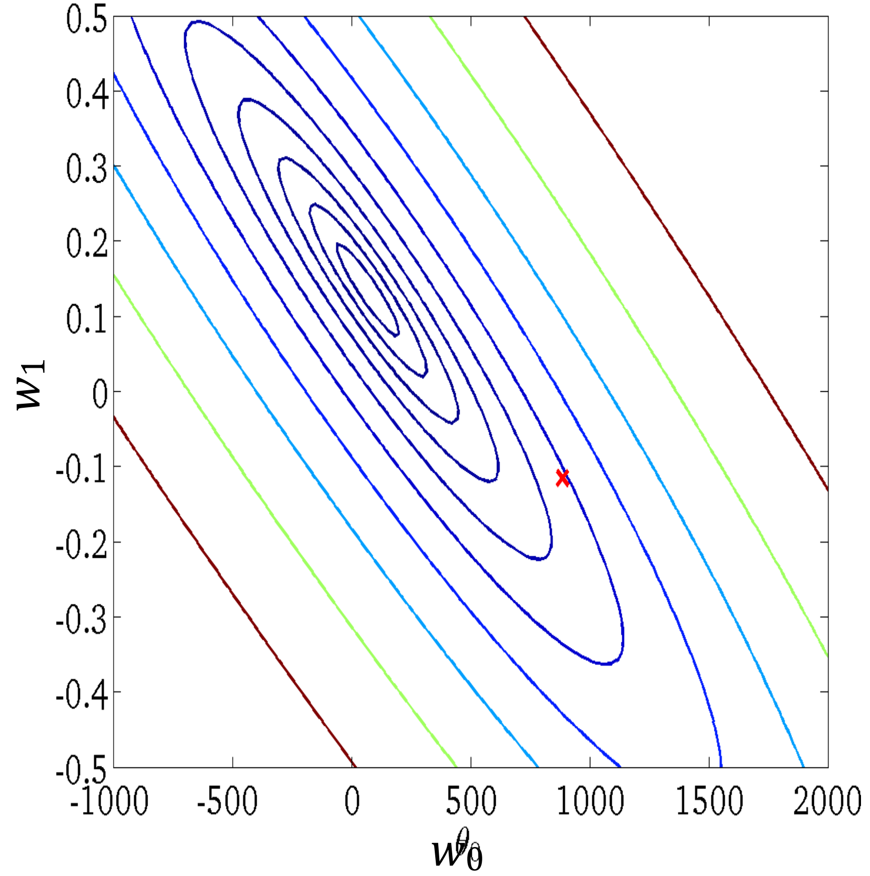
- η: too small → gradient descent can be slow.
- η: too large → gradient descent can overshoot the minimum. It may fail to converge, or even diverge.

$f(x; w_0, w_1) = w_0 + w_1 x$



$J(w_0, w_1)$

(function of the parameters w_0,w_1)



This example has been adopted from: Prof. Ng's slides (ML Online Course, Stanford)

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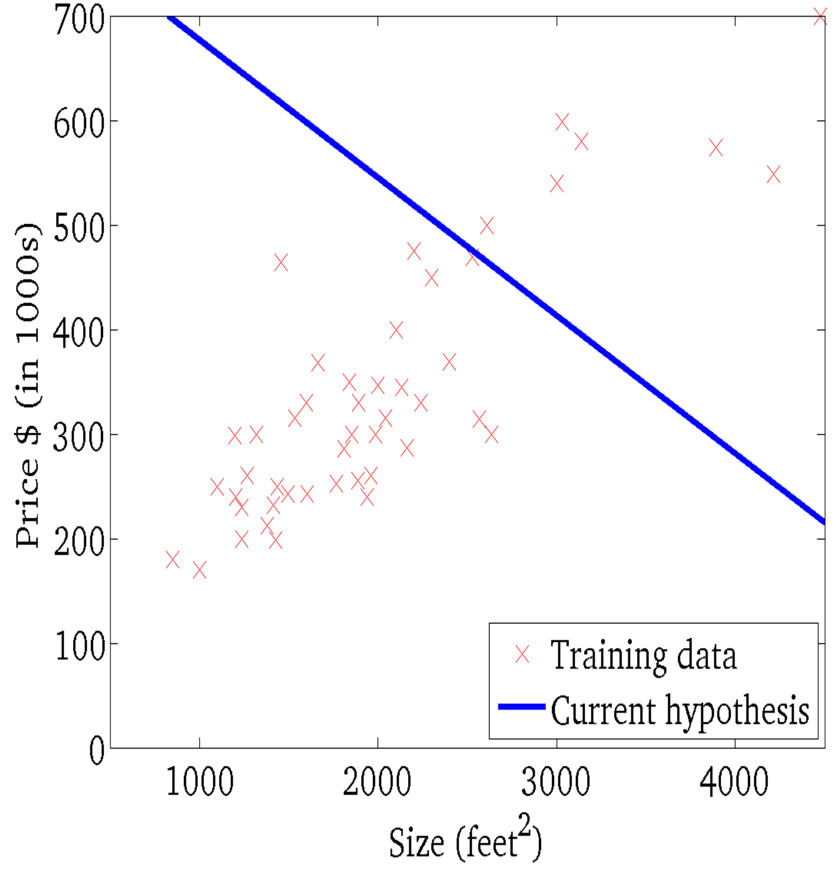

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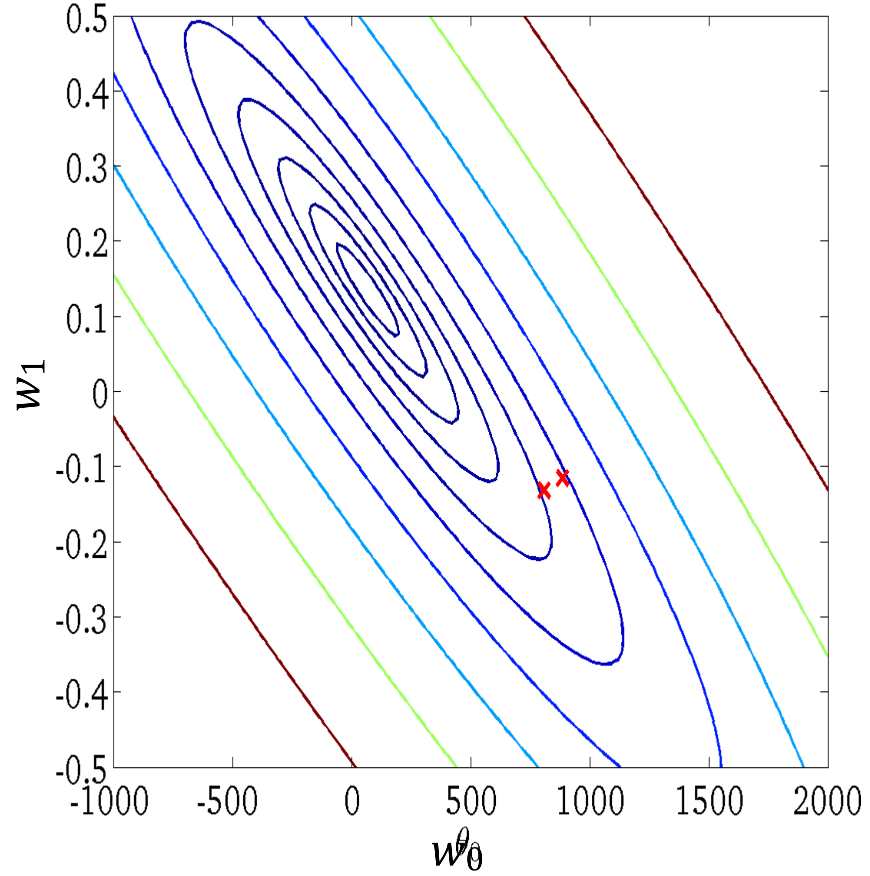

