# Linear Regression

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# Outline

- Introduction
- Single Feature Case
- Multiple Features Case
- Numerical Optimization

# Introduction

- What is regression?

  Based on the given features, predict the values of interested variables

- Example: House price prediction

Features | Interest variable

| Size (feet) $x_1$ | # bedrooms $x_2$ | # floors $x_3$ | # years (Ages) $x_4$ | Price ($ 1000) $y$ |
|---|---|---|---|---|
| 2104 | 5 | 1 | 45 | 460 |
| 1416 | 3 | 2 | 40 | 232 |
| 1534 | 3 | 2 | 30 | 315 |
| 852 | 2 | 1 | 36 | 178 |
| …. | …. | …. | …. | …. |

Features: 1) size, 2) # bedrooms, 3) # floors, 4) # years

- Mathematically, regression aims at building a function $f(\cdot)$ to model the relation between input data $x$ and supervised value $y$

$$\hat{y} = f(x_1, x_2, x_3, x_4)$$

- Linear regression

  Restricting the function $f(\cdot)$ to be of linear form, *i.e.*,

$$f(x_1, x_2 \cdots x_m) = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_m x_m$$

  - $w_k$: model parameters
  - $m$: number of features

- Objective

Find a set of parameters $\{w_k\}_{k=1}^{m}$ so that the prediction

$$\hat{y} = f(x_1, x_2, \cdots, x_m)$$

is as close as possible to the true $y$ values *for all data samples* in the training dataset

| | Size (feet) $x_1$ | # bedrooms $x_2$ | # floors $x_3$ | # years (Ages) $x_4$ | Price ($ 1000) $y$ |
|---|---|---|---|---|---|
| Sample 1 → | 2104 | 5 | 1 | 45 | 460 |
| Sample 2 → | 1416 | 3 | 2 | 40 | 232 |
| Sample 3 → | 1534 | 3 | 2 | 30 | 315 |
| Sample 4 → | 852 | 2 | 1 | 36 | 178 |
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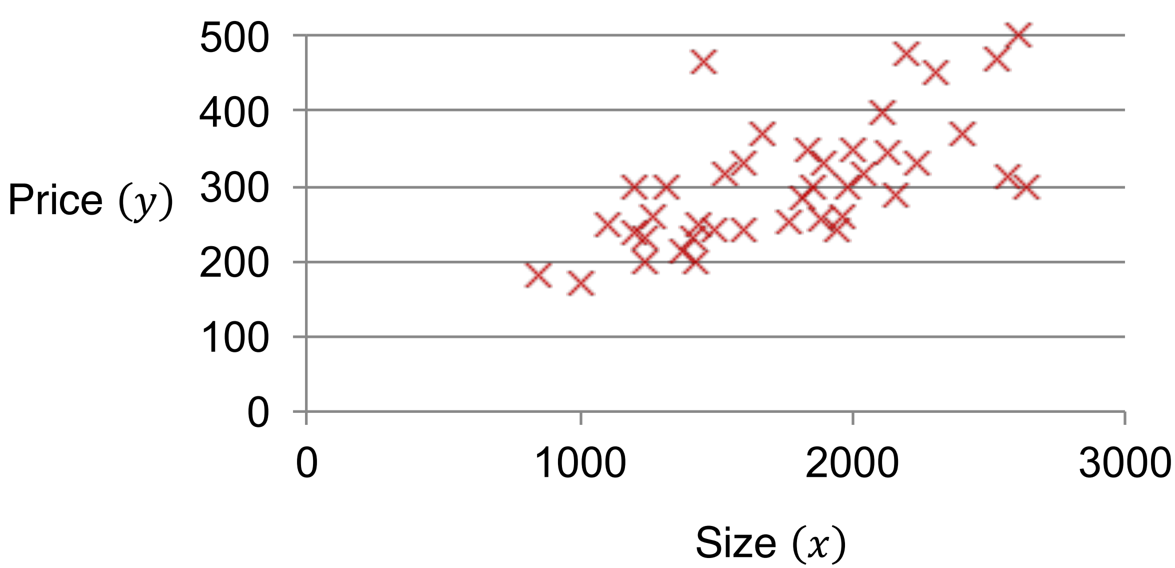
# Model

- For simplicity, first consider only one feature, *e.g.*, *house size*

| Size (feet) $x$ | Price ($ 1000) $y$ |
|---|---|
| 2104 | 460 |
| 1416 | 232 |
| 852 | 178 |
| …. | …. |

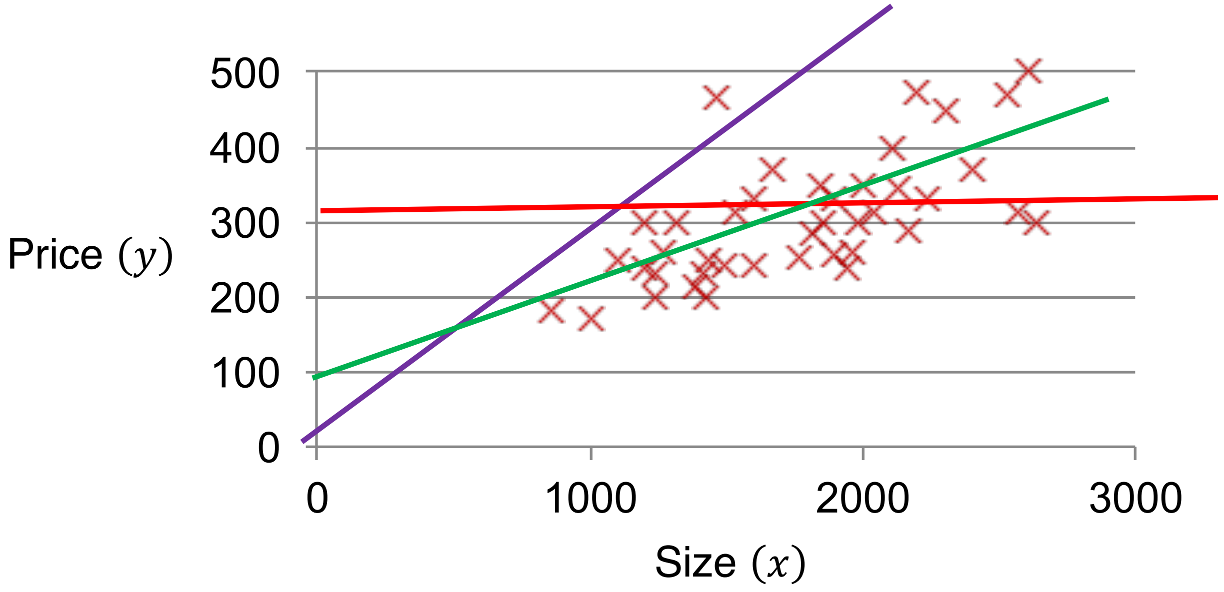
- Plot the $(x, y)$ pairs on a plane



- The prediction function reduces to

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

- For different $w_0$ and $w_1$, the function $f(x)$ represents different straight lines



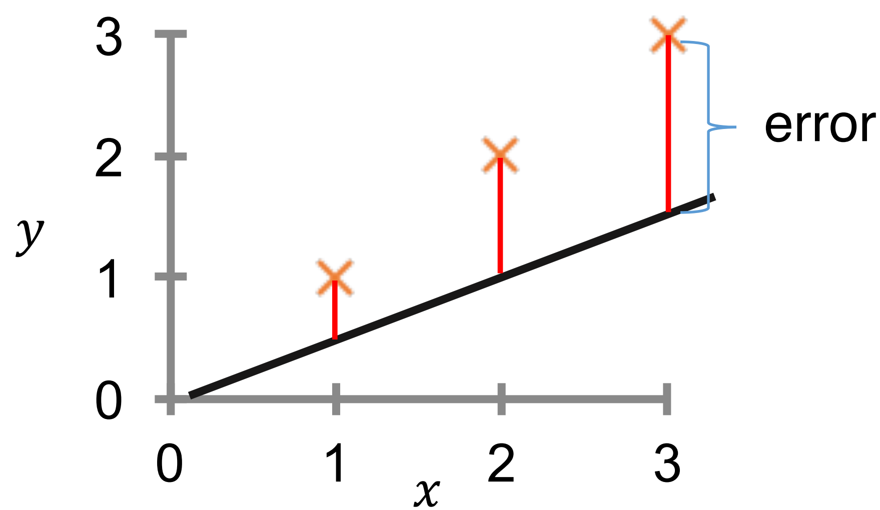

- The objective is to find an appropriate $w_0$ and $w_1$ so that the line is as fit as possible with the true $y$'s of all given $x$

# Cost / Loss Function

- Mathematically, the objective can be described as minimizing the cost (loss) function

