Optimization Introduction

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Outline

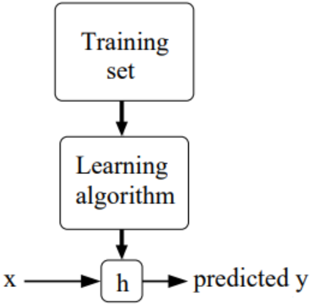
Outline

Formulas in this note

- **Features**: $x^{(i)}$
- "Output" or **target** variable: $y^{(i)}$
- A pair $(x^{(i)}, y^{(i)})$ is called a **training example**
- A list of m training examples $\{(x^{(i)}, y^{(i)}) : i = 1, \ldots, m\}$ is called a **training set**

Supervised Learning Problem

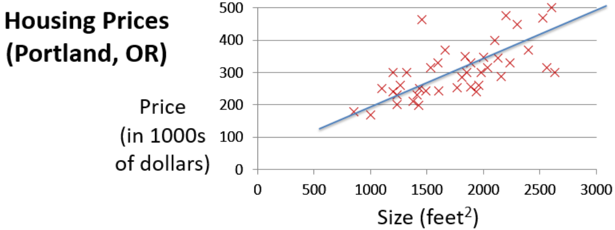
In supervised learning problems, our goal is, given a training set, to learn function $h : \mathcal{X} \mapsto \mathcal{Y}$ so that $h(x)$ is a "good" predictor for the corresponding value of y.



For historical reasons, h is called a **hypothesis**.

Example: regression problem

When y is continuous, we call the learning problem a **regression** problem.



Example: classification problem

When y takes on only a small number of discrete values, we call the learning problem a **classification** problem.

Outline

Learning Regression

We want to predict the house price using living area and number of bedrooms. Here, x's are 2-dimensional.

- $x_1^{(i)}$ is the living area of i-th house in the training set
- $x_2^{(i)}$ is its number of bedrooms

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

Learning Regression

If we approximate y as a linear function of x:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2.$$

- θ_i's are the **parameters** (also called **weights**)
- By letting $x_0 = 1$ (**intercept**), we simplify the notation as

$$h(x) = \sum_{i=0}^{n} \theta_i x_i = \theta^T x.$$

To quantify how close $h(x^{(i)})$'s are to the corresponding $y^{(i)}$'s, we define the **cost function**:

$$J(\theta) = \frac{1}{2} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2.$$

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Target: Minimizing $J(\theta)$

Let's use a search algorithm that starts with some initial guess for θ, and that repeatedly changes θ to make $J(\theta)$ smaller, until hopefully we converge to a value of θ that minimizes $J(\theta)$.

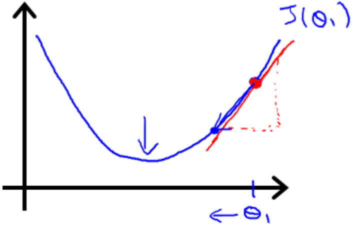
Gradient Descent

Starting with some initial θ, the Gradient Descent algorithm repeatedly performs the update:

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

This update is simultaneously performed for all θ_j $j = 0, \ldots, n$. Here, α is called the **learning rate.**

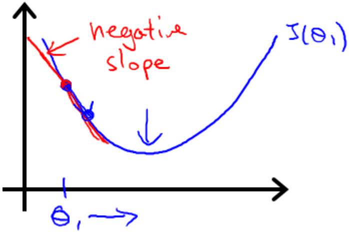
Logic for 1-dimensional GD



$(\theta_1 \in \mathbb{R})$

$$\theta_1 := \theta_1 - \alpha \underbrace{\boxed{\frac{d}{d\theta_1} J(\theta_1)}}_{\geq 0} \qquad \frac{\partial}{\partial \theta_1} \leftarrow$$

$$\theta_1 := \theta_1 - \alpha \cdot (\text{positive number})$$



$$\underbrace{\frac{d}{d\theta_1} J(\theta_1)}_{\leq 0}$$

$$\theta_1 := \theta_1 - \alpha\,(\text{negative number})$$

Calculate $\frac{\partial}{\partial \theta_j} J(\theta)$

In order to update, we need $\frac{\partial}{\partial \theta_j} J(\theta)$.