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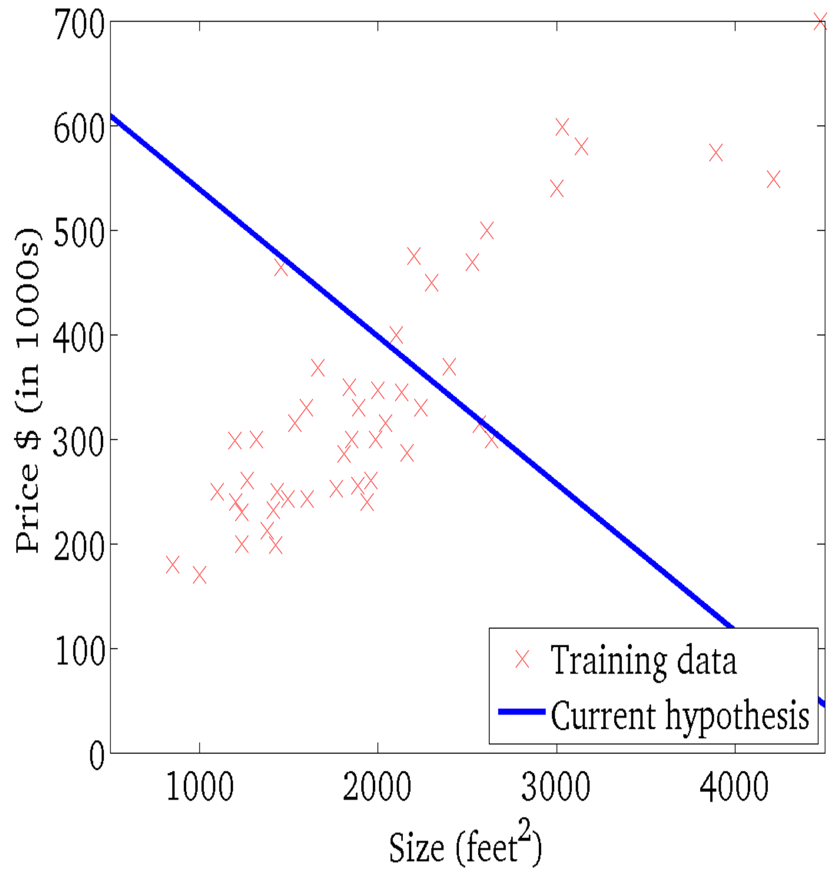

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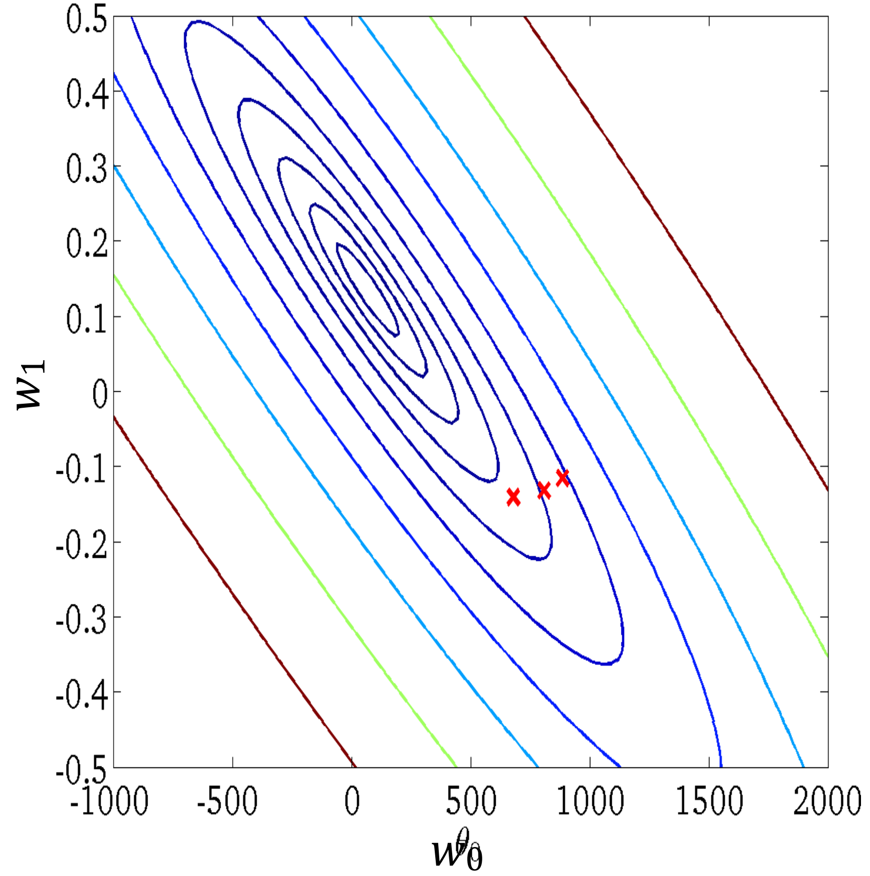

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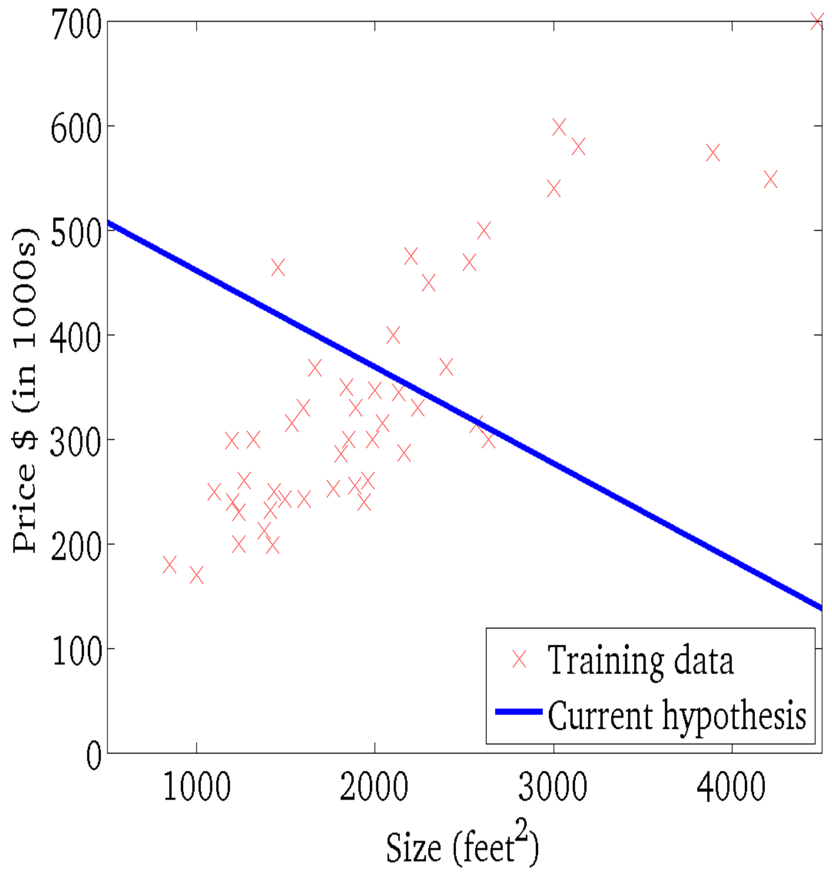

