Gradient Descent and Related Methods

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Objectives

- Explain how **gradient descent** works
- Use gradient descent to optimize the cost function for logistic regression
- Explain the advantage of **stochastic gradient descent**
- Implement stochastic gradient descent
- Implement **Newton's method**

Agenda

- Morning
  1. What is gradient descent and why do we need it?
  2. Examples of gradient descent
  3. What can go wrong?
  4. Using gradient descent to solve logistic regression
- Afternoon
  1. Stochastic Gradient Descent
  2. Newton's Method

Cost Functions

- Machine learning often involves fitting a model to test data
- The best fit is often determined using a *cost function* or *likelihood function*
  - Linear Regression:
$$\sum (y_i - \beta^T \mathbf{x}_i)^2$$
  - Logistic Regression:
$$\sum y_i \log g(\beta^T \mathbf{x}_i) + (1 - y_i) \log(1 - g(\beta^T \mathbf{x}_i))$$
$$\left(g(z) = \frac{1}{1+e^{-z}} \right)$$

Linear Regression

The cost function $\sum(y_i - \beta^T \mathbf{x}_i)^2$ can be represented in matrix format:

$$||\mathbf{y} - X\beta||^2$$

Has a closed-form solution for the minimum

$$\beta = (X^T X)^{-1} X^T \mathbf{y}$$

Why is this infeasible sometimes?

Logistic Regression

The log-likelihood function

$$\sum y_i \log g(\beta^T \mathbf{x}_i) + (1 - y_i) \log(1 - g(\beta^T \mathbf{x}_i))$$

has no such closed form for its maximum.

How will you find the maximum?

Gradient Descent

Basic gradient-descent algorithm to find a minimum

- Choose a point and
- Calculate the gradient (direction of fastest ascent)
- Step in the opposite direction
- Repeat

How would you find a maximum?

Recall

- The *gradient* of a multivariate function $f(x_1, \ldots, x_n)$ is

$$\nabla f(\mathbf{a}) = \left(\frac{\partial f}{\partial x_1}(\mathbf{a}), \ldots, \frac{\partial f}{\partial x_n}(\mathbf{a}) \right)$$

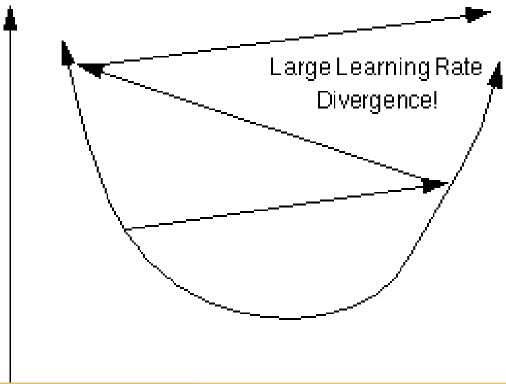
- $\nabla f(\mathbf{a})$ points in the direction of greatest increase of f at $\mathbf{a}$

Gradient Descent

To minimize f

- Choose:
  - a starting point $\mathbf{x}_0$
  - *learning rate* α
  - threshold ϵ
- Move in the direction of $-\nabla f(\mathbf{x})$:
  - Update $\mathbf{x}_{i+1} = \mathbf{x}_i - \alpha \nabla f(\mathbf{x}_i)$
- If $\frac{|f(\mathbf{x}_i) - f(\mathbf{x}_{i+1})|}{|f(\mathbf{x}_i)|} < \epsilon$, return $f(\mathbf{x}_{i+1})$ as the min, and $\mathbf{x}_{i+1}$ as the argmin

- `alpha` is called the *step-size* or *learning rate*
  - If 'alpha' is too small, convergence takes a long time
  - If 'alpha' is too big, can overshoot the minimum



Choosing Alpha

- If the value of

$$\frac{|\nabla f(\mathbf{x}_i) - \nabla f(\mathbf{x}_{i+1})|}{|\mathbf{x}_i - \mathbf{x}_{i+1}|}$$

is bounded above by some number $L(\nabla f)$ then

$$\alpha \leq \frac{1}{L(\nabla f)}$$

will converge.

- For example:
  - $f(x) = x^2$
  - $L(\nabla f) = 2$
  - $\alpha = 1/2$ will be the best value

Adaptive Step Size

- Change α at each iteration
- Barzilai and Borwein, 1998
  - Suppose $\mathbf{x}_i$ is the value of $\mathbf{x}$ at the iteration i
  - $\Delta\mathbf{x} = \mathbf{x}_i - \mathbf{x}_{i-1}$
  - $\Delta g(\mathbf{x}) = \nabla f(\mathbf{x}_i) - \nabla f(\mathbf{x}_{i-1})$
  - At each step

$$\alpha = \frac{\Delta g(\mathbf{x})^T \Delta\mathbf{x}}{||\Delta g(\mathbf{x})||^2}$$

  is a good choice of α

Convergence Criteria

Choices:

- $\frac{|f(\mathbf{x})-f(\mathbf{y})|}{|f(\mathbf{x})|} < \epsilon$
- Max number of iterations
- Magnitude of gradient $|\nabla f| < \epsilon$

Gradient Ascent

- To maximize f, we can minimize $-f$
- Still use almost the same algorithm
  - Just replace

$$\mathbf{x} = \mathbf{x} - \alpha \nabla f(\mathbf{x})$$

with

$$\mathbf{x} = \mathbf{x} + \alpha \nabla f(\mathbf{x})$$

Some Examples

- Examples

What Can Go Wrong

- Where do you think gradient descent fails?

