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

$$\underbrace{x_1 \quad x_2 \quad x_3 \quad x_4}_{\text{Features}} \qquad \overset{\text{Interest variable}}{\downarrow}\, y$$

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 to learn a function $f(\cdot)$ that can model the relation between input data x and output value y

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

- Linear regression

Restricting the function family $f(\cdot)$ to be 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 ground-truth values y *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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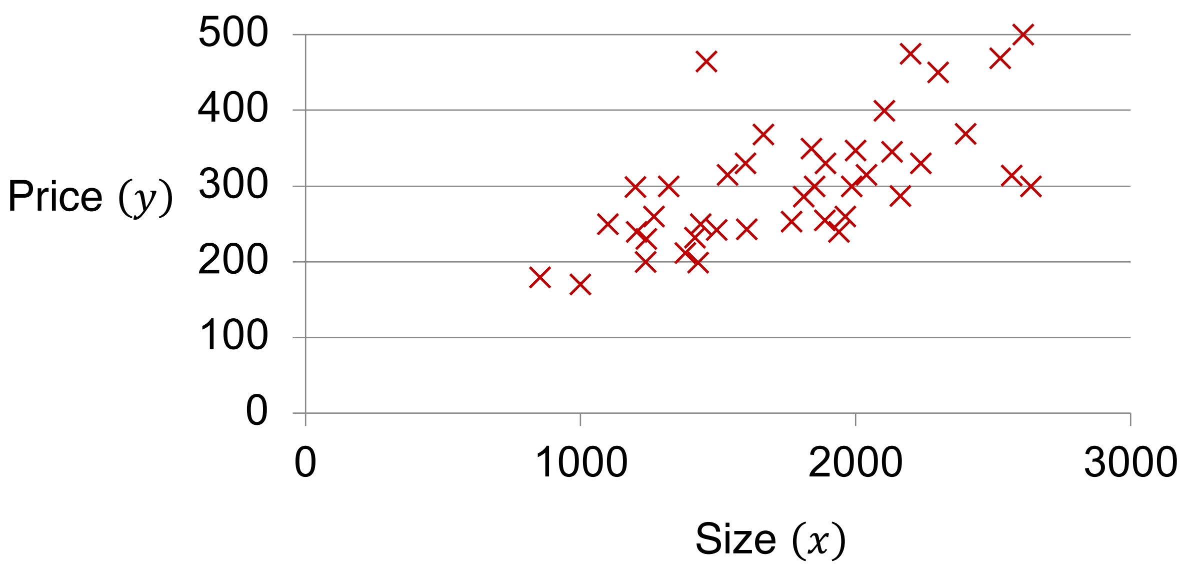
Model

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

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

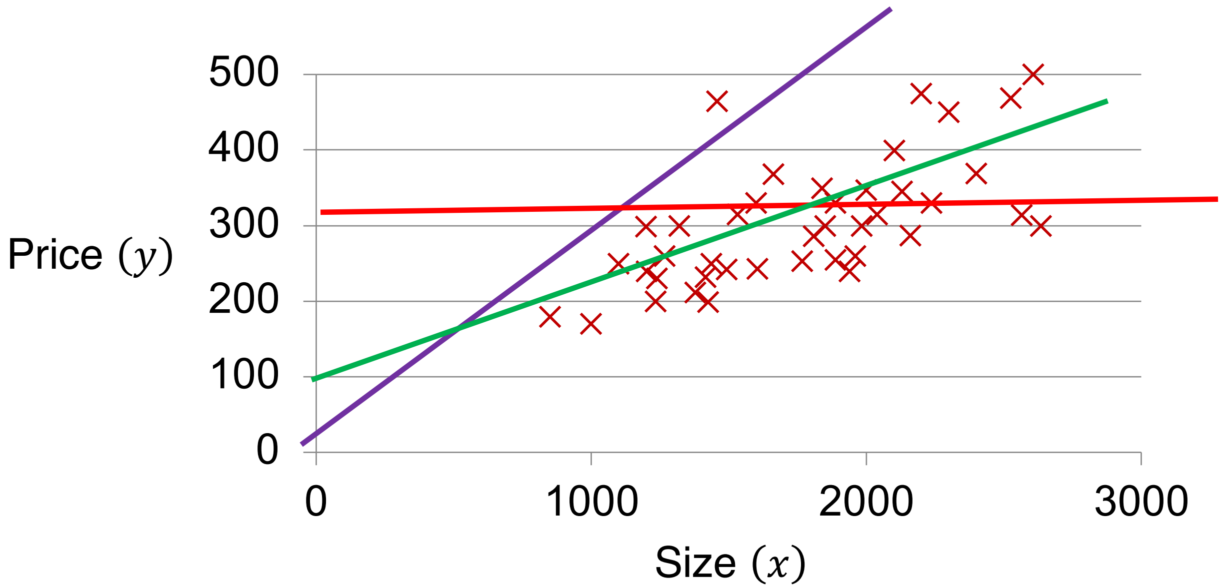
- Plot the (x, y) pairs on a plane



- The prediction function is reduced to

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

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



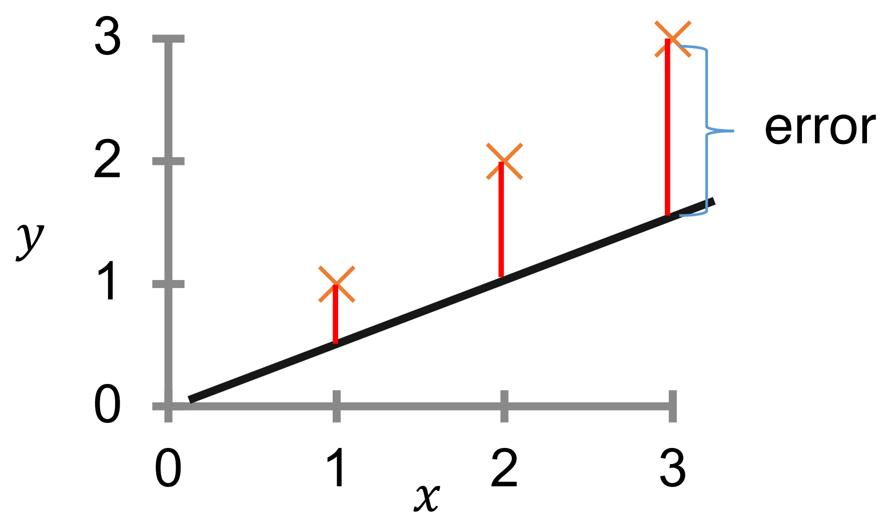
- The goal is to find an appropriate w_0 and w_1 such that the line is as fit as possible to the true y's for all given x

Cost / Loss Function

- Mathematically, the goal can be formulated as minimizing the cost (loss) function

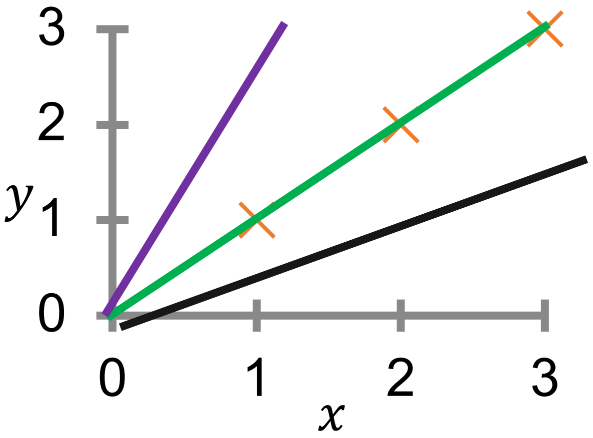
$$L(w_0, w_1) = \frac{1}{n}\sum_{i=1}^{n}\left(f\left(x^{(i)}\right) - y^{(i)}\right)^2$$