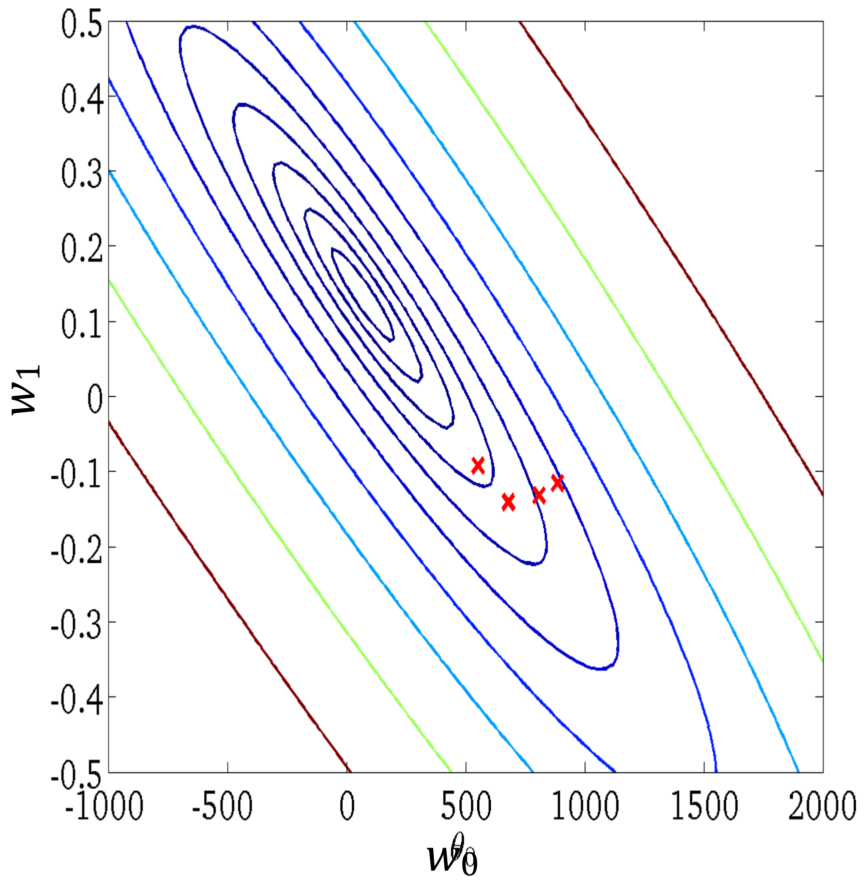

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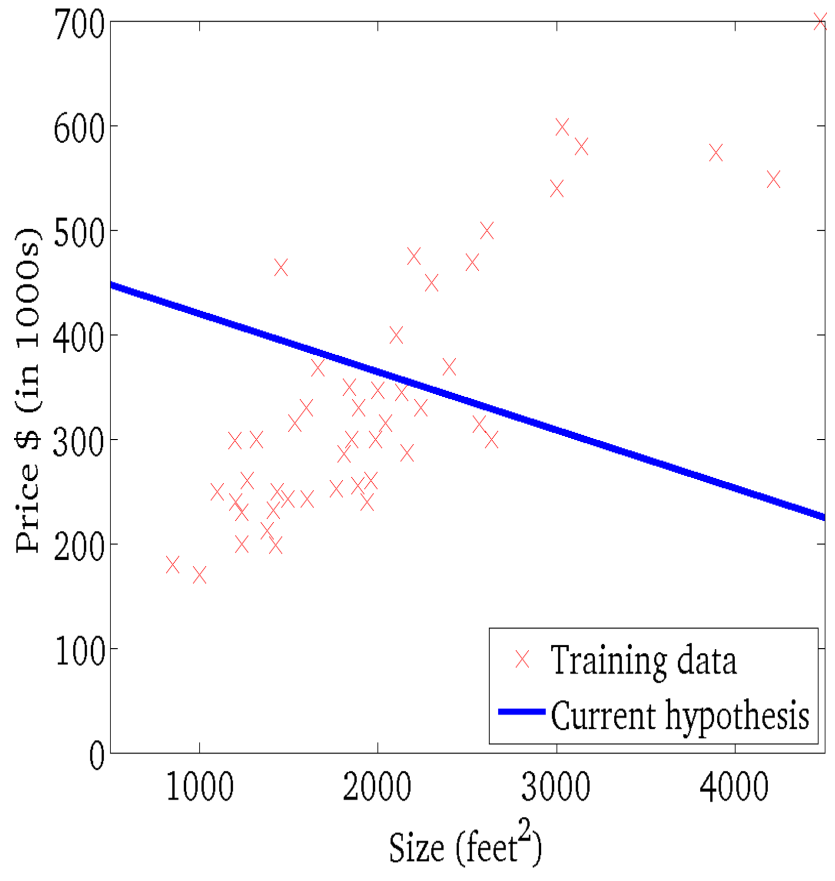

$J(w_0, w_1)$

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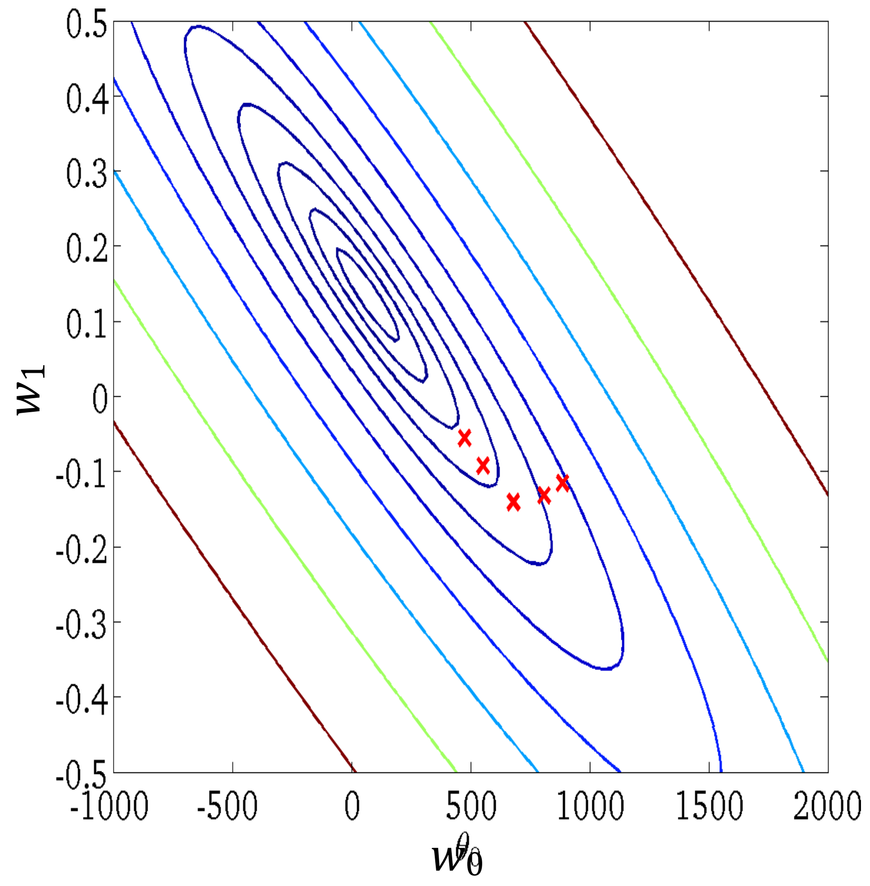

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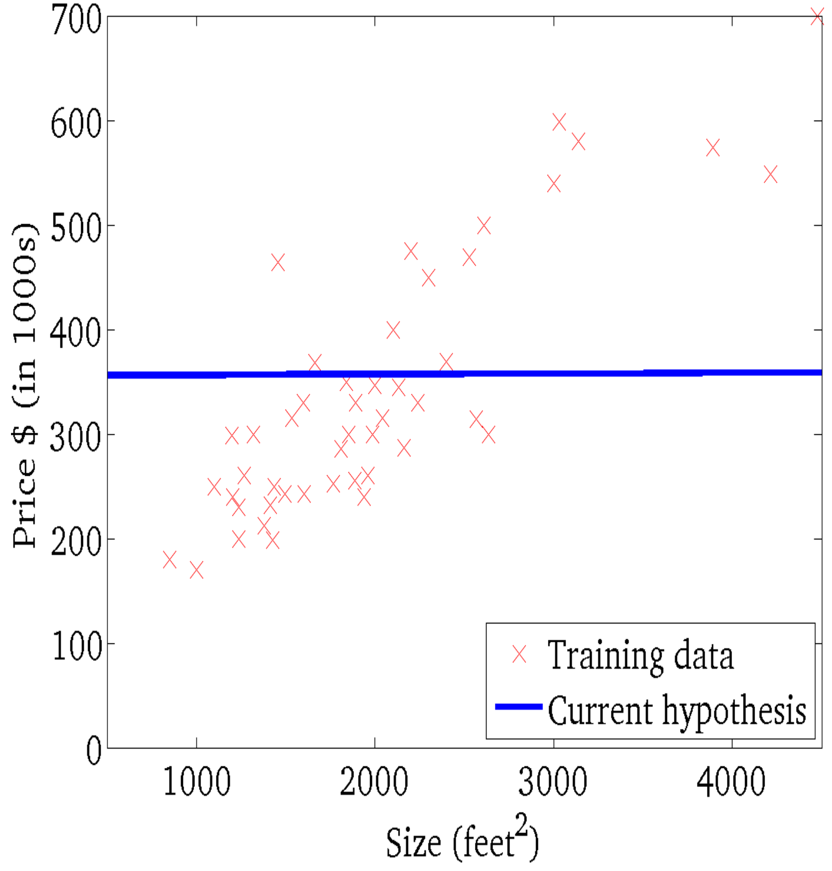