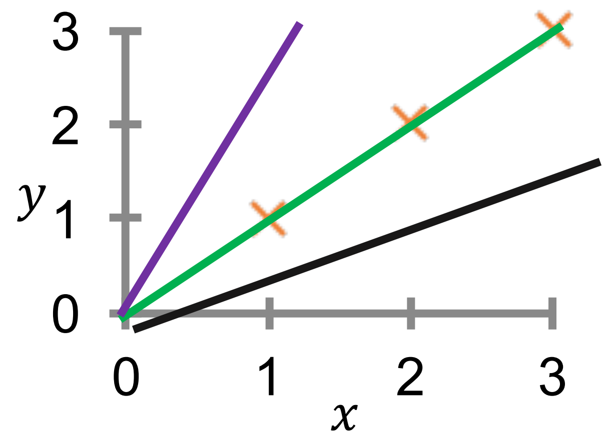
$$L(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}\left(f\left(x^{(i)}\right) - y^{(i)}\right)^2$$

where $x^{(i)}$ and $y^{(i)}$ means the $i$-th feature and target values; $n$ is the number of training examples



- Substituting $f\left(x^{(i)}\right) = w_0 + w_1 x^{(i)}$ into $L(w_0, w_1)$ gives

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



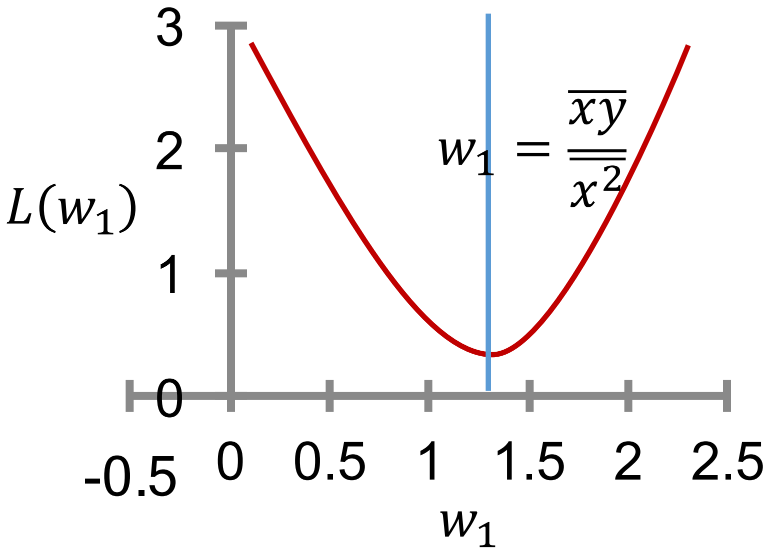

*Remark: To better understand this cost function, we simplify it by setting $w_0 = 0$*

- Then, the cost function becomes

$$\boxed{L(w_1) = \overline{x^2} w_1^2 - 2\overline{xy} w_1 + \overline{y^2}}$$

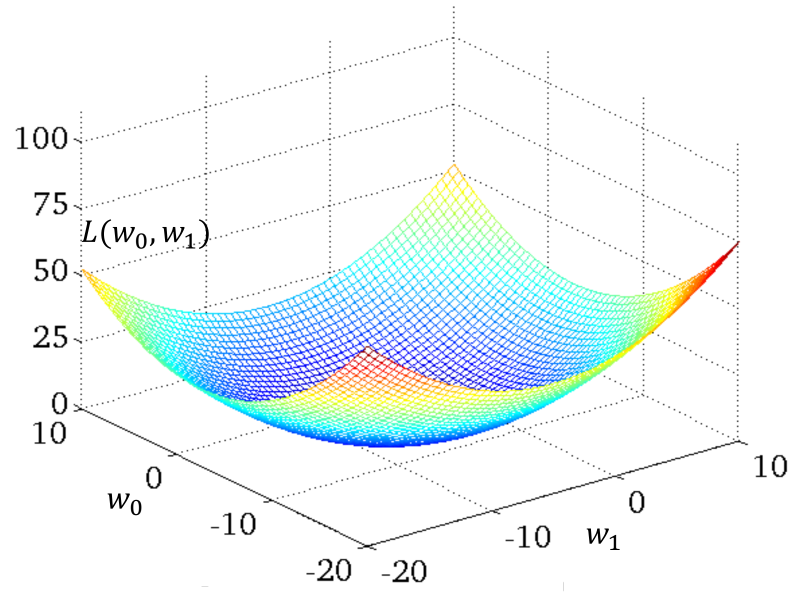
where $\overline{x^2} = \frac{\sum_{i=1}^{n}\left(x^{(i)}\right)^2}{n}$, $\overline{xy} = \frac{\sum_{i=1}^{n} x^{(i)} y^{(i)}}{n}$ and $\overline{y^2} = \frac{\sum_{i=1}^{n}\left(y^{(i)}\right)^2}{n}$

- The cost function is a quadratic function *w.r.t.* $w_1$




$$L(w_1) = \overline{x^2}w_1^2 - 2\overline{xy}w_1 + \overline{y^2}$$

- If $w_0$ is taken into account, the cost function $L(w_0, w_1)$ is still a quadratic function, but is two-dimensional



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

- The best $w_0$ and $w_1$ can be found by setting the derivatives to zero

$$\frac{\partial L}{\partial w_0} = \frac{2}{n}\sum_{i=1}^{n}\left(w_0 + w_1 x^{(i)} - y^{(i)}\right) = 0$$

$$\frac{\partial L}{\partial w_1} = \frac{2}{n}\sum_{i=1}^{n}\left(w_0 + w_1 x^{(i)} - y^{(i)}\right) x^{(i)} = 0$$

- It can be derived that the best $w_0$ and $w_1$ are

$$w_0 = \frac{\overline{xy}\,\bar{x} - \overline{x^2}\,\bar{y}}{\bar{x}^2 - \overline{x^2}}$$

$$w_1 = \frac{\bar{x}\bar{y} - \overline{xy}}{\bar{x}^2 - \overline{x^2}}$$

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- Training data from single feature to multiple feature case

| Size (feet) $x$ | Price ($ 1000) $y$ |
|---|---|
| 2104 | 460 |
| $\boxed{1416}$ $\longrightarrow$ | 232 |
| 1534 | 315 |
| 852 | 178 |
| …. | …. |

$\Downarrow$

| Size (feet) $x_1$ | # bedrooms $x_2$ | # floors $x_3$ | # years (Ages) $x_4$ | Price ($ 1000) $y$ |
|---|---|---|---|---|
| 2104 | 5 | 1 | 45 | 460 |
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| 1534 | 3 | 2 | 30 | 315 |
| 852 | 2 | 1 | 36 | 178 |
| …. | …. | …. | …. | …. |

- The function of a general linear regression is

$$f(x_1, x_2 \cdots x_m) = w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_m x_m$$

  - $x_i$ is the $i$-th feature

- Working with the scalar form is cumbersome. Reformulating it into a matrix-form gives

$$f(\boldsymbol{x}) = \boldsymbol{x}\boldsymbol{w}$$

  - $\boldsymbol{x} = [1, x_1, x_2, \cdots, x_m]$ is the feature row vector
  - $\boldsymbol{w} = [w_0, w_1, w_2, \cdots, w_m]^T$ is the parameter column vector

*By setting the first element in $x$ to be 1, $w_0$ can be treated the same as the other parameters $w_k$*

# Cost Function

- The objective is still to find a $\boldsymbol{w}$ such that the prediction

$$f\left(\boldsymbol{x}^{(i)}\right) = \boldsymbol{x}^{(i)}\boldsymbol{w}$$

is close to the true value $y^{(i)}$, where $\boldsymbol{x}^{(i)}$ and $y^{(i)}$ is the $i$-th feature vector and target value

| Size (feet) $x_1$ | # bedrooms $x_2$ | # floors $x_3$ | # years (Ages) $x_4$ | Price ($ 1000) $y$ |
|---|---|---|---|---|
| 2104 | 5 | 1 | 45 | 460 |
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| …. | …. | …. | …. | …. |

- Thus, the cost function can be represented as

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

- The cost function can be further written as

$$L(\boldsymbol{w}) = \frac{1}{n}\|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2$$

where $\boldsymbol{X}$ is the feature matrix defined as

$$\boldsymbol{X} \triangleq \begin{bmatrix} \boldsymbol{x}^{(1)} \\ \vdots \\ \boldsymbol{x}^{(n)} \end{bmatrix}$$

$\boldsymbol{X} =$

| | Size (feet) | # bedrooms | # floors | # years (Ages) | Price ($ 1000) |
|---|---|---|---|---|---|
| $x_0$ | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $y$ |
| 1 | 2104 | 5 | 1 | 45 | 460 |
| 1 | 1416 | 3 | 2 | 40 | 232 |
| 1 | 1534 | 3 | 2 | 30 | 315 |
| 1 | 852 | 2 | 1 | 36 | 178 |
| 1 | …. | …. | …. | …. | …. |