Example

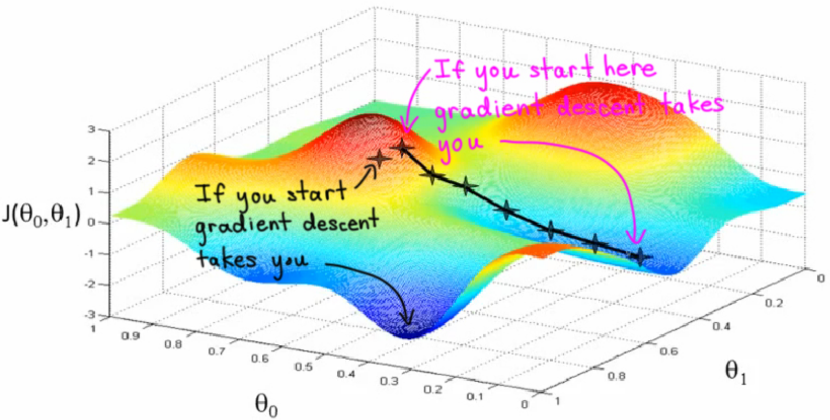


Figure 2:Non-convex function

More Bad Things

Gradient descent has limitations.

- Need differentiable and convex cost/likelihood function
- Only finds local extrema
- Poor performance without feature scaling

Back to Logistic Regression

Trying to maximize the log-likelihood function

$$\ell(\beta) = \sum_i y_i \log g(\beta^T \mathbf{x}_i) + (1 - y_i) \log(1 - g(\beta^T \mathbf{x}_i))$$

To use gradient ascent: need to compute $\nabla \ell(\beta)$

More Logistic Regression

First, let's compute the derivative of the sigmoid function g:

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

More Logistic Regression

Using this and the chain rule, and writing $g = g(\beta^T \mathbf{x}_i)$ compute $\frac{\partial \ell}{\partial \beta_i}$,

$$\begin{aligned}
\frac{\partial \ell}{\partial \beta_j} &= \frac{\partial}{\partial \beta_i} \sum_i y_i \log g(\beta^T \mathbf{x}_i) + (1 - y_i) \log(1 - g(\beta^T \mathbf{x}_i)) \\
&= \frac{\partial}{\partial \beta_j} \sum_i y_i \log g + (1 - y_i) \log(1 - g) \\
&= \sum_i y_i \frac{1}{g} g(1 - g) \mathbf{x}_i - (1 - y_i) \frac{1}{1 - g} g(1 - g) x_{ij} \\
&= \sum_i (y_i - y_i g - g + y_i g) x_{ij} \\
&= \sum_i (y_i - g(\beta^T \mathbf{x}_i)) x_{ij}
\end{aligned}$$

This is what you'll use to update the value of β in each iteration of gradient descent

Stochastic Gradient Descent

Why Not Regular Gradient Descent?

What are the problems with gradient descent?

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- Memory constrained
  - Need to store all data in memory
- CPU constrained
  - Cost function is a function of *all* data
- What if you are getting new data continuously?

Solution

Only use a single data point, or a small subset of your data, at in each step!

Algorithm

Same as gradient descent except

- at each step compute the cost function by using **just one observation**
- For example in linear regression, instead of computing the gradient of

$$\sum_i (y_i - \beta^T \mathbf{x}_i)^2$$

randomly select some $\mathbf{x}_i, y_i$ and compute the gradient of

$$(y_i - \beta^T \mathbf{x}_i)^2$$

Properties

- Faster than *batch* (regular) Gradient Descent on average
- Prone to oscillation around an optimum
- Only requires one observation in memory at once

Variants

There are a couple variants.

- "Minibatch" SGD: use a small subset of your data instead of a single observations
- "Online" SGD: update the model by performing a gradient descent step each time a new observation is collected

Newton's Method

What Is It?

- Optimization technique similar to gradient descent
- Uses a root-finding method applied to $f'(x)$

Algorithm in One Dimension

Algorithm

- Choose initial x_0
- While $f'(x) > \epsilon$:

$$x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)}$$

Higher Dimensions

For higher dimentions, change

$$x_{i+1} = x_i - \frac{f'(x_i)}{f''(x_i)}$$

to

$$\mathbf{y}_{i+1} = \mathbf{y}_i - H(\mathbf{y}_i)^{-1} \nabla f(\mathbf{y}_i)$$

where $H(\mathbf{a}) = \left[\frac{\partial f}{\partial x_i \partial x_j}(\mathbf{a}) \right]$ is the *Hessian* matrix, the matrix of second partial derivatives at $\mathbf{a}$

Problems

- Hessian might be singular, or computation can be slow
- Can diverge with a bad starting guess