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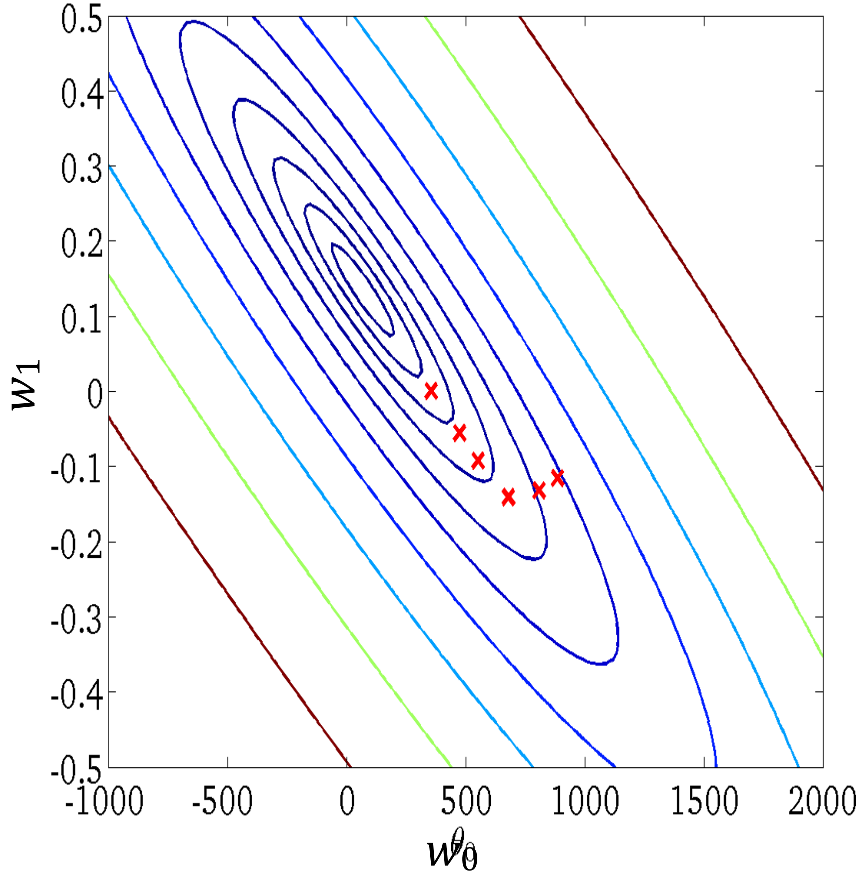

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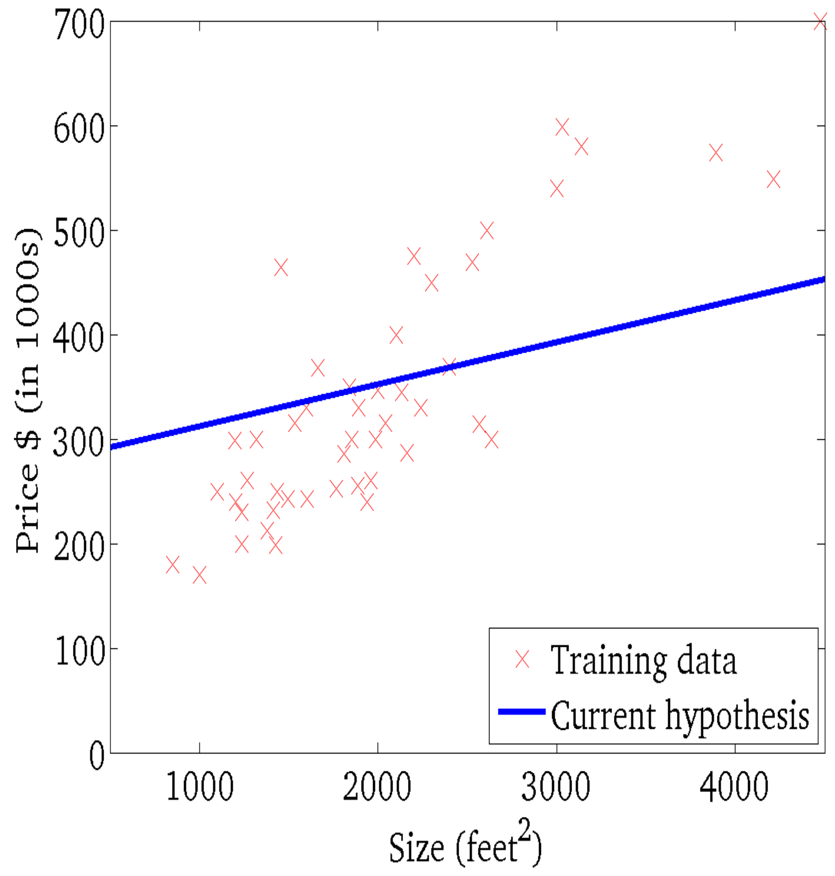
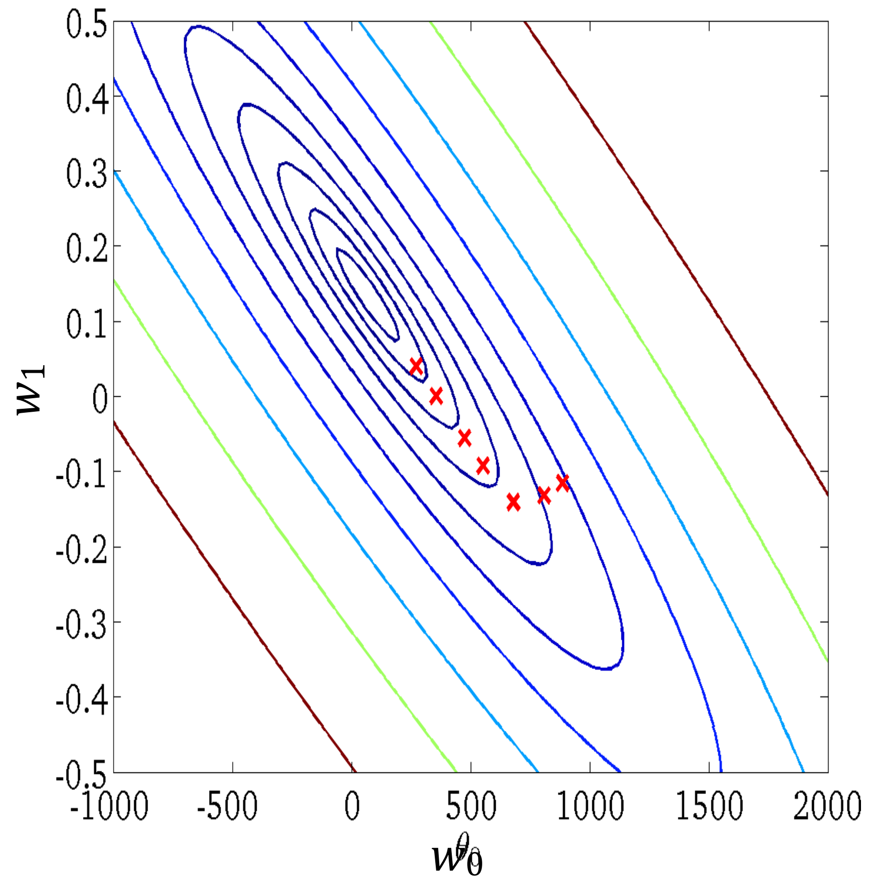