- The gradient of the cost function w.r.t. $\boldsymbol{w}$ is

$$\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{2}{n} \boldsymbol{X}^T (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$$

- Since $L(\boldsymbol{w})$ is a convex function, its optima can be found by setting

$$\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{2}{n} \boldsymbol{X}^T (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}) = 0$$

- Solving the equation gives

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

- It can be verified that when the number of feature is 1, the result reduces to

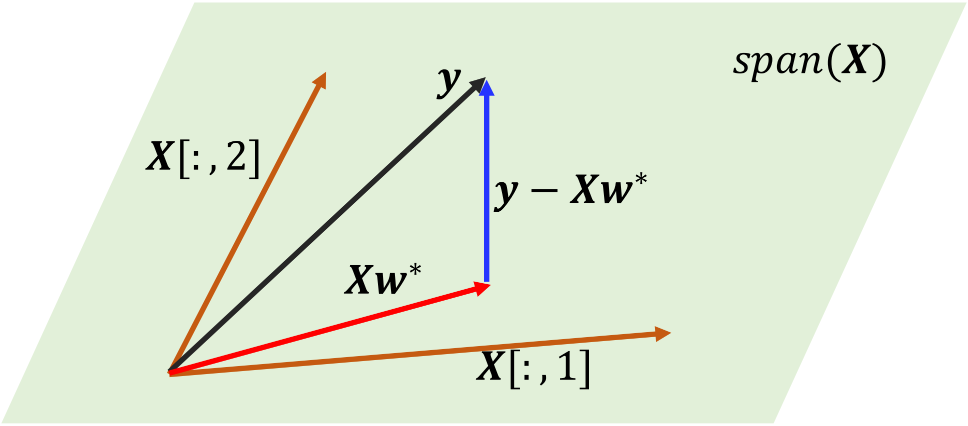
$$w_0 = \frac{\overline{xy}\bar{x} - \overline{x^2}\bar{y}}{\bar{x}^2 - \overline{x^2}}, \qquad w_1 = \frac{\bar{x}\bar{y} - \overline{xy}}{\bar{x}^2 - \overline{x^2}}$$

# Geometric Interpretation

- From the requirement of $\boldsymbol{X}^T(\boldsymbol{X}\boldsymbol{w}^* - \boldsymbol{y}) = \boldsymbol{0}$, we can see that

$$\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}^* \perp span(\boldsymbol{X})$$

- The result suggests that $\boldsymbol{X}\boldsymbol{w}^*$ can be understood as *the projection of $\boldsymbol{y}$ onto the space spanned by $\boldsymbol{X}$*



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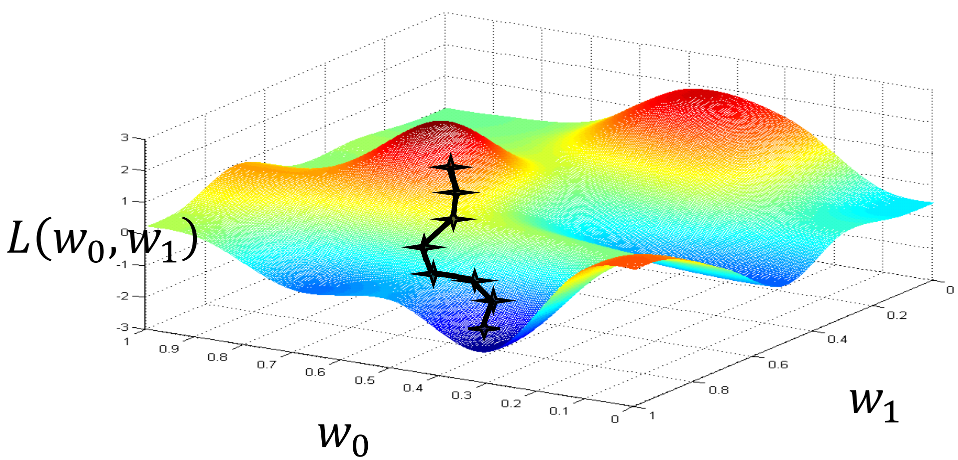
# Gradient Descent

- Analytical solutions do *not always exist*, or evaluating the analytical expression is *computational expensive*
- Then, we should resort to numerical methods, *e.g.*, the gradient descent

$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} - r \cdot \left.\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}}\right|_{\boldsymbol{w}=\boldsymbol{w}^{(t)}}$$

  - $r$: the learning rate

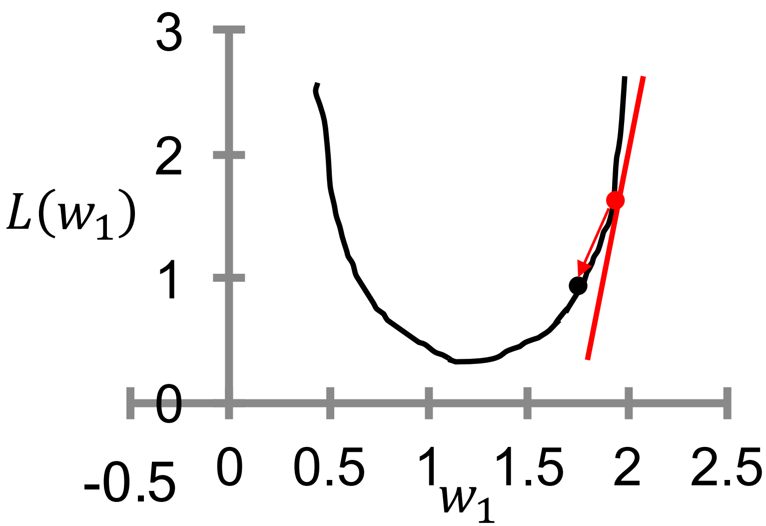


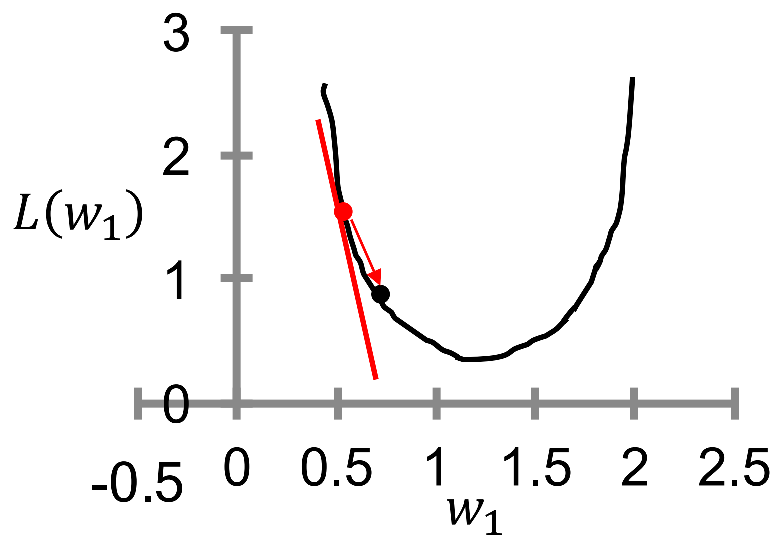
- Let us take the single-feature case and set $w_0 = 0$ as an example, in which the loss function becomes

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

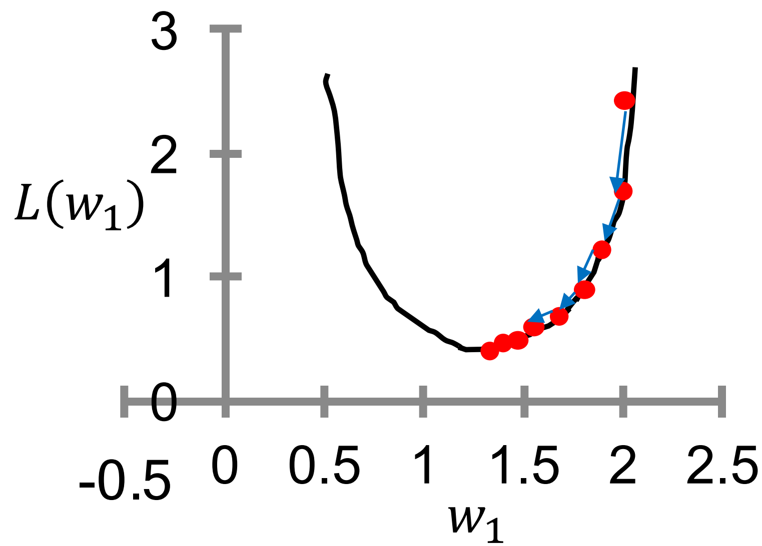
- The parameter $w_1$ can be updated as

$$w_1^{(t+1)} = w_1^{(t)} - r \cdot \left.\frac{\partial L(w_1)}{\partial w_1}\right|_{w_1 = w_1^{(t)}}$$