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

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



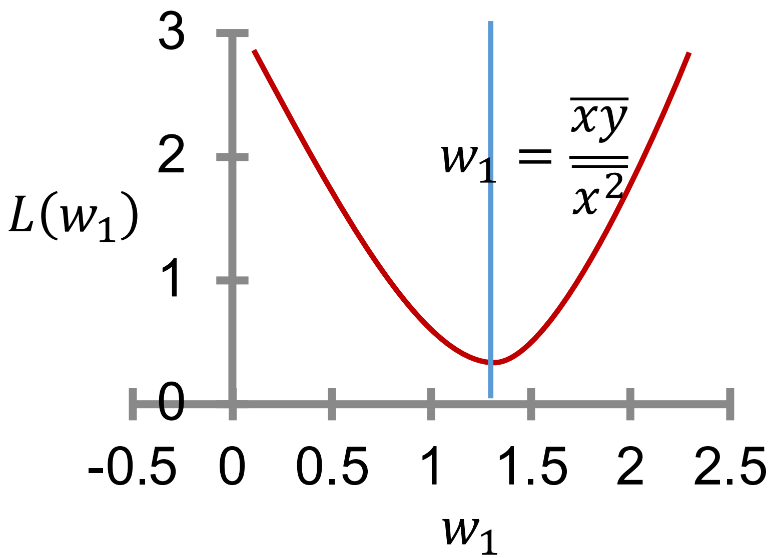
Remark: To better understand this cost function, we simplify it by setting $w_0 = 0$

- Then, the cost function becomes

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

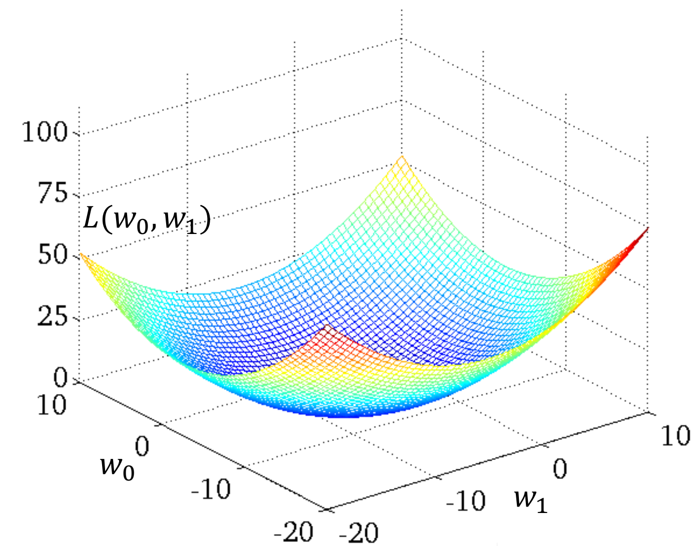
where $\overline{x^2} = \frac{\sum_{i=1}^{n} \left(x^{(i)}\right)^2}{n}$, $\overline{xy} = \frac{\sum_{i=1}^{n} x^{(i)} y^{(i)}}{n}$ and $\overline{y^2} = \frac{\sum_{i=1}^{n} \left(y^{(i)}\right)^2}{n}$

- 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

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

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

- By solving the linear equation system, the optimal w_0 and w_1 can be derived as

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

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

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- Training data from single-feature to multiple-feature case

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

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
….	….	….	….	….

- 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 in the same way as the other parameters w_k

Cost Function

- The goal 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
1416	3	2	40	232
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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

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

	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	....	....	....	....	....
		$\boldsymbol{X}$			$\boldsymbol{y}$

- 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

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

Supplement: gradient of a function w.r.t. a vector or matrix

- The meaning of gradient w.r.t a vector or matrix
  - $L(\cdot)$ is a scalar function

$$\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} \triangleq \begin{bmatrix} \frac{\partial L(\boldsymbol{w})}{\partial w_1} \\ \vdots \\ \frac{\partial L(\boldsymbol{w})}{\partial w_m} \end{bmatrix} \qquad \frac{\partial L(\boldsymbol{X})}{\partial \boldsymbol{X}} \triangleq \begin{bmatrix} \frac{\partial L(\boldsymbol{X})}{\partial x_{11}} & \cdots & \frac{\partial L(\boldsymbol{X})}{\partial x_{1m}} \\ \vdots & \ddots & \vdots \\ \frac{\partial L(\boldsymbol{X})}{\partial x_{m1}} & \cdots & \frac{\partial L(\boldsymbol{X})}{\partial x_{mm}} \end{bmatrix}$$

The gradient *w.r.t.* a vector or matrix is just the compact notation of gradients of the function *w.r.t.* every element

  - $L(\cdot)$ could be any function, *e.g.*, norm $\|\cdot\|^2$, sum $\sum_{i=1}^{m} w_i$, matrix trace $trace(\cdot)$, matrix determinant $\det(\cdot)$ etc.

$$\frac{\partial \|\boldsymbol{w}\|^2}{\partial \boldsymbol{w}} = 2\boldsymbol{w} \qquad \frac{\partial \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2}{\partial (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})} = 2(\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})$$

- When $\boldsymbol{L}(\cdot) = \left[L_1(\boldsymbol{w}), \cdots, L_p(\boldsymbol{w})\right]$ is a row vector function

$$\frac{\partial \boldsymbol{L}(\boldsymbol{w})}{\partial \boldsymbol{w}} \triangleq \left[\frac{\partial L_1(\boldsymbol{w})}{\partial \boldsymbol{w}} \quad \cdots \quad \frac{\partial L_p(\boldsymbol{w})}{\partial \boldsymbol{w}}\right] = \begin{bmatrix} \frac{\partial L_1(\boldsymbol{w})}{\partial w_1} & \cdots & \frac{\partial L_p(\boldsymbol{w})}{\partial w_1} \\ \vdots & \cdots & \vdots \\ \frac{\partial L_1(\boldsymbol{w})}{\partial w_m} & \cdots & \frac{\partial L_p(\boldsymbol{w})}{\partial w_m} \end{bmatrix}$$

It is still a compact notation

- Then, we can see that

chain rule

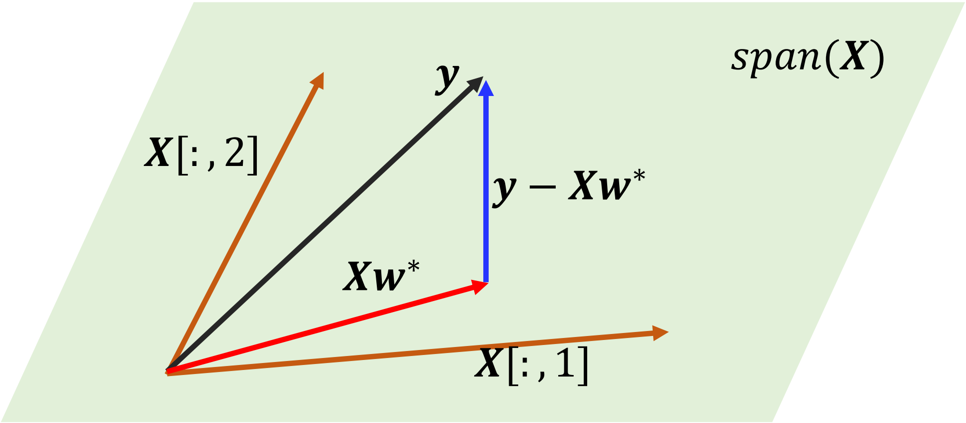
$$\frac{\partial \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2}{\partial \boldsymbol{w}} = \boxed{\frac{\partial (\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y})^T}{\partial \boldsymbol{w}} \frac{\partial \|\boldsymbol{X}\boldsymbol{w} - \boldsymbol{y}\|^2}{\partial (\boldsymbol{X}\boldsymbol{w}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