$J(w_0, w_1)$

(function of the parameters w_0,w_1)



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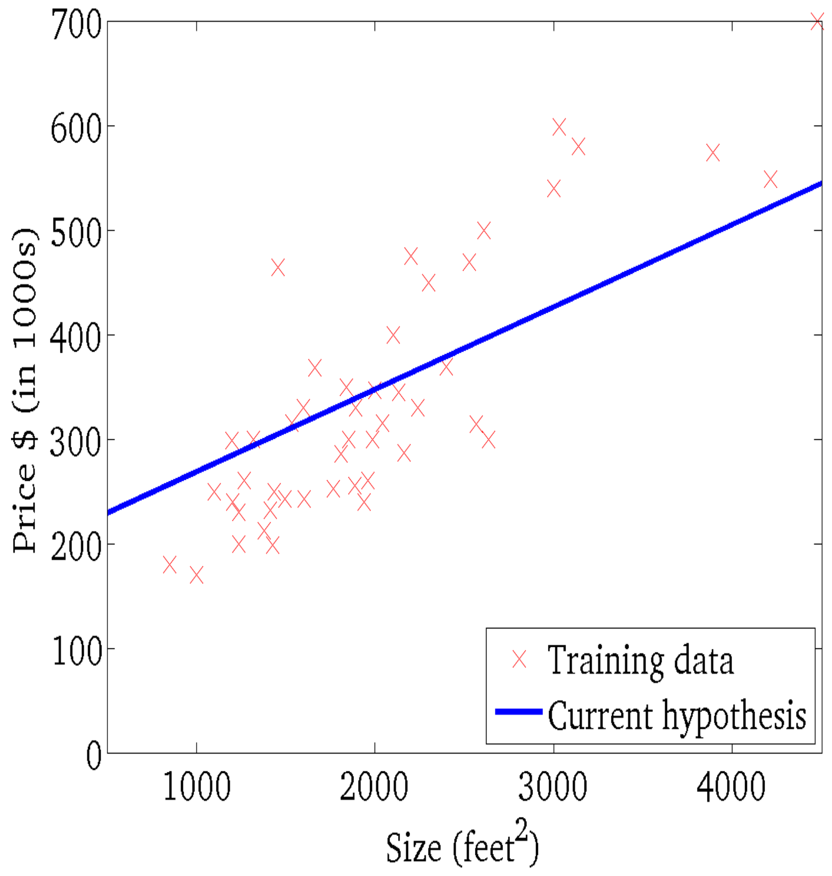

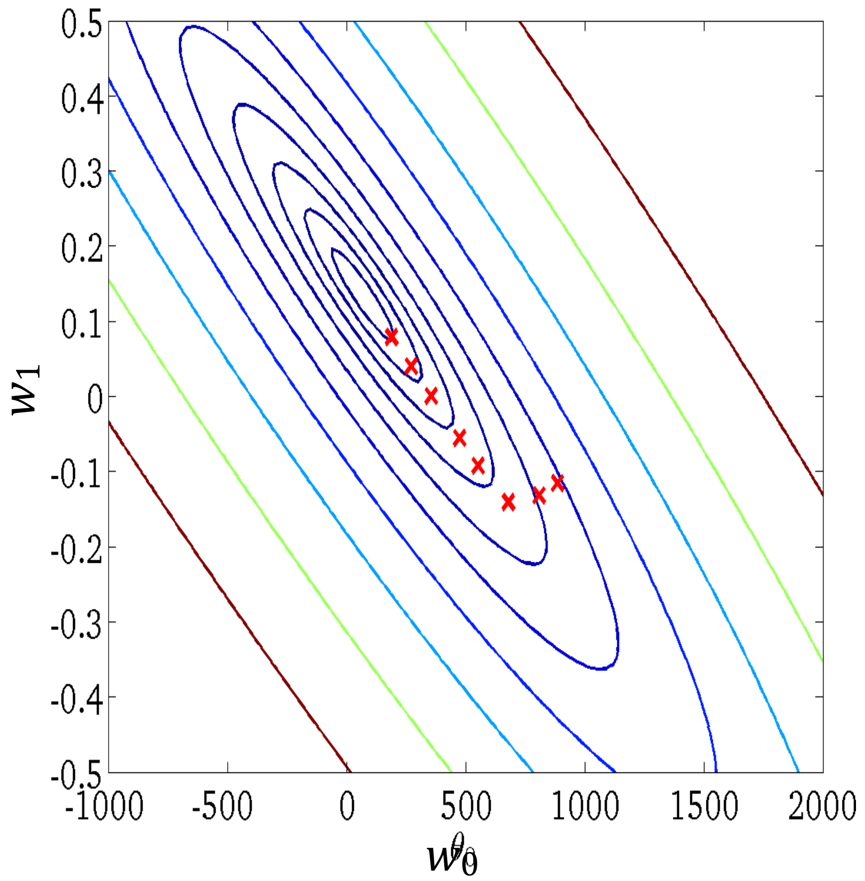

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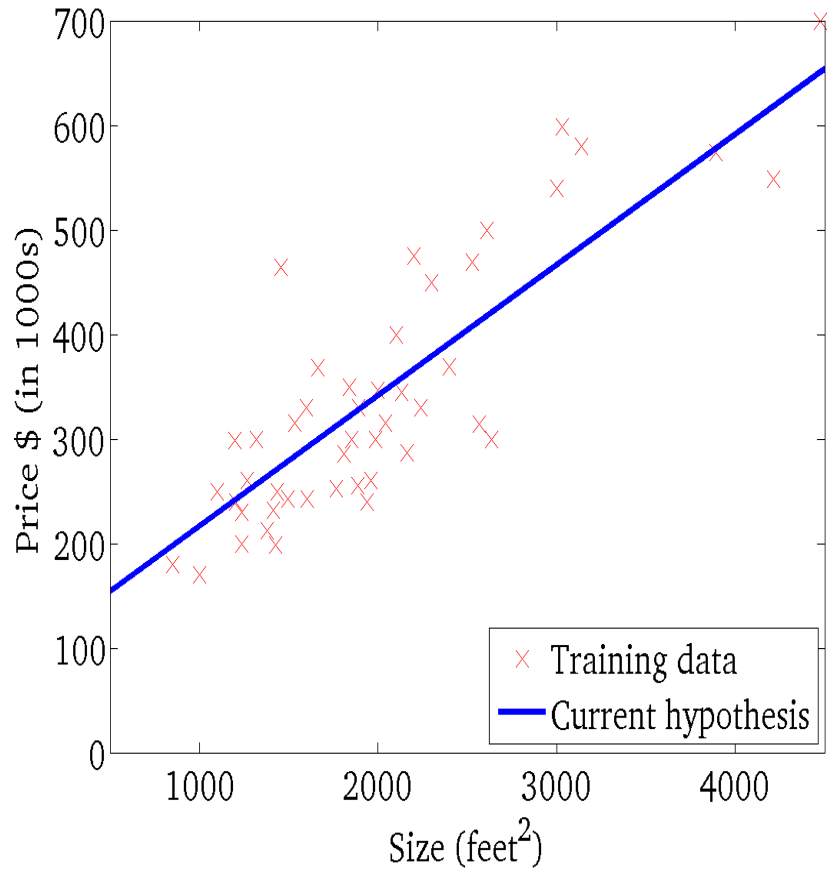
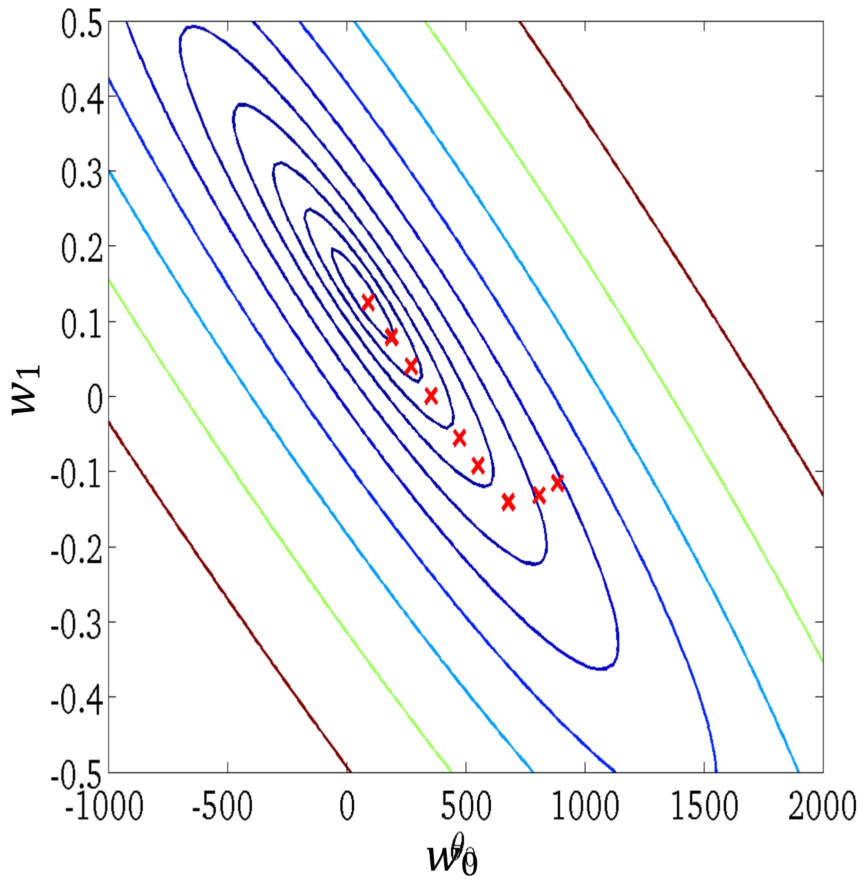