$$
\begin{aligned}
\frac{\partial}{\partial \theta_j} J(\theta) &= \frac{\partial}{\partial \theta_j} \frac{1}{2} \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)})^2 \\
&= \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \frac{\partial}{\partial \theta_j} (h_\theta(x^{(i)}) - y^{(i)}) \\
&= \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) \frac{\partial}{\partial \theta_j} \left[\sum_{k=0}^{n} \theta_k x_k^{(i)} - y^{(i)} \right] \\
&= \sum_{i=1}^{m} (\theta^T x^{(i)} - y^{(i)}) x_j^{(i)}
\end{aligned}
$$

Gradient Descent for LMS

Batch Gradient Descent for LMS

Repeat until convergence $\{$

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m} (y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)} \qquad \text{for every } j$$

$\}$

This method looks at every example in the entire training set on every step, and is called **batch gradient descent.**

Supervised Learning

Learning Regression

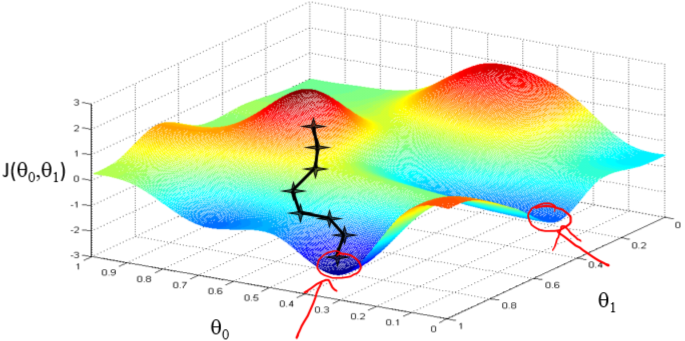
Gradient Descent

Normal Equations

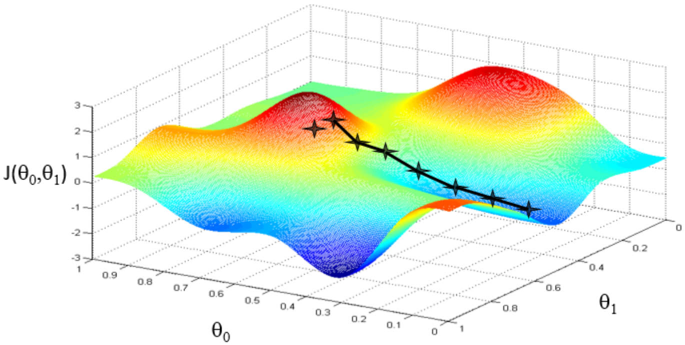
Logistic Regression

Newton's Method

Local minimum in 2-dimensional $J(\theta)$

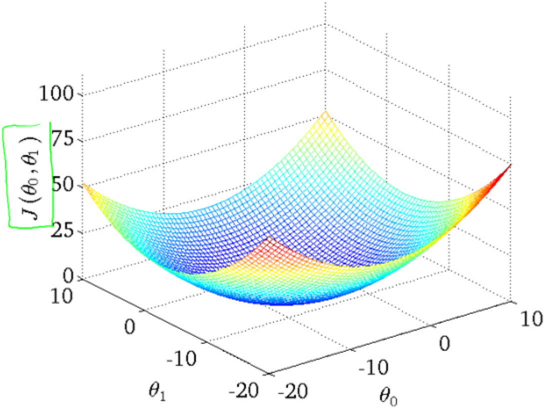


Local minimum in 2-dimensional $J(\theta)$



Global minimum in 2-dimensional $J(\theta)$

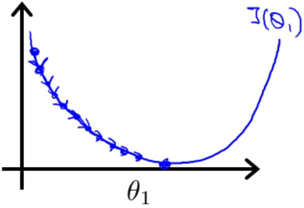
In order to avoid the local minimum, $J(\theta)$ needs to be "**convex**" (or "**convex downward**" or "**concave upward**").



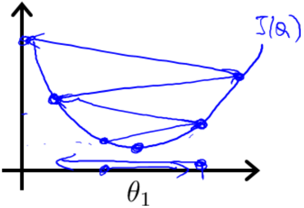
Learning Rate

$$\boxed{\theta_1 := \theta_1 - \alpha \frac{\partial}{\partial \theta_1} J(\theta_1)}$$

If α is too small, gradient descent can be slow.



If α is too large, gradient descent can overshoot the minimum. It may fail to converge, or even diverge.