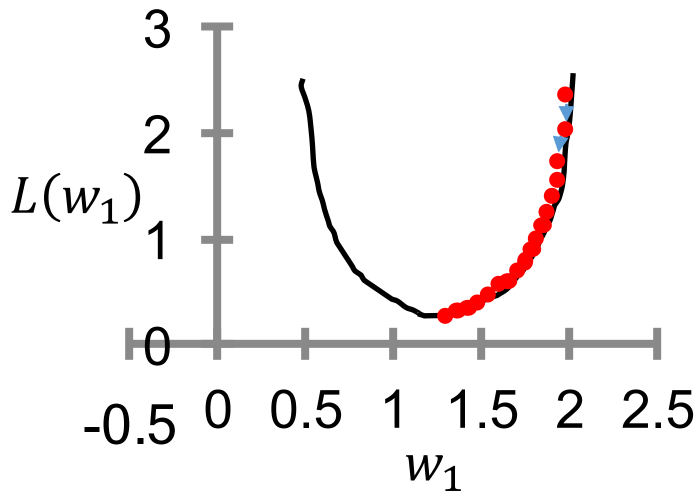



- With appropriate learning rate, the model parameter is iteratively updated, and will eventually converge to the optima

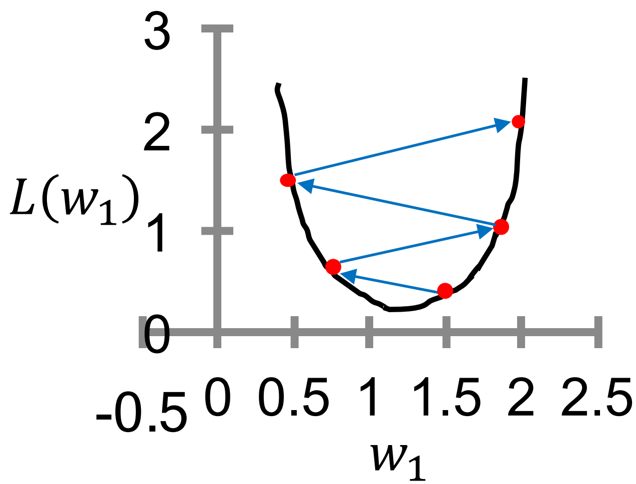



- As approaching the optimal value, the gradient becomes smaller and smaller. Thus, *even if the learning rate is fixed*, the updating intervals also approach 0 as the iteration proceeds, as long as the rate is set appropriately

- If the learning rate is too small, the convergence speed will be very slow




- If the learning rate is too large, the iteration may diverge

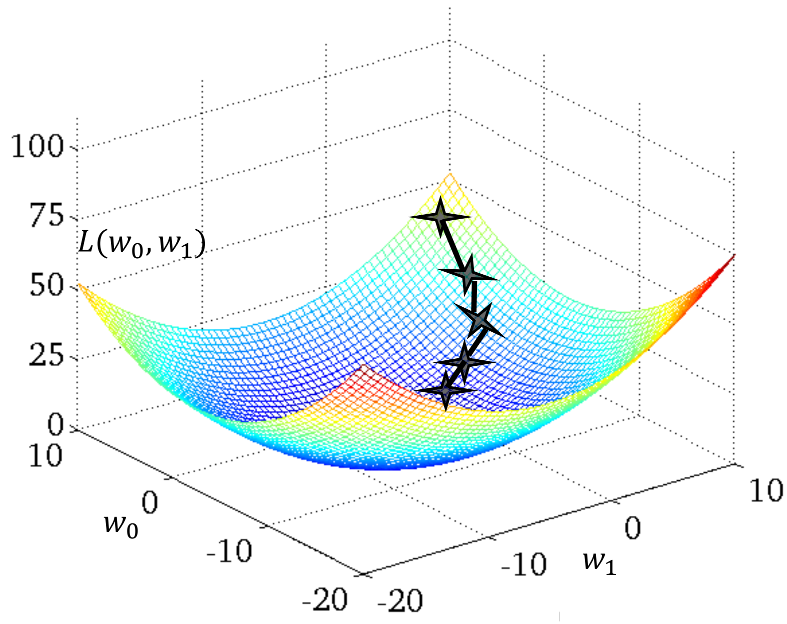



- So, setting appropriate learning rate is important

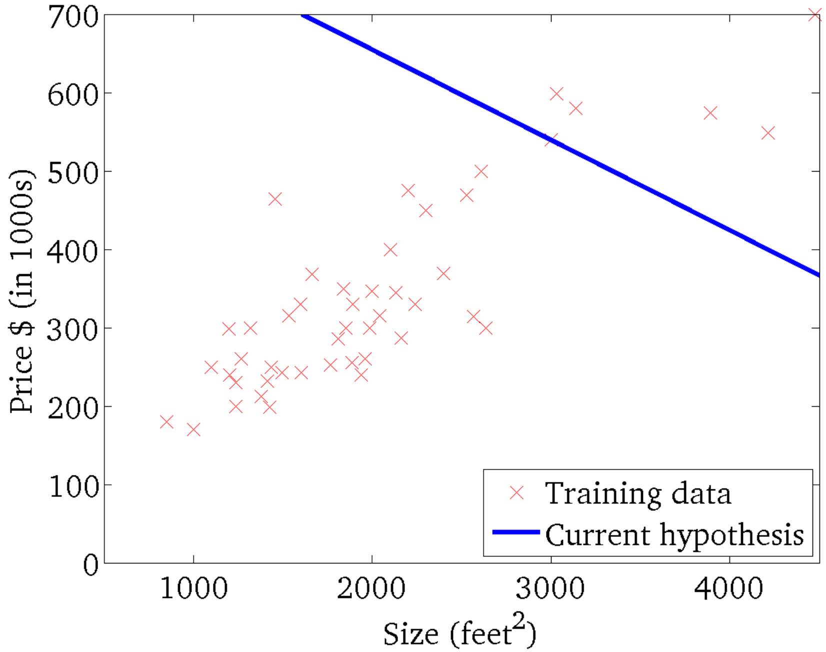
- Now consider the case with both $w_0$ and $w_1$

$$w_0^{(t+1)} = w_0^{(t)} - r \cdot \left. \frac{\partial L(w_0, w_1)}{\partial w_0} \right|_{w_0 = w_0^{(t)},\, w_1 = w_1^{(t)}}$$

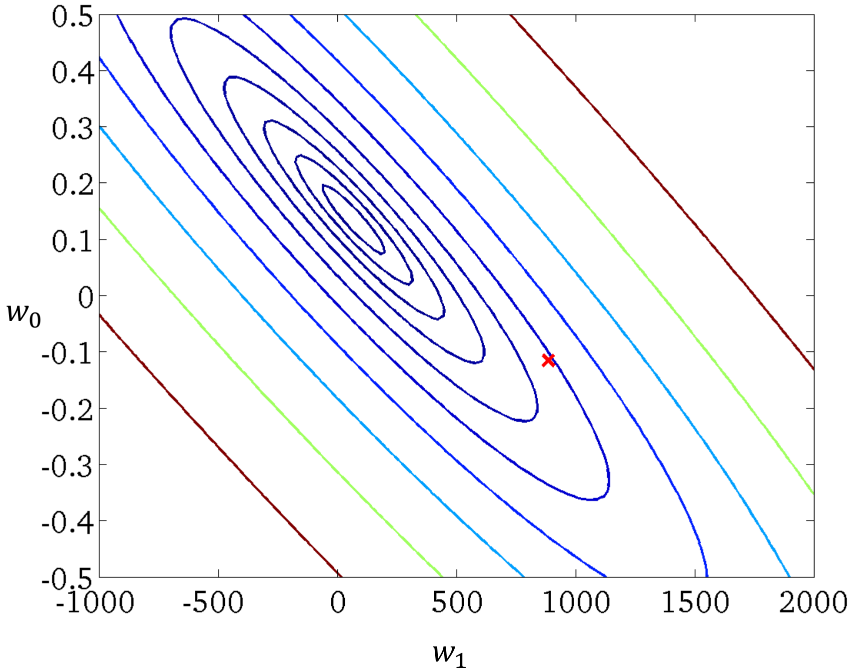
$$w_1^{(t+1)} = w_1^{(t)} - r \cdot \left. \frac{\partial L(w_0, w_1)}{\partial w_1} \right|_{w_0 = w_0^{(t)},\, w_1 = w_1^{(t)}}$$



The function $f(x) = w_0^{(t)} + w_1^{(t)} x$




The contours of $L(w_0, w_1)$ and the track of $\left((w_0^{(t)}, w_1^{(t)}\right)$