This example has been adopted from: Prof. Ng's slides (ML Online Course, Stanford)

Stochastic gradient descent

- Example: Linear regression with SSE cost function

$$J^{(i)}(\boldsymbol{w}) = \left(y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)}\right)^2$$

$$\boldsymbol{w}^{t+1} = \boldsymbol{w}^t - \eta \nabla_{\boldsymbol{w}} J^{(i)}(\boldsymbol{w})$$

$$\boxed{\boldsymbol{w}^{t+1} = \boldsymbol{w}^t + \eta \left(y^{(i)} - \boldsymbol{w}^T \boldsymbol{x}^{(i)}\right) \boldsymbol{x}^{(i)}}$$

Least Mean Squares (LMS)

It is proper for sequential or online learning

Stochastic gradient descent: online learning

- Sequential learning is also appropriate for real-time applications
  - data observations are arriving in a continuous stream
  - and predictions must be made before seeing all of the data

- The value of η needs to be chosen with care to ensure that the algorithm converges

Evaluation and generalization

- Why minimizing the cost function (based on only training data) while we are interested in the performance on new examples?

$$\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} Loss\left(y^{(i)}, f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})\right) \longrightarrow \text{Empirical loss}$$

- **Evaluation**: After training, we need to measure how well the learned prediction function can predicts the target for unseen examples

Training and test performance

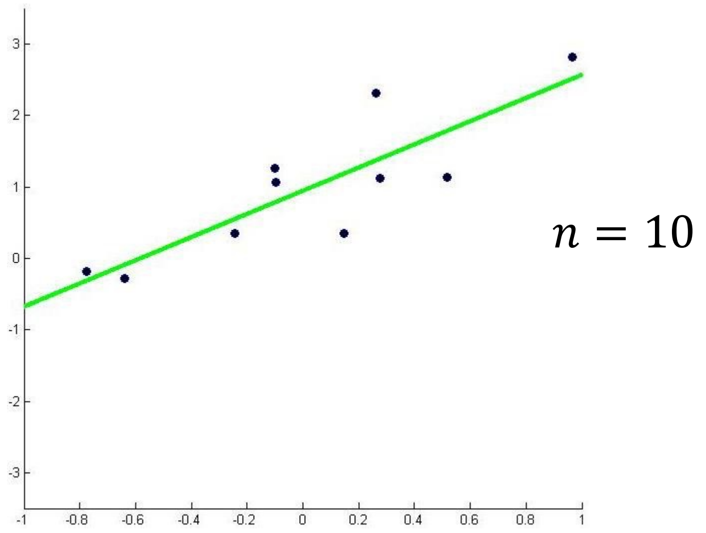
- Assumption: training and test examples are drawn independently at random from the same but unknown distribution.
  - Each training/test example $(\boldsymbol{x}, y)$ is a sample from joint probability distribution $P(\boldsymbol{x}, y)$, i.e., $(\boldsymbol{x}, y) \sim P$

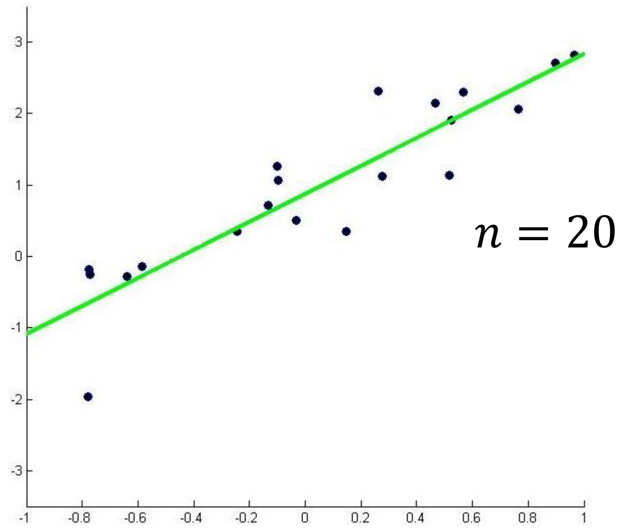
Empirical (training) loss = $\frac{1}{n}\sum_{i=1}^{n} Loss\left(y^{(i)}, f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta})\right)$

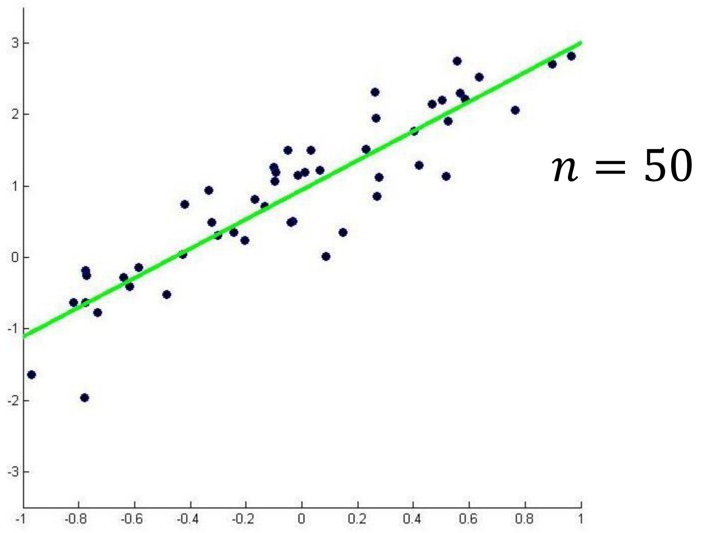
Expected (test) loss = $E_{\boldsymbol{x},y}\left\{Loss(y, f(\boldsymbol{x}; \boldsymbol{\theta}))\right\}$