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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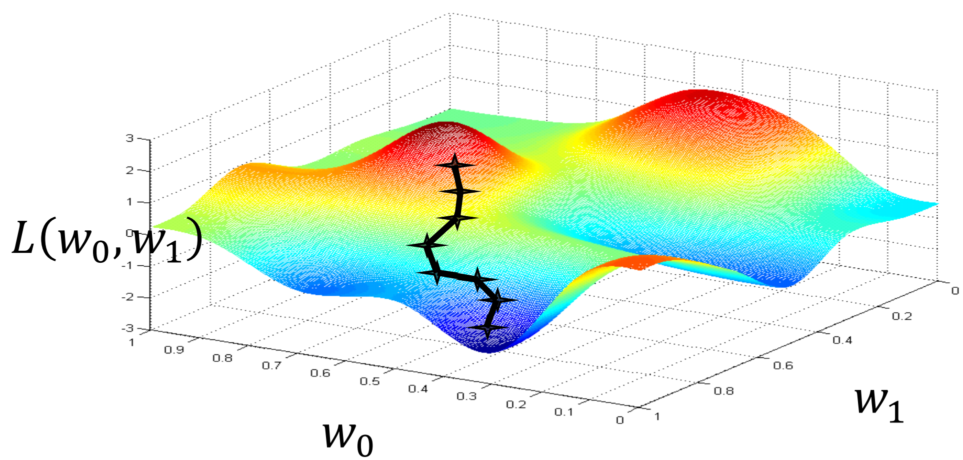
Gradient Descent

- Close-form solutions do *not always exist*, or computing the close-form expression is *too expensive*
- Under such circumstances, we can 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

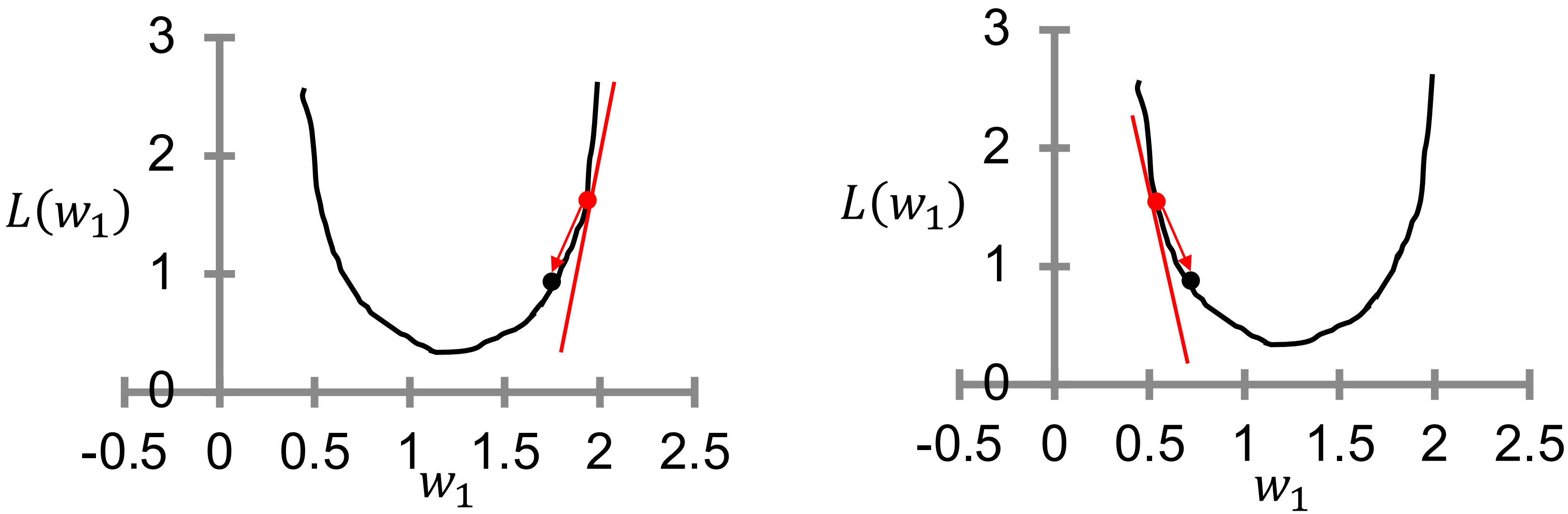


- Let us take the single-feature case and set $w_0 = 0$ as an example, under which the loss function becomes

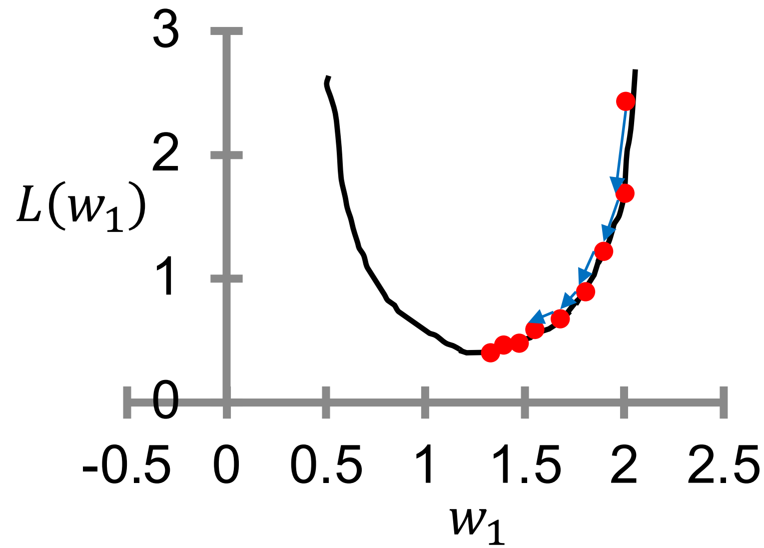
$$L(w_1) = \frac{1}{n}\sum_{i=1}^{n}\left(w_1 x^{(i)} - y^{(i)}\right)^2$$

- The parameter w_1 can be updated as

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

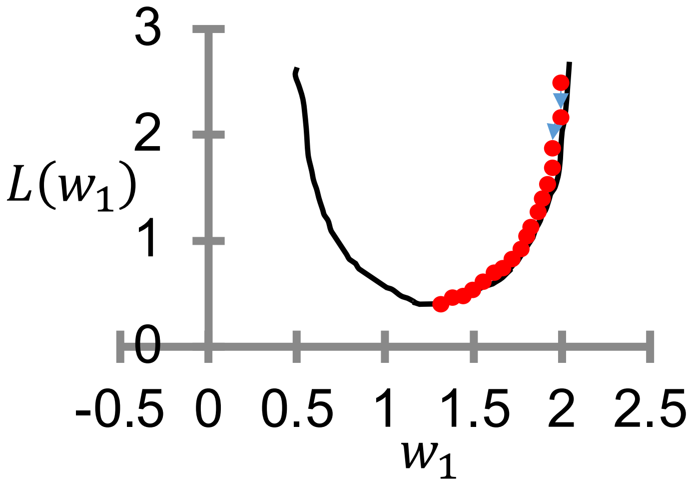


- With appropriate learning rate, the model parameter is iteratively updated, and will eventually converge to the optima

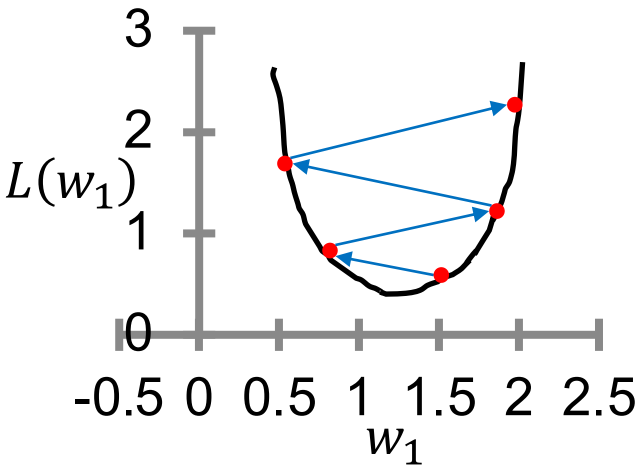


- When approaching the optima, the gradient becomes smaller and smaller. Thus, *even if the learning rate is fixed*, the updating intervals also approach 0 as the iteration proceeds, as long as the rate is set appropriately