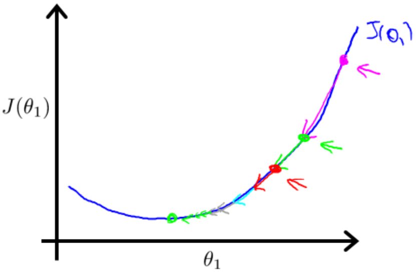


Learning Rate

Gradient descent can converge to a local minimum, even with the learning rate α fixed.

$$\theta_1 := \theta_1 - \alpha \boxed{\frac{d}{d\theta_1} J(\theta_1)}$$

As we approach a local minimum, gradient descent will automatically take smaller steps. So, no need to decrease α over time.



Stochastic Gradient Descent for LMS

Supervised Learning
Learning Regression
Gradient Descent
Normal Equations
Logistic Regression
Newton's Method

Stochastic Gradient Descent (Mini Batch GD) for LMS

Repeat until convergence {
for $i = 1$ to m {

$$\theta_j := \theta_j + \alpha(y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)} \qquad \text{for every } j$$

}
}

Batch Gradient Descent for LMS

Repeat until convergence {

$$\theta_j := \theta_j + \alpha \sum_{i=1}^{m}(y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)} \qquad \text{for every } j$$

}

Stochastic Gradient Descent for LMS

Stochastic Gradient Descent for LMS

Repeat until convergence {

for $i = 1$ to m {

$$\theta_j := \theta_j + \alpha(y^{(i)} - h_\theta(x^{(i)}))x_j^{(i)} \qquad \text{for every } j$$

}

}

Whereas **batch gradient descent** has to scan the entire training set before taking a single step (a costly operation if m is large), **stochastic gradient descent** starts making progress right away.

SGD vs. batch gradient descent

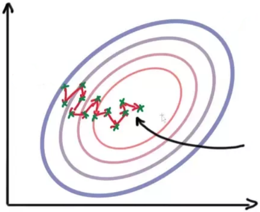


Figure: SGD

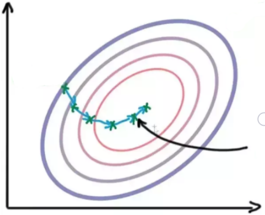


Figure: batch gradient descent

More on SGD

- Often, **SGD** is much faster than **batch gradient descent**.
- Note however that **SGD** may never "converge" to the minimum, and the parameters θ will keep oscillating around the minimum of $J(\theta)$.
- In practice, **SGD** often performs better than **batch gradient descent**.
- An alternative is **mini-batch gradient descent** which seeks a balance between **SGD** and **batch GD.**
  - **mini-batch gradient descent** splits the training set into batches, and apply **SGD** on each batch.

Outline

LMS Revisit

We all learned the closed form solution to LMS in STA 603. Let X be the design matrix, then

$$J(\theta) = \frac{1}{2}(X\theta - y)^T(X\theta - y)$$
$$\nabla_\theta J(\theta) = X^T X\theta - X^T y.$$

To minimize $J(\theta)$, we set the derivatives to zero and obtain the **normal equations**:

$$X^T X\theta = X^T y.$$

Thus the value of θ that minimizes $J(\theta)$ is given in a closed form by the equation

$$\theta = (X^T X)^{-1} X^T y.$$

Gradient Descent vs. Normal Equation

m **training examples,** n **features.**

Gradient Descent

- Need to choose α.
- Needs many iterations.
- Works well even when n is large.

Normal Equation

- No need to choose α.
- Don't need to iterate.
- Need to compute $(X^T X)^{-1}$
- Slow if n is very large, sometimes even unable to compute.

Outline

Logistic Regression

Logistic Regression Model

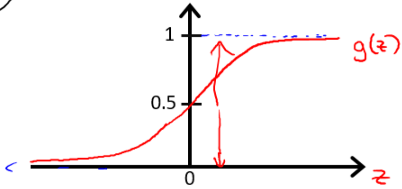
Want $\boxed{0 \leq h_\theta(x) \leq 1}$

$$h_\theta(x) = g(\theta^T x)$$

$$\rightarrow g(z) = \frac{1}{1+e^{-z}}$$

$\theta^T x$

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



Sigmoid function
Logistic function

Parameters θ.