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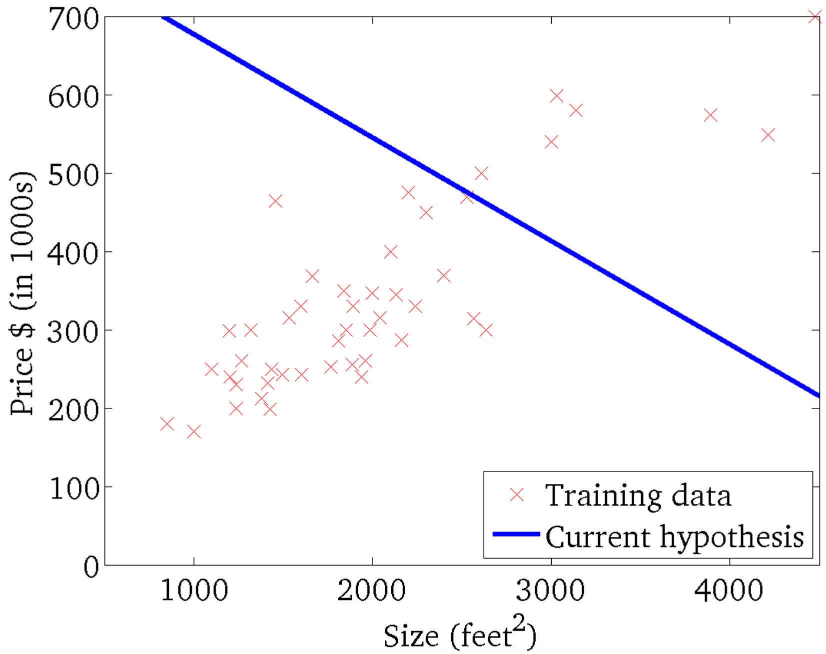


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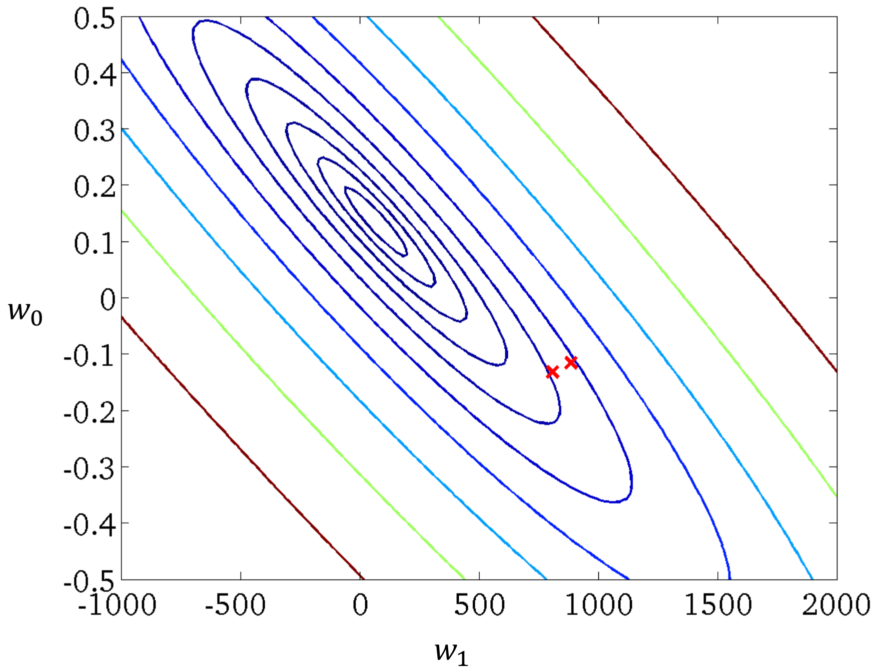

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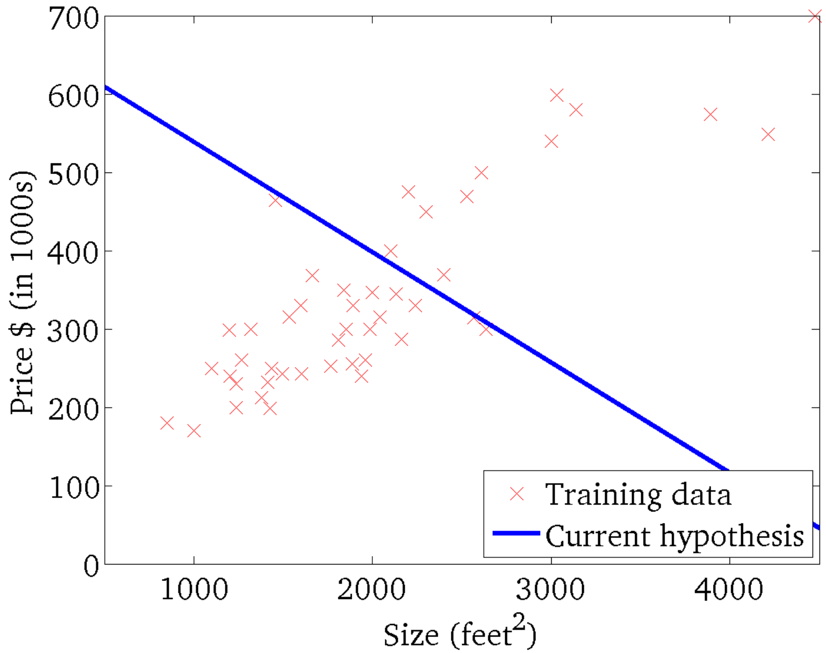


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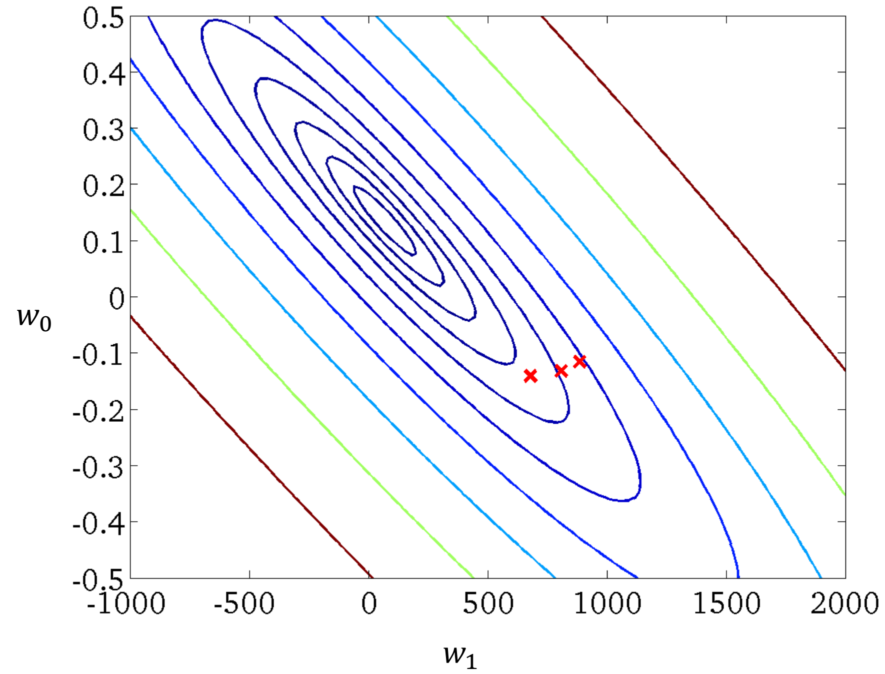

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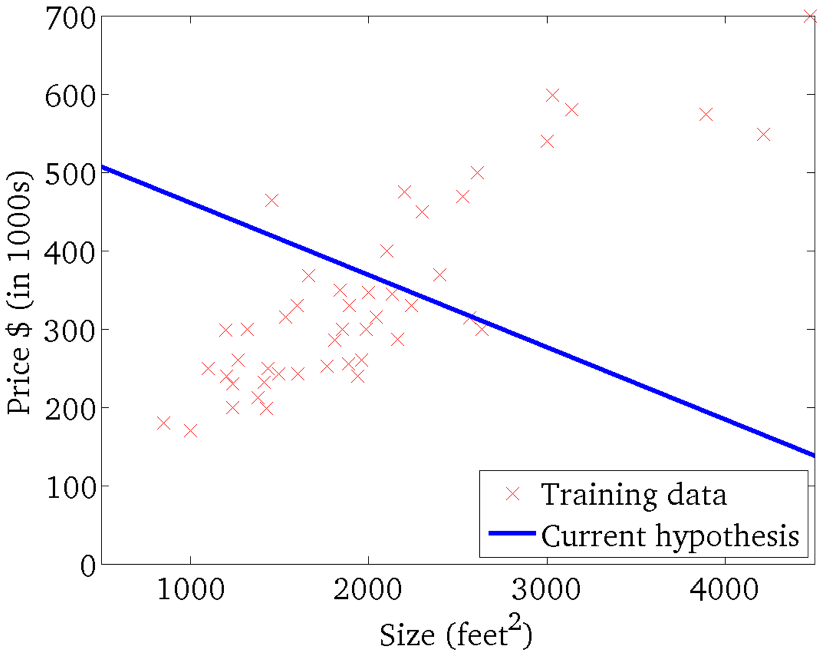