- 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

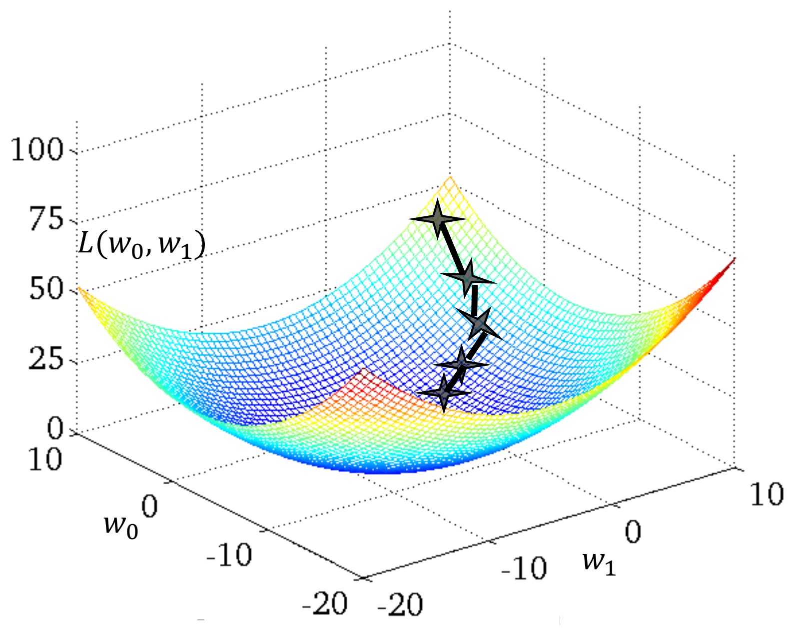


- So, setting appropriate learning rate is important

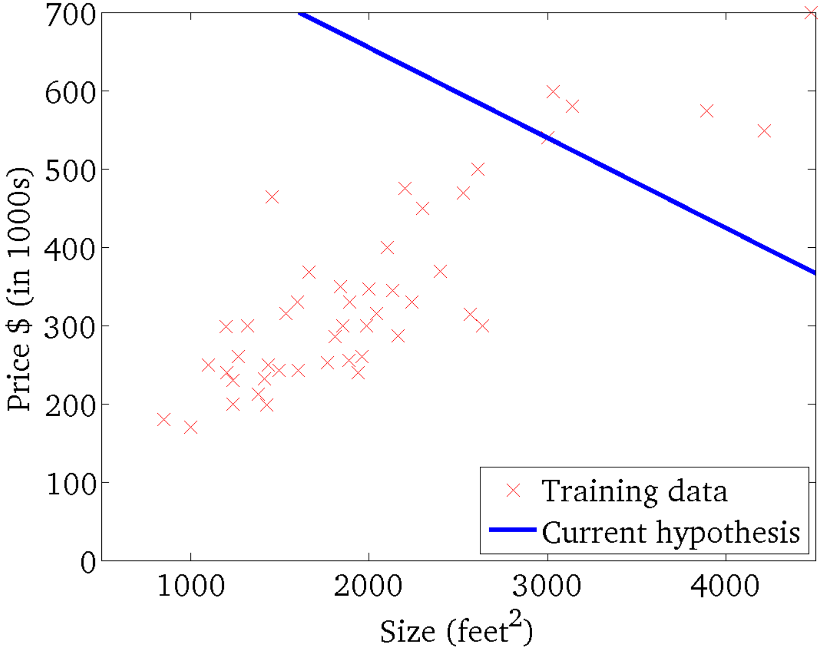
- Now consider the case with both w_0 and w_1

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

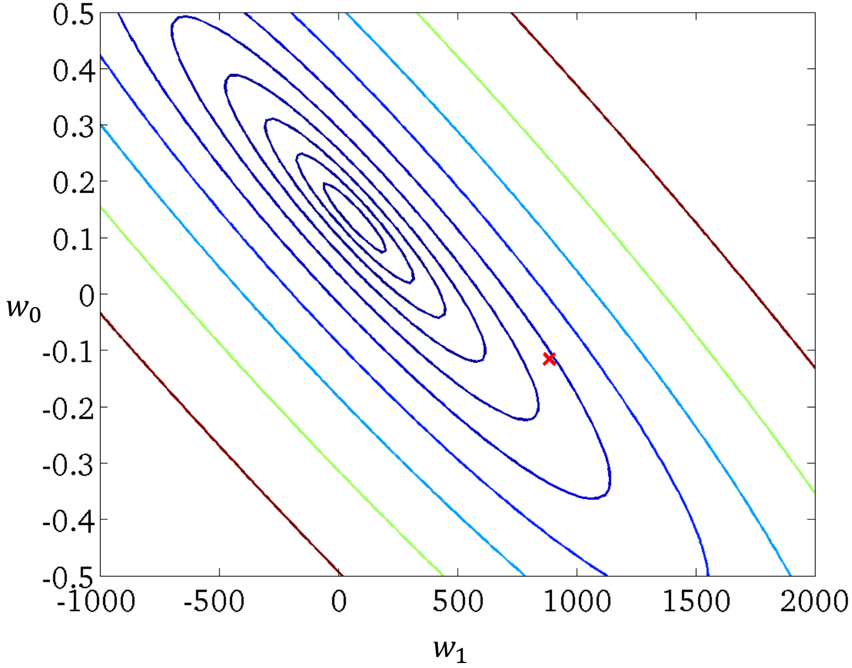
$$w_1^{(t+1)} = w_1^{(t)} - r \cdot \left. \frac{\partial L(w_0, w_1)}{\partial w_1} \right|_{w_0 = w_0^{(t)},\, w_1 = w_1^{(t)}}$$



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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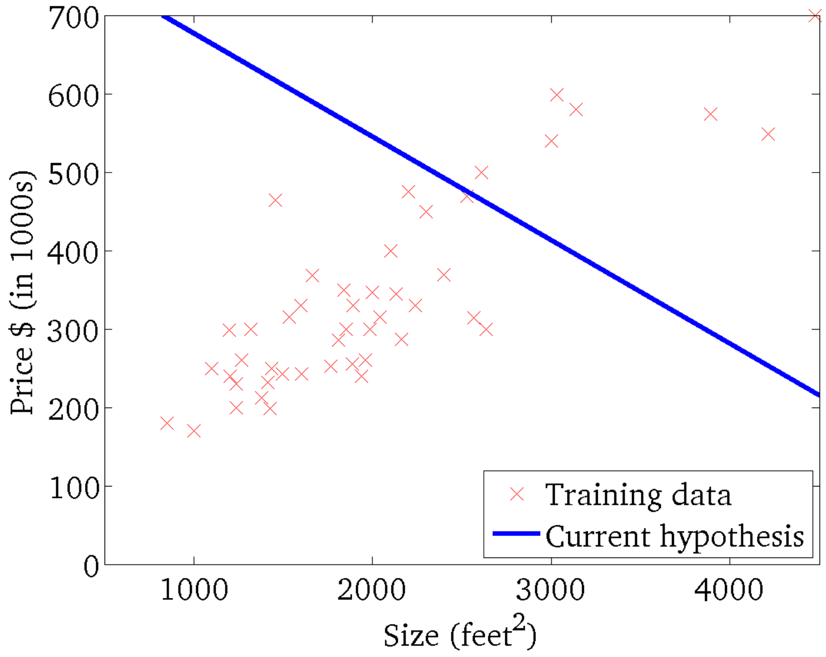