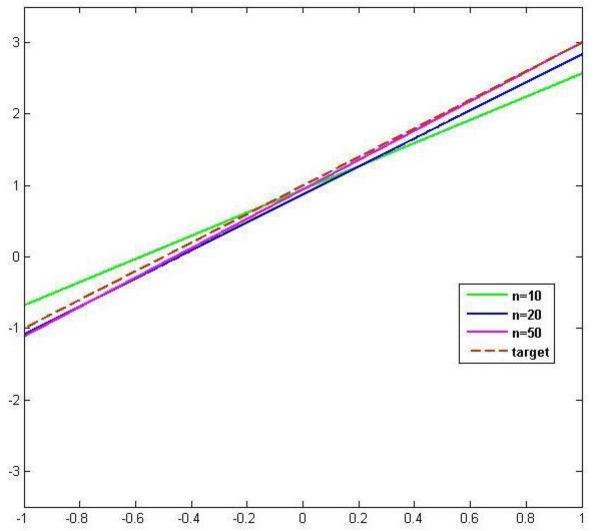
- We minimize empirical loss (on the training data) and expect to also find an acceptable expected loss
  - Empirical loss as a proxy for the performance over the whole distribution.

Linear regression: number of training data



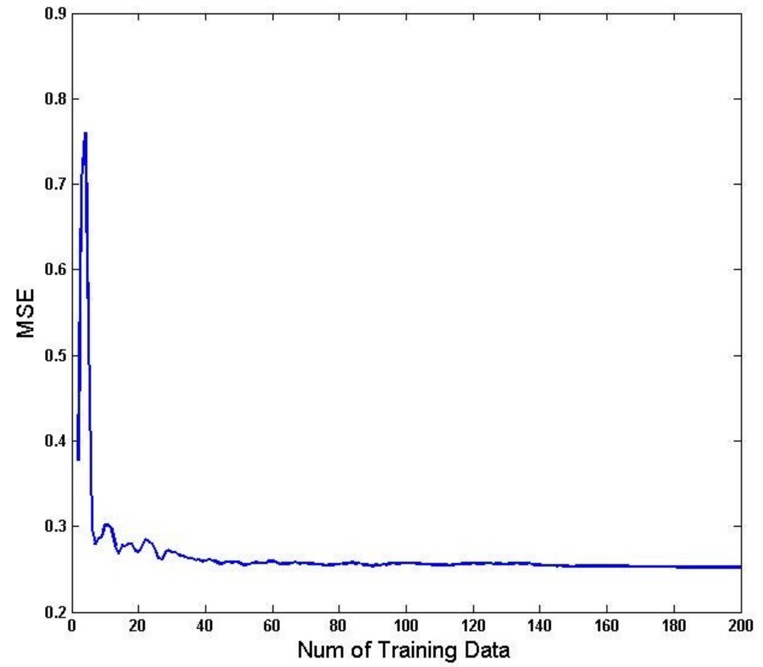






Linear regression: generalization

- By increasing the number of training examples, will solution be better?
- Why the mean squared error does not decrease more after reaching a level?



Linear regression: types of errors

- Structural error: the error introduced by the limited function class (infinite training data):

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}}\, E_{\boldsymbol{x},y}[(y - \boldsymbol{w}^T\boldsymbol{x})^2]$$

$$\text{Structural error:} E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x}\right)^2\right]$$

where $\boldsymbol{w}^* = (w_0^*, \cdots, w_d^*)$ are the optimal linear regression parameters (infinite training data)

Linear regression: types of errors

- Approximation error measures how close we can get to the optimal linear predictions with limited training data:

$$\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}}\, E_{\boldsymbol{x},y}[(y - \boldsymbol{w}^T\boldsymbol{x})^2]$$

$$\boldsymbol{w} = \underset{\boldsymbol{w}}{\operatorname{argmin}} \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{w}^T\boldsymbol{x}^{(i)}\right)^2$$

Approximation error: $E_{\boldsymbol{x}}\left[\left(\boldsymbol{w}^{*T}\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{x}\right)^2\right]$

Where $\boldsymbol{w}$ are the parameter estimates based on a small training set (so themselves are random variables).

Linear regression: error decomposition

- The expected error can decompose into the sum of structural and approximation errors

$$E_{\boldsymbol{x},y}[(y - \boldsymbol{w}^T\boldsymbol{x})^2]$$
$$= E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x}\right)^2\right] + E_{\boldsymbol{x}}\left[\left(\boldsymbol{w}^{*T}\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{x}\right)^2\right]$$

- Derivation

$$E_{\boldsymbol{x},y}[(y - \boldsymbol{w}^T\boldsymbol{x})^2] = E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x} + \boldsymbol{w}^{*T}\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{x}\right)^2\right]$$
$$= E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x}\right)^2\right] + E_{\boldsymbol{x}}\left[\left(\boldsymbol{w}^{*T}\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{x}\right)^2\right]$$
$$+ 2E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x}\right)\left(\boldsymbol{w}^{*T}\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{x}\right)\right]$$

Linear regression: error decomposition

- The expected error can decompose into the sum of structural and approximation errors

$$
\begin{aligned}
&E_{\boldsymbol{x},y}[(y - \boldsymbol{w}^T\boldsymbol{x})^2] \\
&= E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x}\right)^2\right] + E_{\boldsymbol{x}}\left[\left(\boldsymbol{w}^{*T}\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{x}\right)^2\right]
\end{aligned}
$$

- Derivation

$$
\begin{aligned}
&E_{\boldsymbol{x},y}[(y - \boldsymbol{w}^T\boldsymbol{x})^2] = E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x} + \boldsymbol{w}^{*T}\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{x}\right)^2\right] \\
&= E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x}\right)^2\right] + E_{\boldsymbol{x}}\left[\left(\boldsymbol{w}^{*T}\boldsymbol{x} - \boldsymbol{w}^T\boldsymbol{x}\right)^2\right] \\
&+ 0
\end{aligned}
$$

Note: Optimality condition for $\boldsymbol{w}^*$ give us $E_{\boldsymbol{x},y}\left[\left(y - \boldsymbol{w}^{*T}\boldsymbol{x}\right)\boldsymbol{x}\right] = 0$
since $\nabla_{\boldsymbol{w}} E_{\boldsymbol{x},y}[(y - \boldsymbol{w}^T\boldsymbol{x})^2]_{\ \boldsymbol{w}^*} = 0$

Recall: Linear regression (squared loss)

- Linear regression functions

$$f : \mathbb{R} \rightarrow \mathbb{R} \quad f(x; \boldsymbol{w}) = w_0 + w_1 x$$

$$f : \mathbb{R}^{\mathrm{d}} \rightarrow \mathbb{R} \quad f(\boldsymbol{x}; \boldsymbol{w}) = w_0 + w_1 x_1 + \ldots w_d x_d$$

$\boldsymbol{w} = [w_0, w_1, \ldots, w_d]^T$ are the parameters we need to set.