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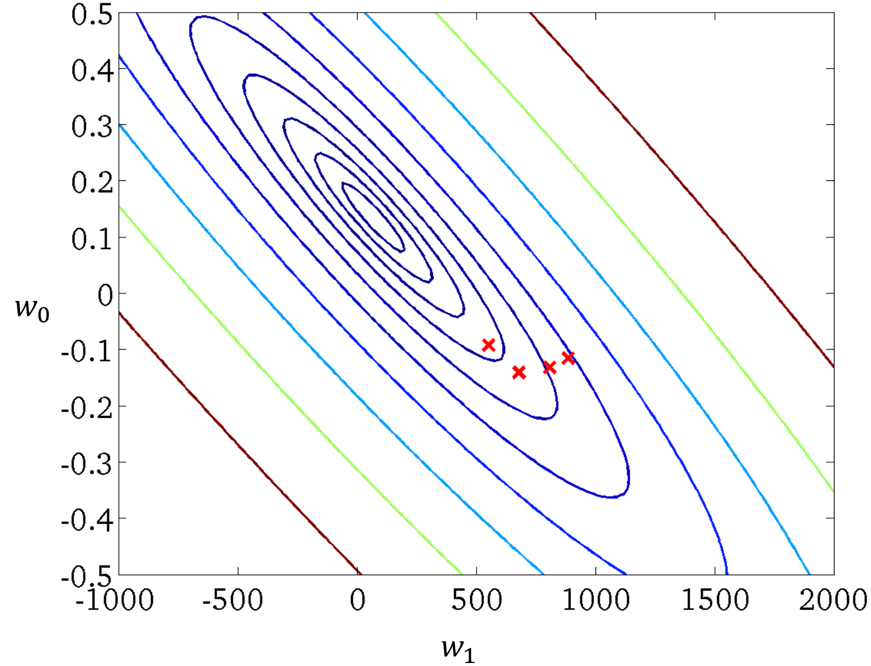

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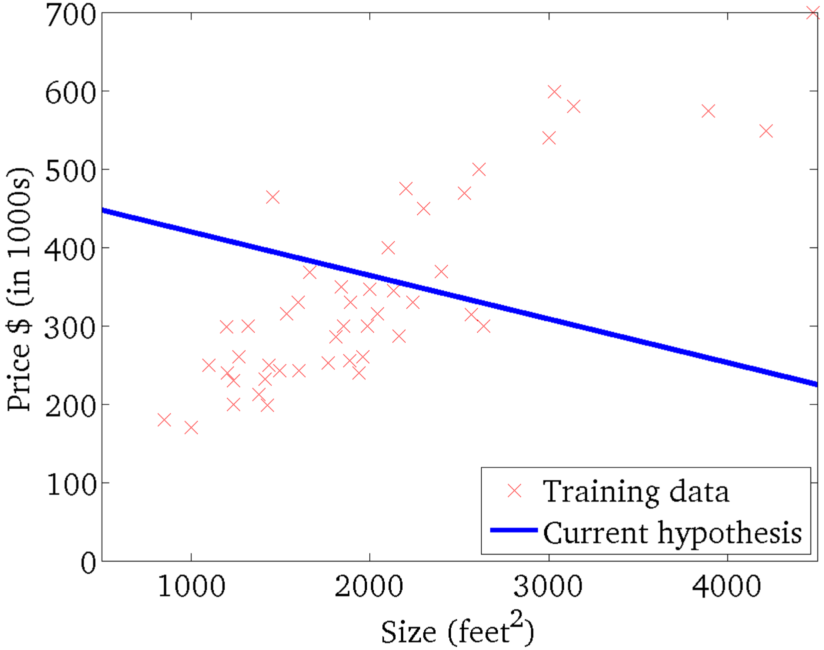


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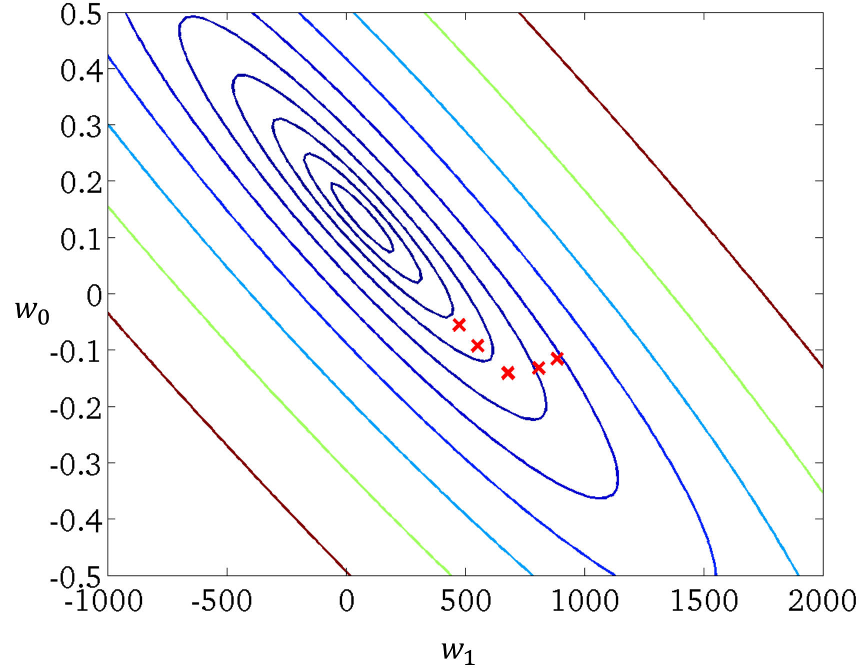

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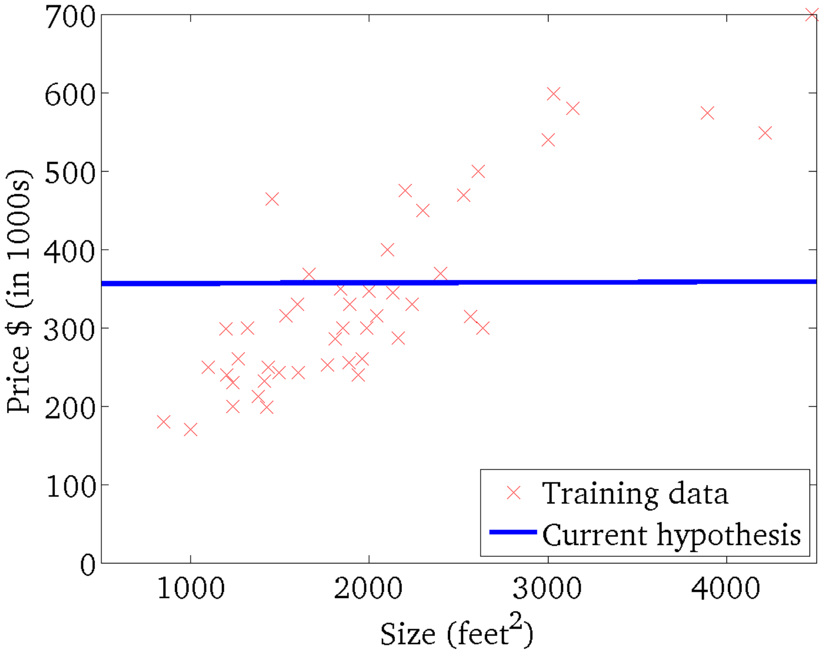