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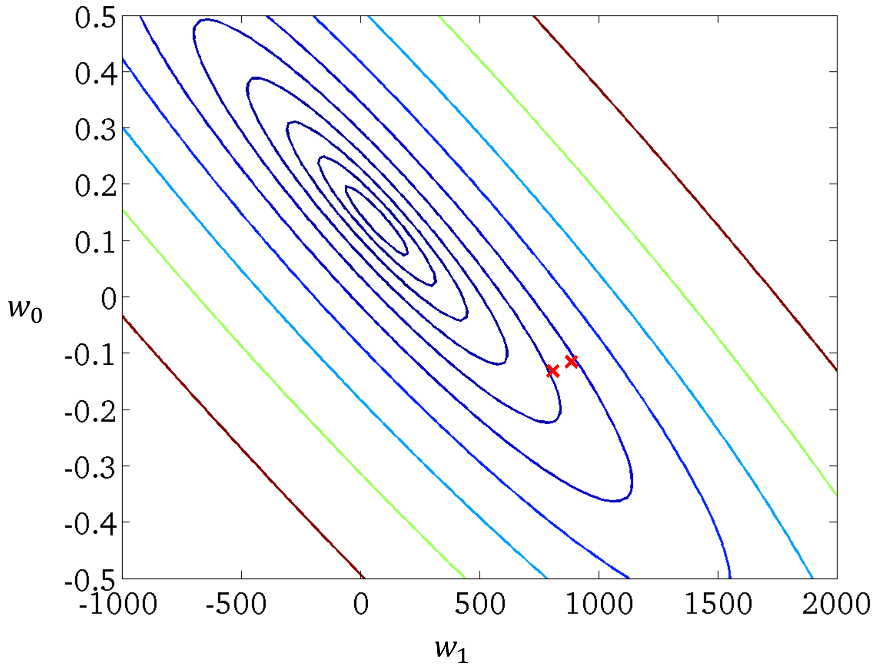

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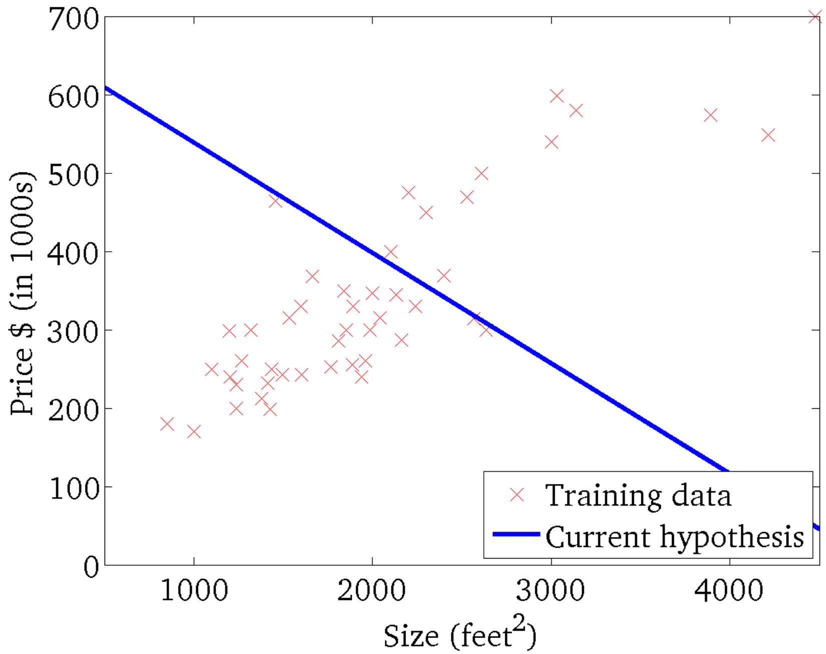

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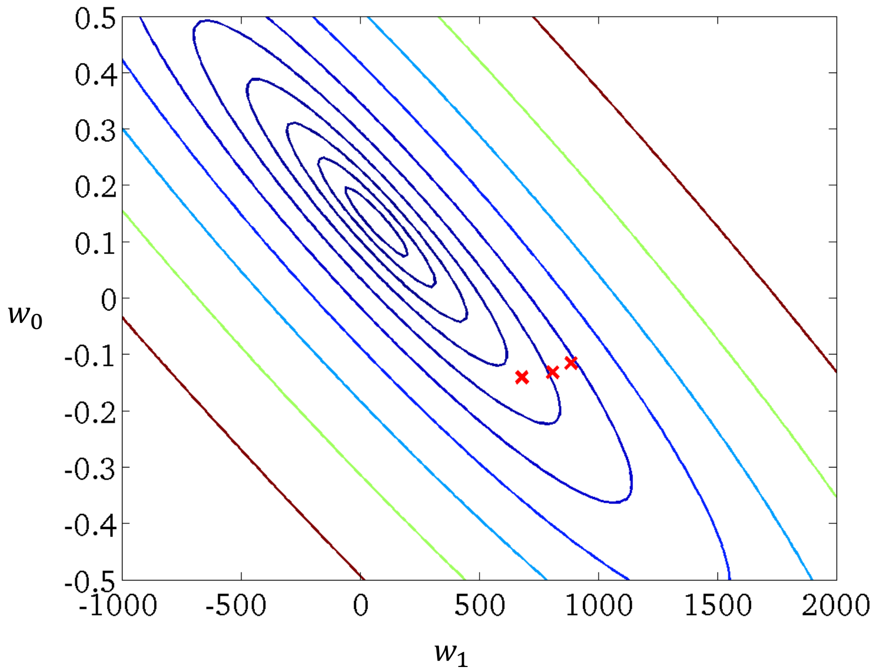

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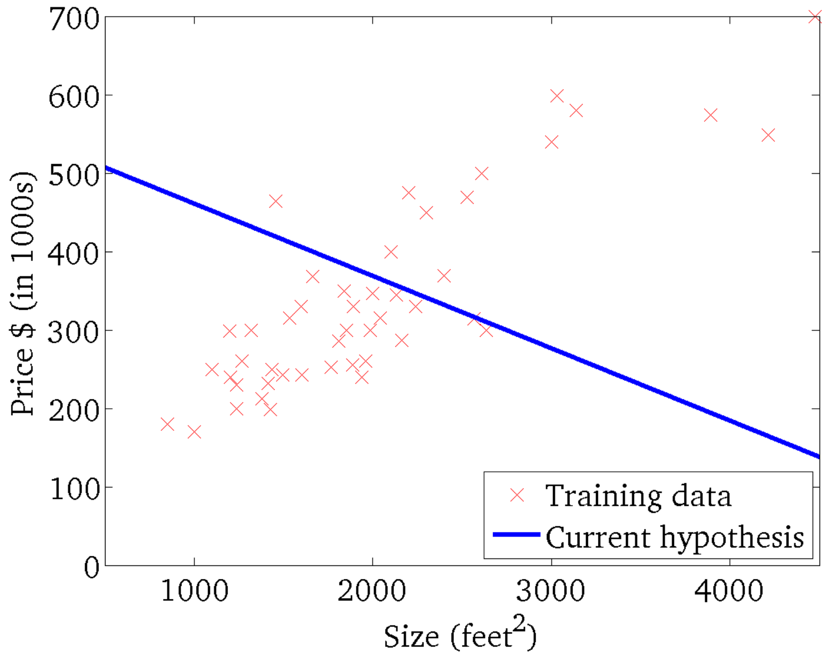

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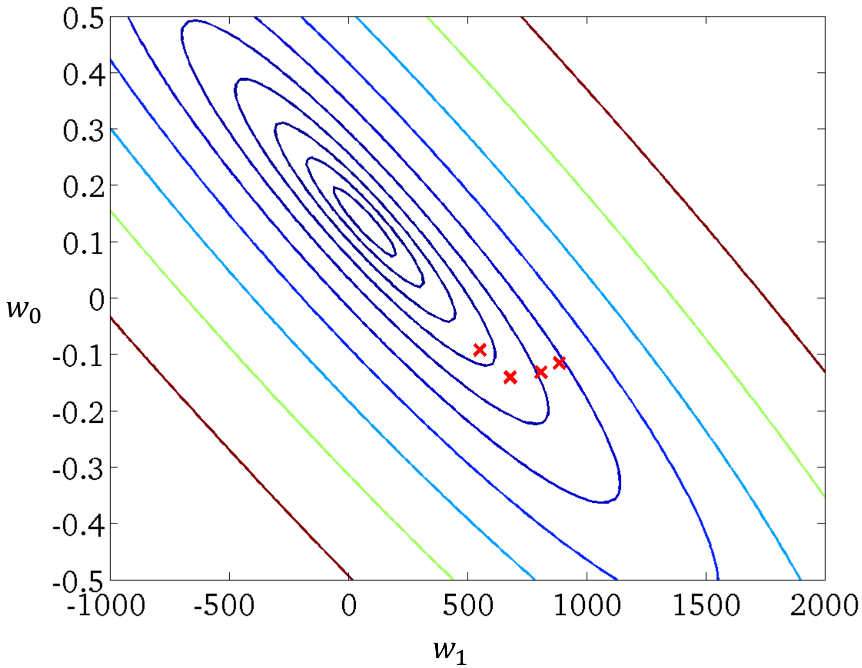