Logistic Regression

Supervised Learning

Learning Regression

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Newton's Method

Useful property of the sigmoid function:

$$
\begin{aligned}
g'(z) &= \frac{d}{dz}\frac{1}{1+e^{-z}} \\
&= \frac{e^{-z}}{(1+e^{-z})^2} \\
&= \frac{1}{1+e^{-z}} \cdot \left(1 - \frac{1}{1+e^{-z}}\right) \\
&= g(z)(1-g(z)).
\end{aligned}
$$

Logistic Regression

Question: Which cost function should we use? Same as the square loss in linear regression?

Logistic Regression

Assume that

$$P(y=1|x,\theta) = h_\theta(x)$$
$$P(y=0|x,\theta) = 1 - h_\theta(x).$$

Then we can write down the likelihood as

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

The log likelihood is

$$\ell(\theta) = \log \ell(\theta) = \sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1-y^{(i)}) \log(1-h_\theta(x^{(i)})).$$

Logistic Regression

Calculate the derivative of $\ell(\theta)$:

$$\frac{\partial}{\partial\theta_j}\ell(\theta) = \sum_{i=1}^{m}\left[y^{(i)}\frac{1}{g(\theta^T x^{(i)})} - (1-y^{(i)})\frac{1}{1-g(\theta^T x^{(i)})}\right]\frac{\partial}{\partial\theta_j}g(\theta^T x^{(i)})$$

$$= \sum_{i=1}^{m}\left[y^{(i)}\frac{1}{g(\theta^T x^{(i)})} - (1-y^{(i)})\frac{1}{1-g(\theta^T x^{(i)})}\right]$$

$$\cdot\, g(\theta^T x^{(i)})[1-g(\theta^T x^{(i)})]\frac{\partial}{\partial\theta_j}\theta^T x^{(i)}$$

$$= \sum_{i=1}^{m}[y^{(i)}(1-g(\theta^T x^{(i)})) - (1-y^{(i)})g(\theta^T x^{(i)})]x_j^{(i)}$$

$$= \sum_{i=1}^{m}[y^{(i)} - h_\theta(x^{(i)})]x_j$$

Then we could apply batch gradient descent to calculate the MLE for logistic regression. But in practice, people use BFGS or L-BFGS instead, why?

Outline

Newton's Method

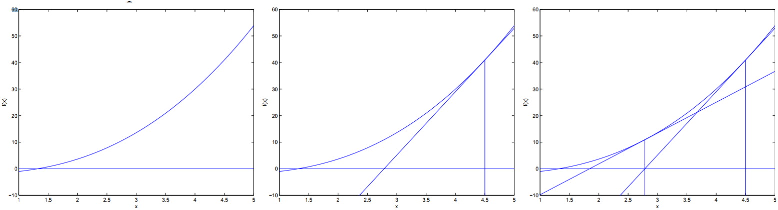
Suppose we have some function $f : \mathbb{R} \mapsto \mathbb{R}$, and we wish to find a value of θ so that $f(\theta) = 0$ ($\theta \in \mathbb{R}$). Newton's Method performs the following update:

$$\theta := \theta - \frac{f(\theta)}{f'(\theta)}.$$

Logic:

- Approximate f via a linear function that is tangent to f at the current guess θ.
- Solving for where that linear function equals to zero.
- Let the next guess for θ be where that linear function is zero.

Newton's Method



Apply Newton's method to log likelihood

We can use Newton's method to solve for $\ell'(\theta) = 0$ in order to get the maixima. Then the update rule is:

$$\theta := \theta - \frac{\ell'(\theta)}{\ell''(\theta)}.$$

We can generalize this to multidimensional setting (called **Newton-Raphson method**):

$$\theta := \theta - H^{-1}\nabla_\theta \ell(\theta).$$

Here, $\nabla_\theta \ell(\theta)$ is, as usual, the vector of partial derivatives of $\ell(\theta)$ with respect to θ_i's. And H is called the **Hessian** matrix, whose entries are given by

$$H_{ij} = \frac{\partial^2 \ell(\theta)}{\partial\theta_i \partial\theta_j}.$$

Newton's method vs. Gradient Descent

Newton's Method:

Pros:

- Faster convergence than (batch) gradient descent
- Requires many fewer iterations to get very close to the minimum.

Cons:

- Requires finding and inverting an n-by-n Hessian
- Slower when n becomes larger.

[6pt] Different quasi Newton's method (BFGS, L-BFGS) varies in how they calculate and update the (local) Hessian matrix at each step.