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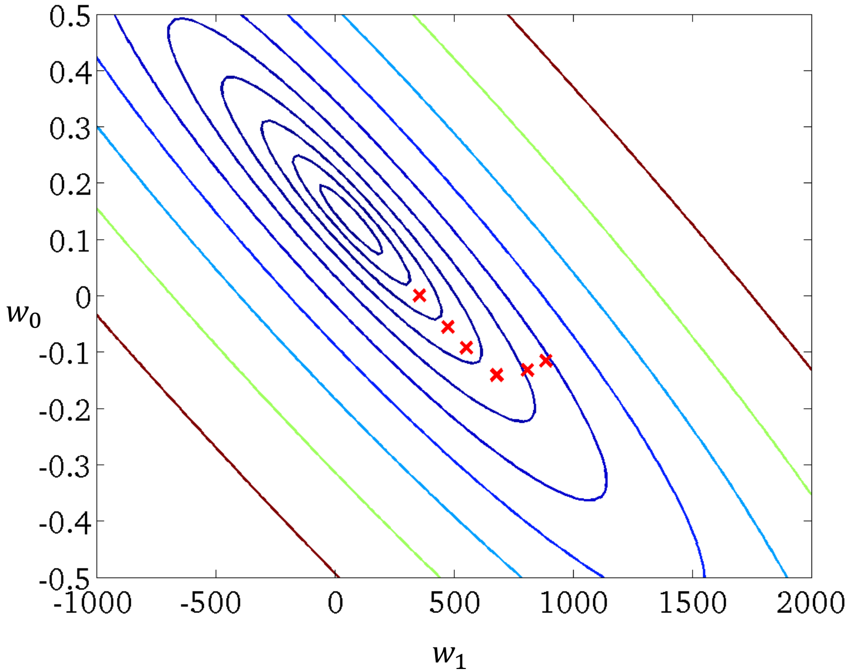

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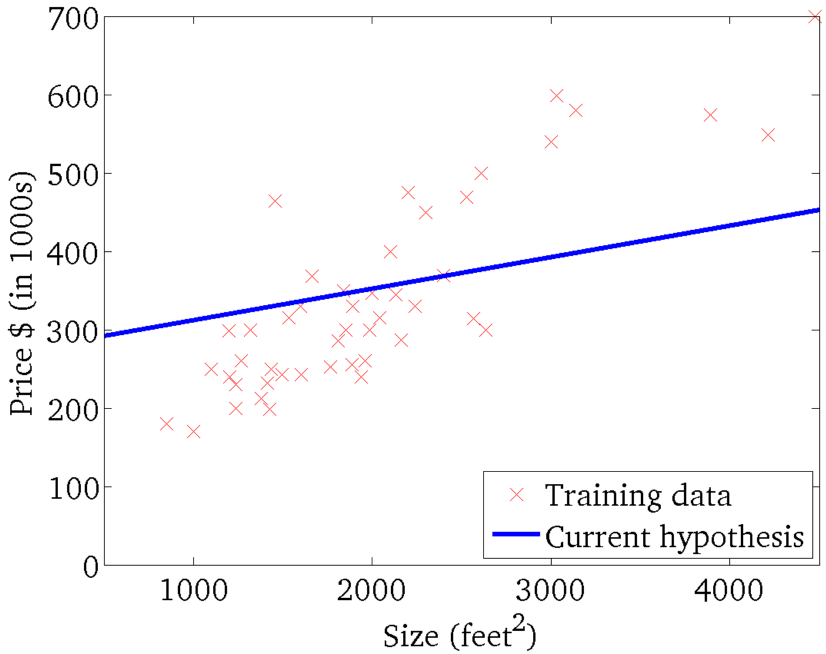


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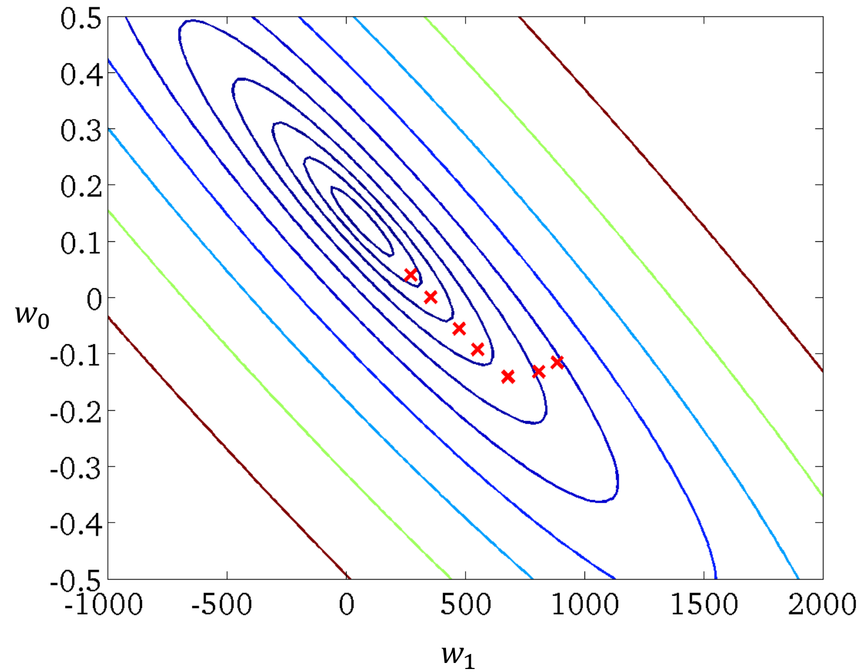

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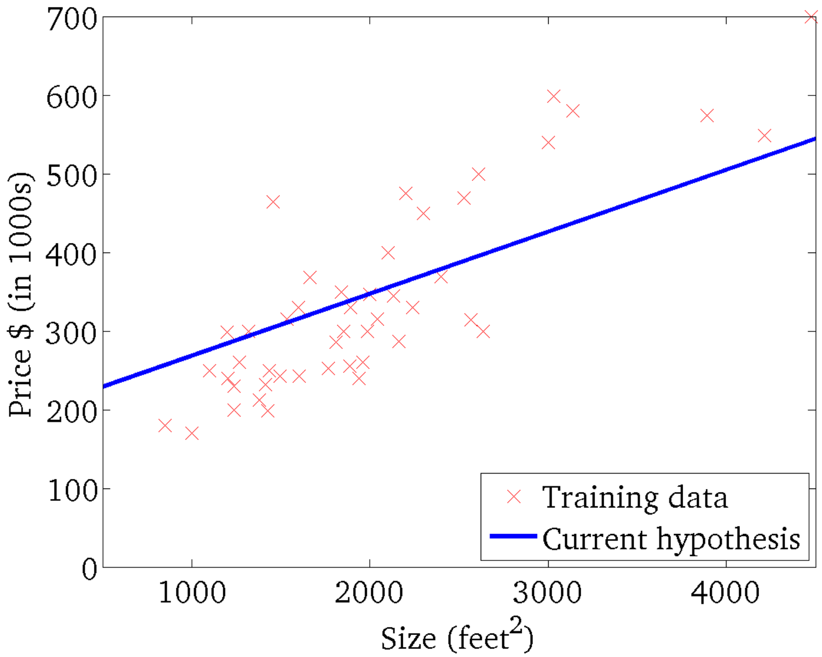


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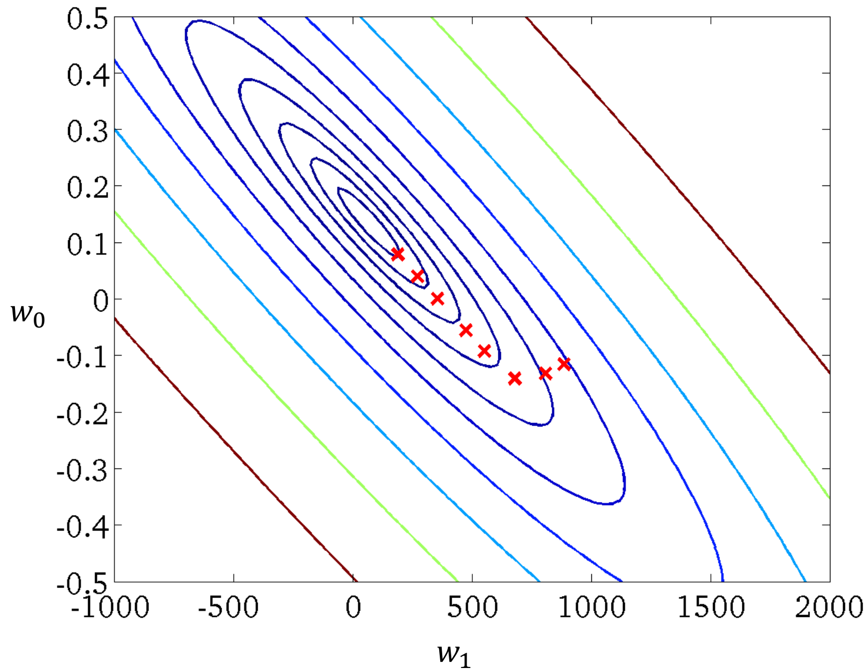