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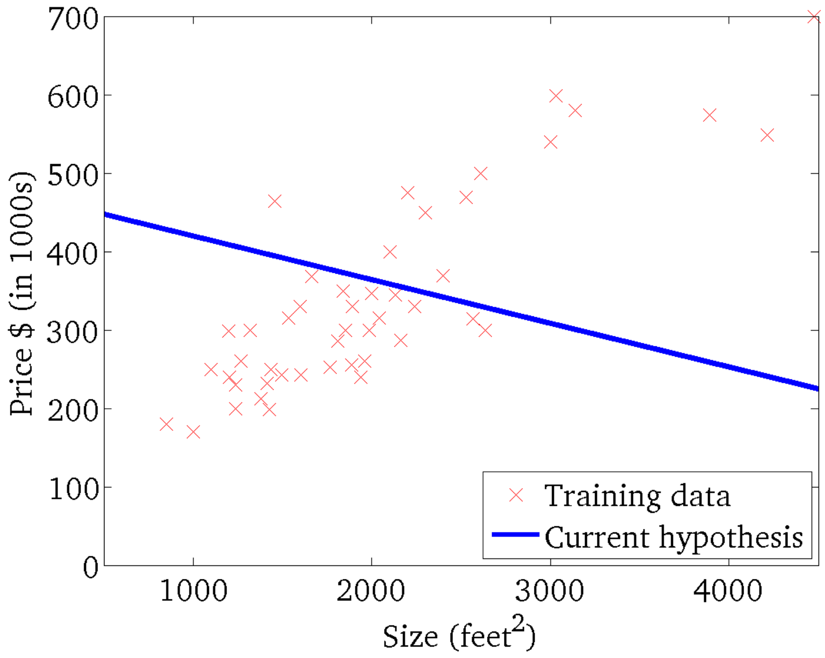

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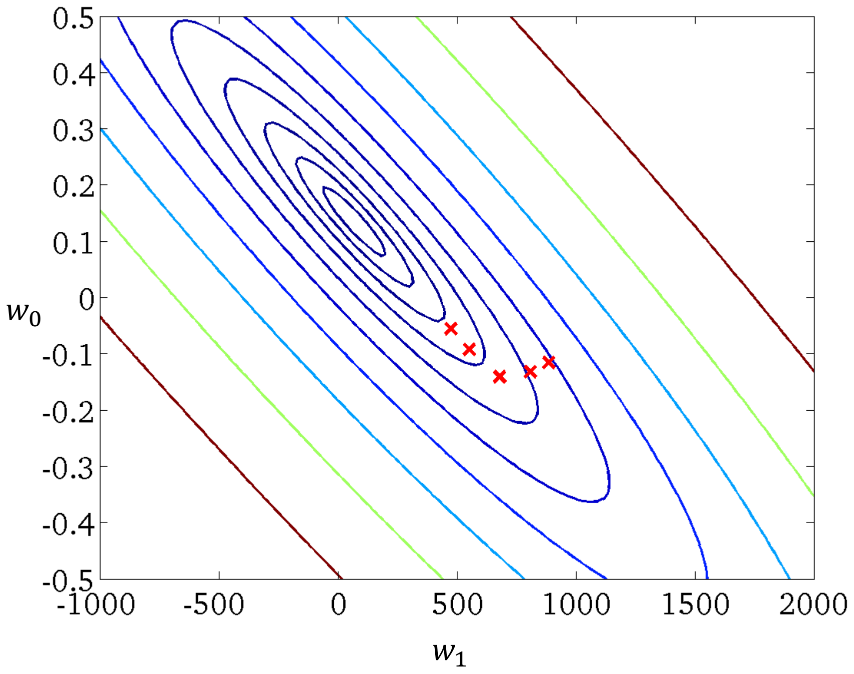

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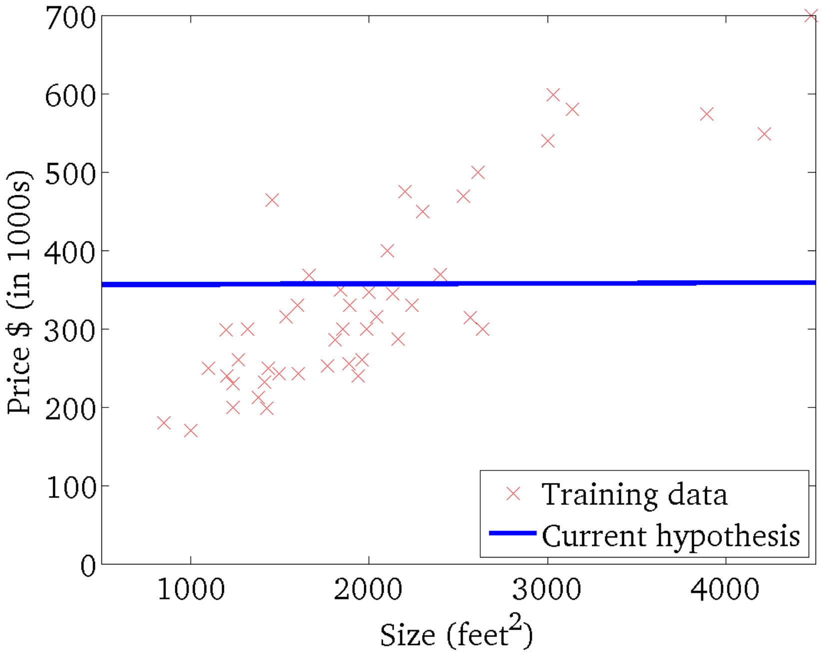

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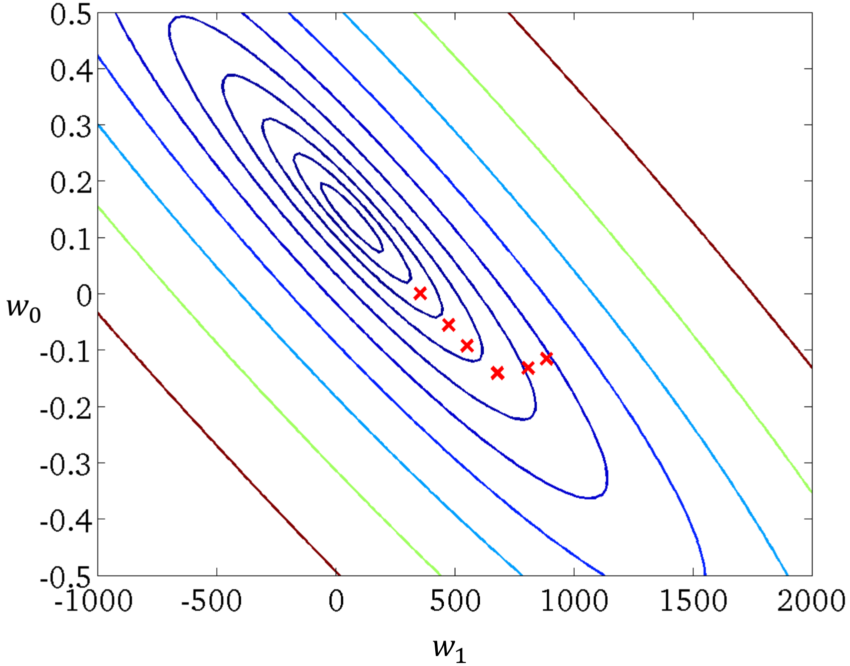