- Minimizing the squared loss for linear regression

$$J(\boldsymbol{w}) = \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2$$

- We obtain $\boldsymbol{w} = (\boldsymbol{X}^T\boldsymbol{X})^{-\mathbf{1}} \boldsymbol{X}^T\boldsymbol{y}$

Beyond linear regression

- How to extend the linear regression to non-linear functions?
  - Transform the data using basis functions
  - Learn a linear regression on the new feature vectors (obtained
  - by basis functions)

Beyond linear regression

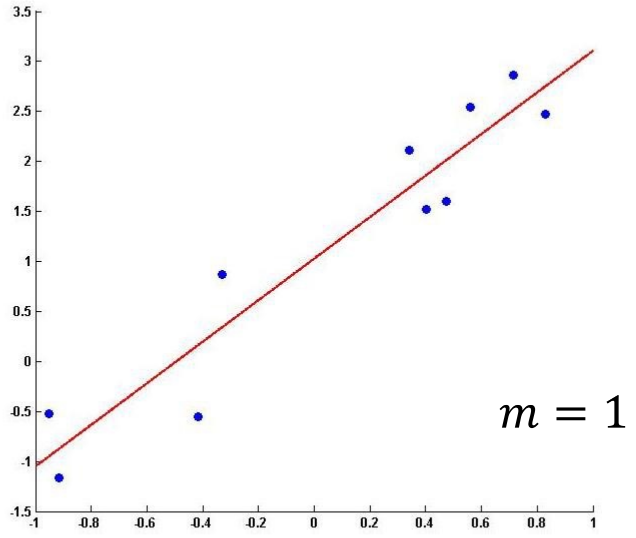
- m^{th} order polynomial regression (univariate $f : \mathbb{R} \longrightarrow \mathbb{R}$)

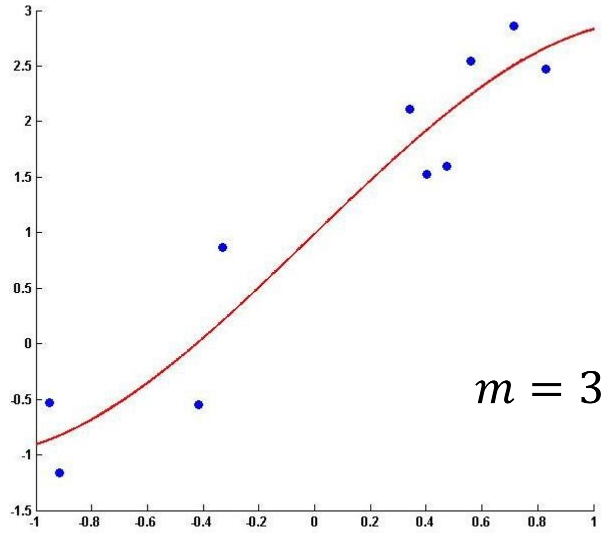
$$f(x; \boldsymbol{w}) = w_0 + w_1 x + \ldots + w_{m-1} x^{m-1} + w_m \, x^m$$

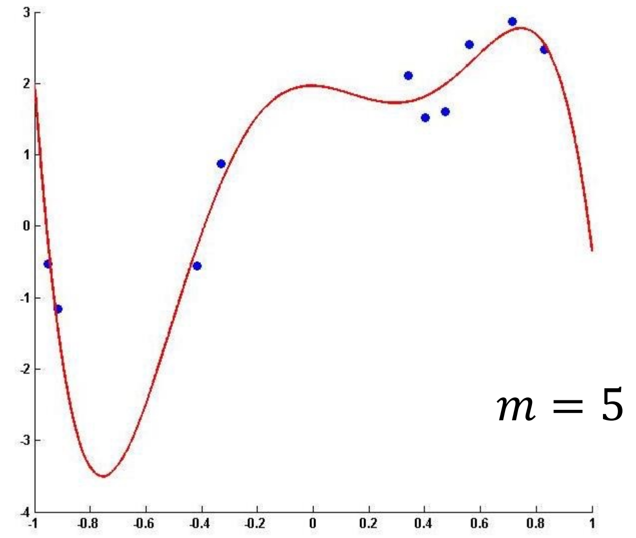
- Solution: $\boldsymbol{w} = \left(\boldsymbol{X}'^T \boldsymbol{X}'\right)^{-\mathbf{1}} \boldsymbol{X}'^T \boldsymbol{y}$

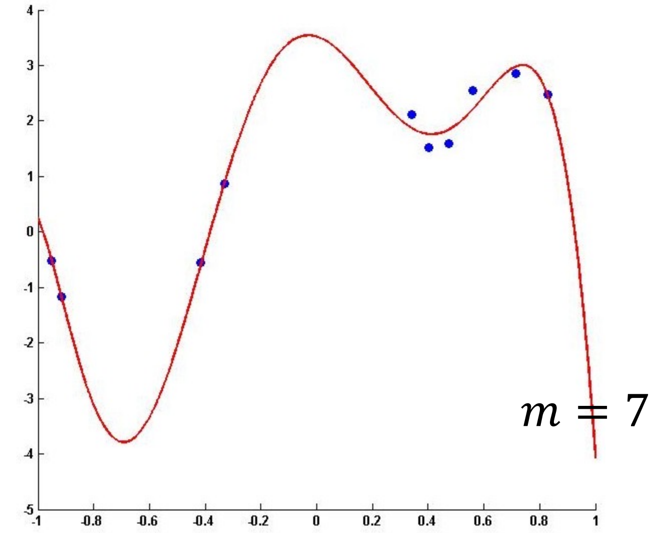
$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \quad \boldsymbol{X}' = \begin{bmatrix} 1 & x^{(1)^1} & x^{(1)^2} & \cdots & x^{(1)^m} \\ 1 & x^{(2)^1} & x^{(2)^2} & \cdots & x^{(2)^m} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x^{(n)^1} & x^{(n)^2} & \cdots & x^{(n)^1} \end{bmatrix} \boldsymbol{w} = \begin{bmatrix} \boldsymbol{w}_0 \\ \boldsymbol{w}_1 \\ \vdots \\ \boldsymbol{w}_m \end{bmatrix}$$

Polynomial regression: example









Generalized linear

- Linear combination of fixed non-linear function of the input vector

$$f(\boldsymbol{x};\boldsymbol{w}) \;= w_0 + w_1\phi_1(\boldsymbol{x}) + \dots w_m\phi_m(\boldsymbol{x})$$

$\{\phi_1(\boldsymbol{x}), \dots, \phi_m(\boldsymbol{x})\}$: set of basis functions (or features)

$$\phi_i(\boldsymbol{x}): \mathbb{R}^d \to \mathbb{R}$$

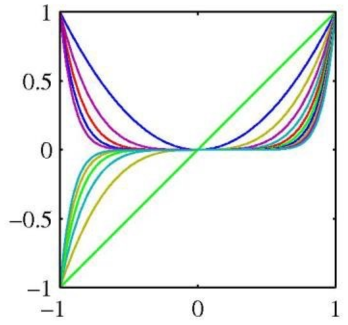
Basis functions: examples

- Linear

If $m = d$, $\phi_i(\mathbf{x}) = x_i$, $i = 1, \ldots, d$, then

$$f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d$$

- Polynomial (univariate)



If $\phi_i(x) = x^i$, $i = 1, \ldots, m$, then

$$f(x; \mathbf{w}) = w_0 + w_1 x + \ldots + w_{m-1} x^{m-1} + w_m x^m$$

Generalized linear: optimization

$$J(\boldsymbol{w}) = \sum_{i=1}^{n} \left(y^{(i)} - f\left(\boldsymbol{x}^{(i)}; \boldsymbol{w}\right)\right)^2$$

$$= \sum_{i=1}^{n} \left(y^{(i)} - \boldsymbol{w}^T \boldsymbol{\phi}\left(\boldsymbol{x}^{(i)}\right)\right)^2$$

$$\boldsymbol{y} = \begin{bmatrix} y^{(1)} \\ \vdots \\ y^{(n)} \end{bmatrix} \boldsymbol{\Phi} = \begin{bmatrix} 1 & \phi_1(\boldsymbol{x}^{(1)}) & \cdots & \phi_m(\boldsymbol{x}^{(1)}) \\ 1 & \phi_1(\boldsymbol{x}^{(2)}) & \cdots & \phi_m(\boldsymbol{x}^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \phi_1(\boldsymbol{x}^{(n)}) & \cdots & \phi_m(\boldsymbol{x}^{(n)}) \end{bmatrix} \quad \boldsymbol{w} = \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_m \end{bmatrix}$$

$$\boldsymbol{w} = \left(\boldsymbol{\Phi}^T \boldsymbol{\Phi}\right)^{\boldsymbol{-1}} \boldsymbol{\Phi}^T \boldsymbol{y}$$

Resource

1 C. M. Bishop, *Pattern Recognition and Machine Learning*.

2 Y. S. Abu-Mostafa, “Machine learning.” California Institute of Technology, 2012.