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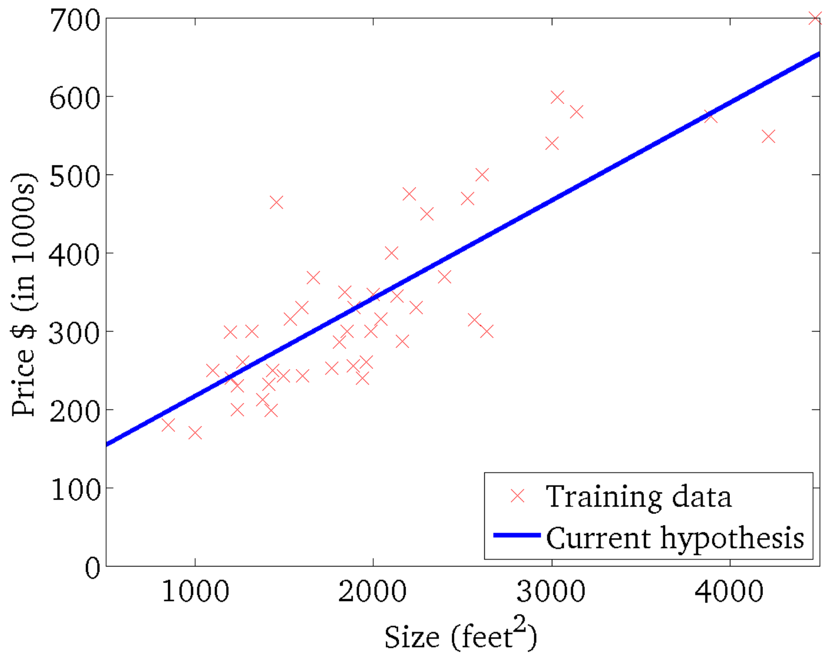


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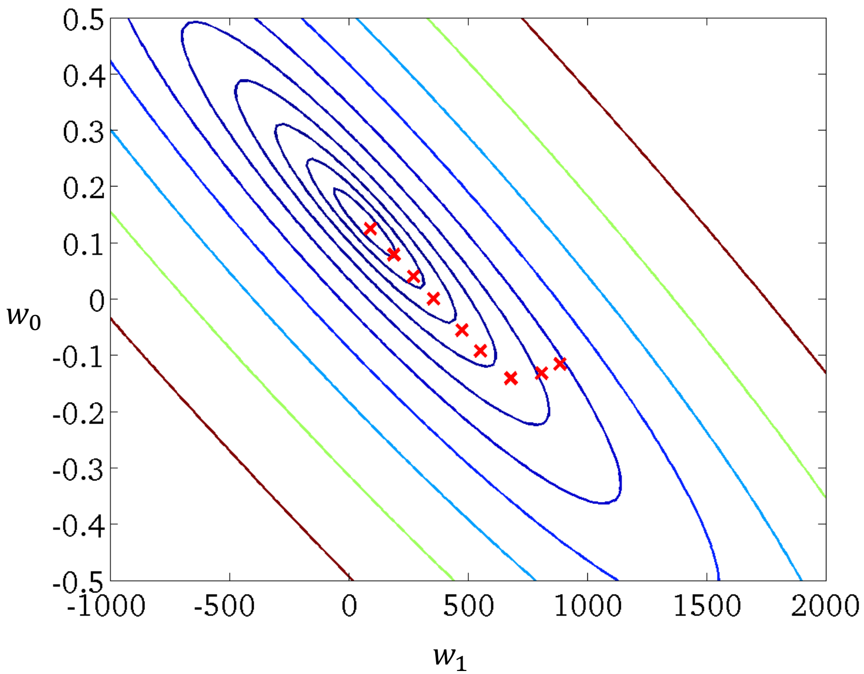


# Stochastic Gradient Descent

- The GD algorithm need to evaluate the gradient of loss w.r.t. model parameters $\boldsymbol{w}$ *at every iteration*

- Generally, the gradient takes the form

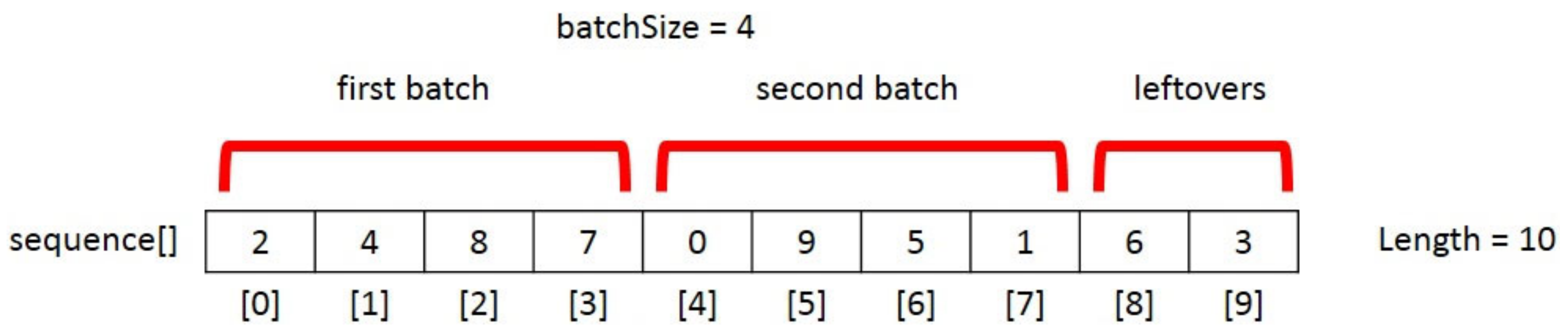
$$\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial \ell\left(\boldsymbol{w}, \boldsymbol{x}^{(i)}, y^{(i)}\right)}{\partial \boldsymbol{w}}$$

- Every iteration requires computing the gradient for all *data samples in the training dataset*

| The complexity would be extremely high for large datasets |
|---|

- To reduce the complexity, we can estimate the gradient $\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}}$ using a small portion of the dataset, *i.e.* *mini-batch*

- How to obtain the mini-batches?
  - Reshuffling
  - Segmenting




- Update:

A noisy estimate to the true gradient

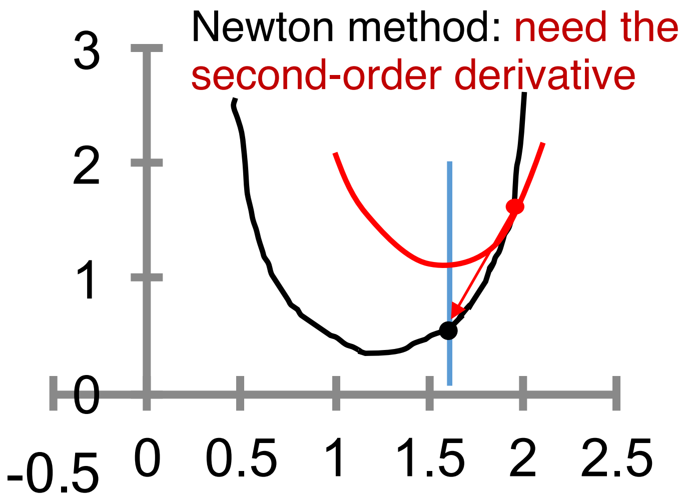
$$\boldsymbol{w}^{(t+1)} = \boldsymbol{w}^{(t)} + r \cdot \boxed{\frac{1}{|\mathcal{B}_t|} \sum_{i \in \mathcal{B}_t} \frac{\partial \ell\left(\boldsymbol{w}, \boldsymbol{x}^{(i)}, y^{(i)}\right)}{\partial \boldsymbol{w}}}$$

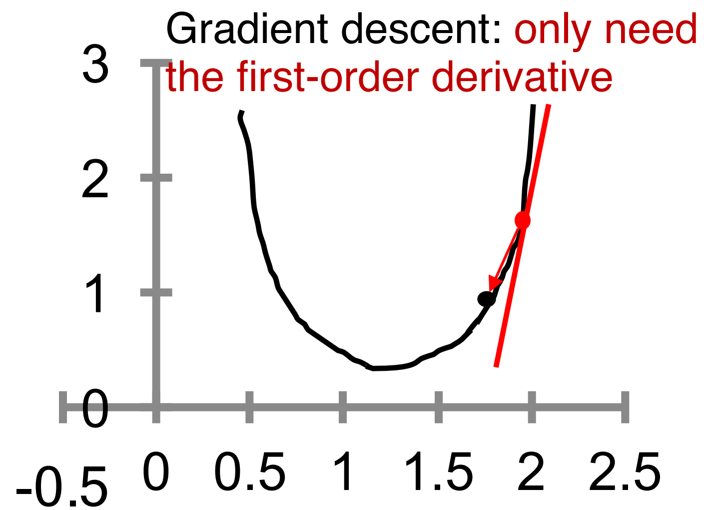
where $\mathcal{B}_t$ is a mini-batch of the dataset at the $t$-th iteration

# Other Optimization Methods

- There also exist many other optimization methods

  1) Newton method




Advantages

- No need to manually choose the learning rate
- Faster convergence rate

Disadvantages

- More expensive

2) Quasi-Newton methods

3) Conjugate gradient method

4) Coordinated descent method

⋮

These methods generally converge faster than the gradient method, but are more computationally expensive