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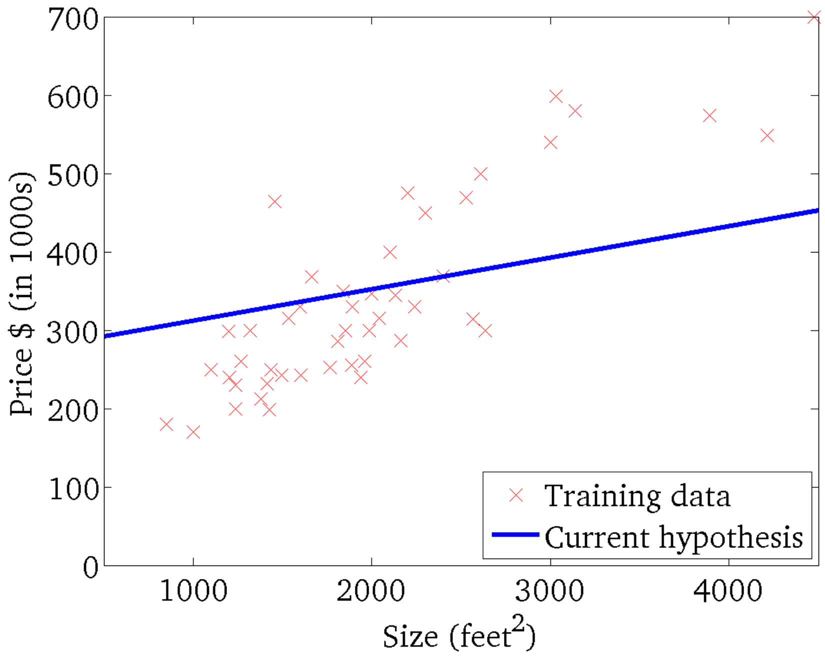

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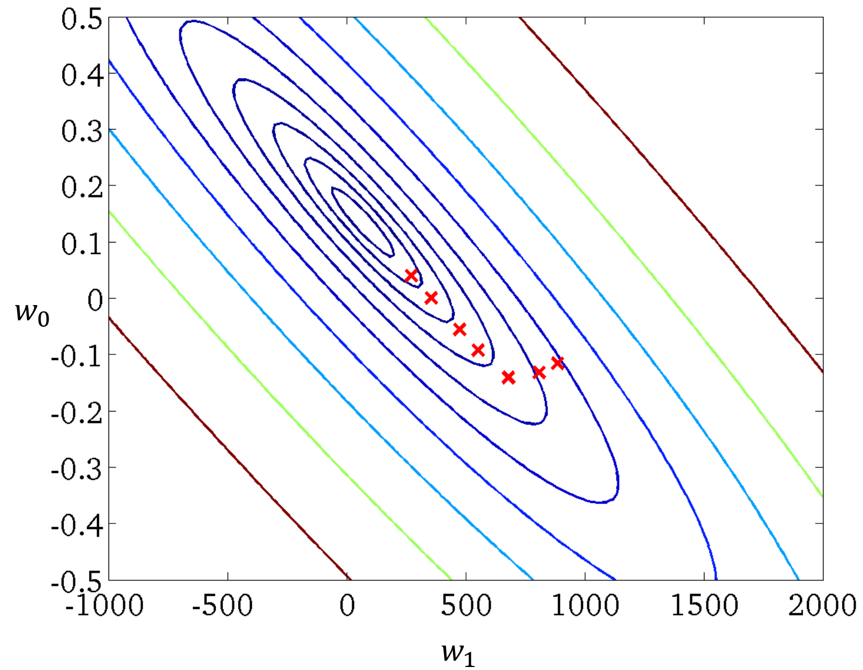

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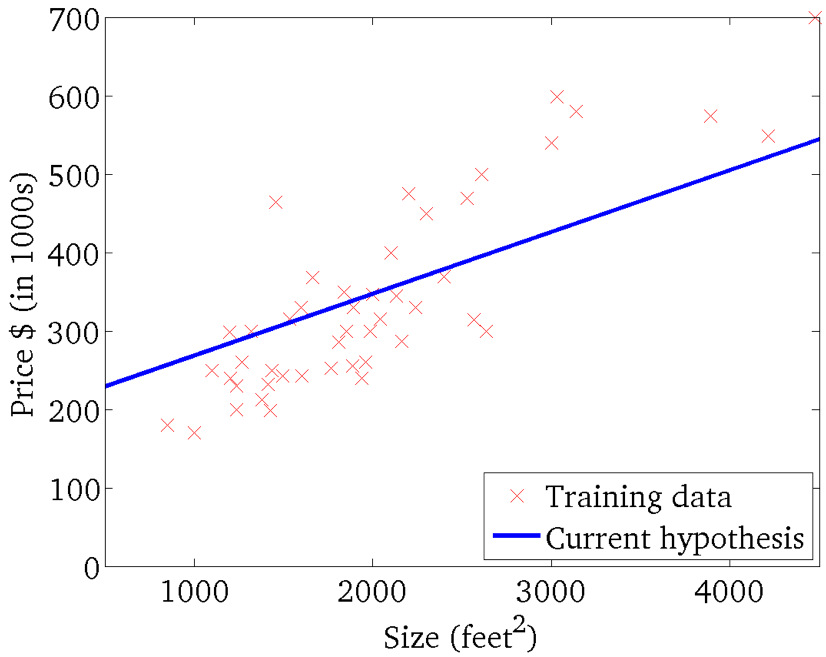

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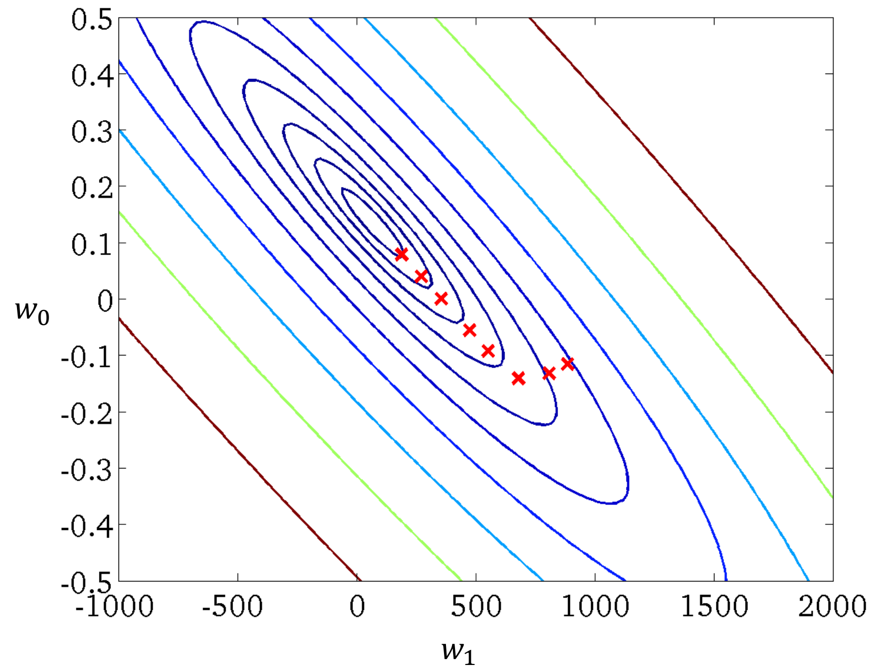

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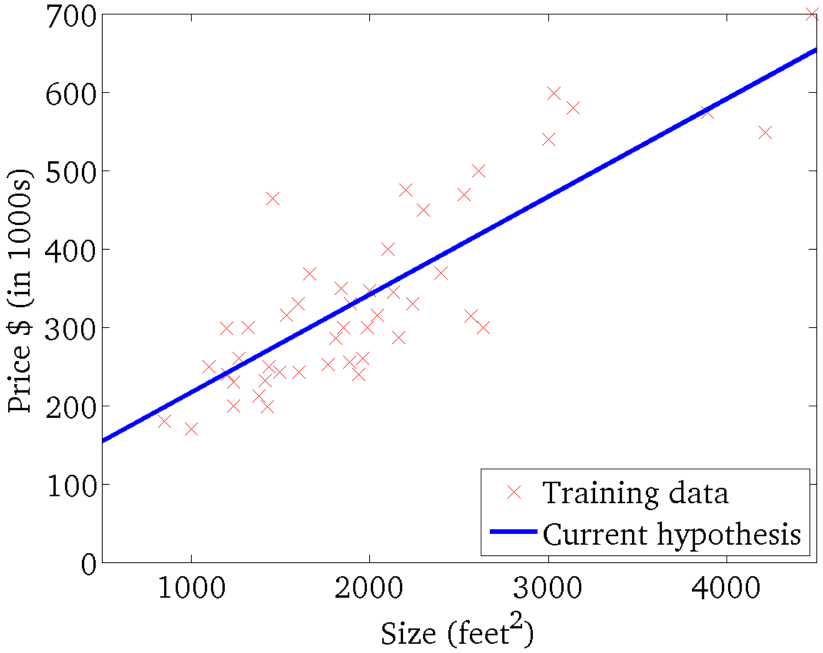

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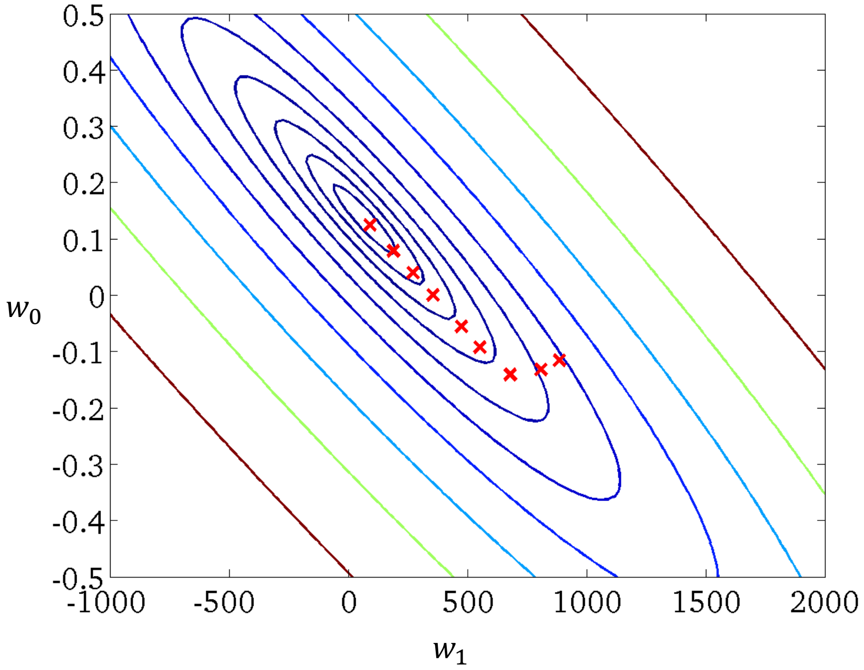


Stochastic Gradient Descent

- 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

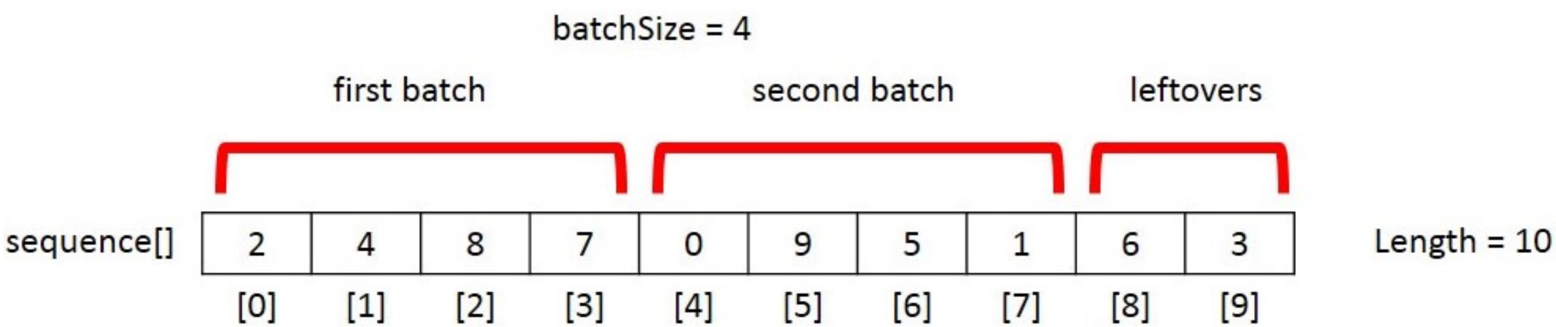
$$\frac{\partial L(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{1}{n} \sum_{i=1}^{n} \frac{\partial \ell\left(\boldsymbol{w}, \boldsymbol{x}^{(i)}, y^{(i)}\right)}{\partial \boldsymbol{w}}$$

- Every iteration requires computing the gradient on 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

- Question: What's the relation between the stochastic gradient

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

and the ground-truth gradient below?

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

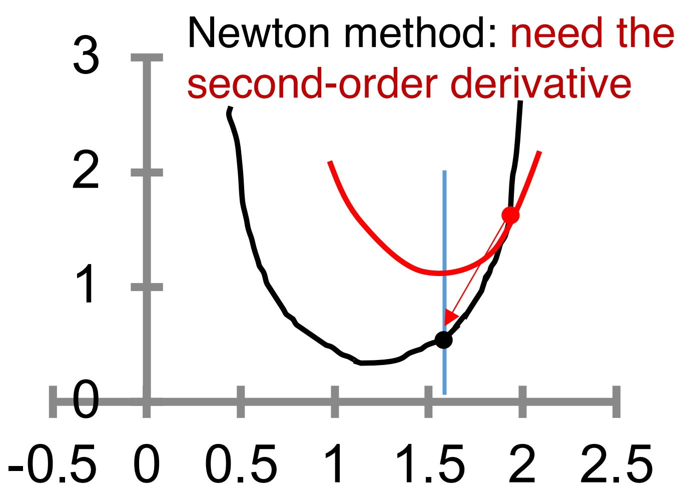
- $\frac{1}{|\mathcal{B}_t|}\sum_{i\in\mathcal{B}_t}\frac{\partial\ell\left(\boldsymbol{w},\boldsymbol{x}^{(i)},y^{(i)}\right)}{\partial\boldsymbol{w}}$ is an unbiased estimate to the true $\frac{\partial L(\boldsymbol{w})}{\partial\boldsymbol{w}}$, *i.e.*,

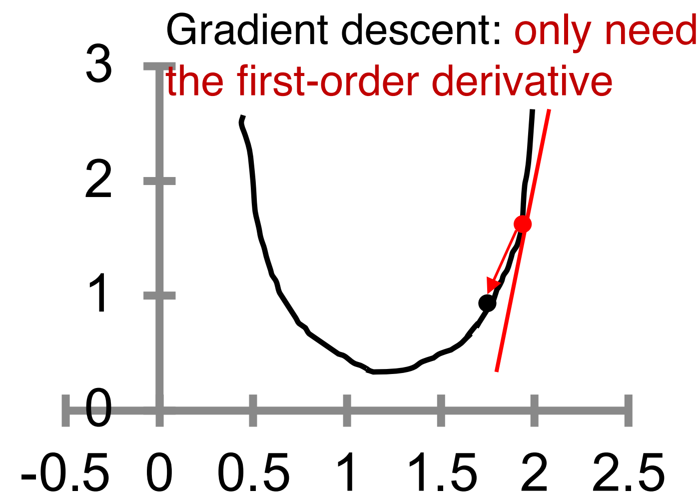
$$\mathbb{E}_{\mathcal{B}_t}\left[\frac{1}{|\mathcal{B}_t|}\sum_{i\in\mathcal{B}_t}\frac{\partial\ell\left(\boldsymbol{w},\boldsymbol{x}^{(i)},y^{(i)}\right)}{\partial\boldsymbol{w}}\right]=\frac{\partial L(\boldsymbol{w})}{\partial\boldsymbol{w}}$$

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 gradient descent methods, but are more expensive computationally