Optimization: gradient descent and Newton's method
Outline of the lecture

Many machine learning problems can be cast as optimization problems. This lecture introduces optimization. The objective is for you to learn:

- The definitions of gradient and Hessian.
- The gradient descent algorithm.
- Newton’s algorithm.
- The stochastic gradient descent algorithm for online learning.
- How to apply all these algorithms to linear regression.
Gradient vector

Let $\mathbf{\theta}$ be an $d$-dimensional vector and $f(\mathbf{\theta})$ a scalar-valued function. The gradient vector of $f(\cdot)$ with respect to $\mathbf{\theta}$ is:

$$\nabla_{\mathbf{\theta}} f(\mathbf{\theta}) = \begin{bmatrix} \frac{\partial f(\mathbf{\theta})}{\partial \theta_1} \\ \frac{\partial f(\mathbf{\theta})}{\partial \theta_2} \\ \vdots \\ \frac{\partial f(\mathbf{\theta})}{\partial \theta_n} \end{bmatrix}$$
The **Hessian** matrix of $f(\cdot)$ with respect to $\theta$, written $\nabla_{\theta}^2 f(\theta)$ or simply as $H$, is the $d \times d$ matrix of partial derivatives,

$$
\nabla_{\theta}^2 f(\theta) = \begin{bmatrix}
\frac{\partial^2 f(\theta)}{\partial \theta_1^2} & \frac{\partial^2 f(\theta)}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2 f(\theta)}{\partial \theta_1 \partial \theta_n} \\
\frac{\partial^2 f(\theta)}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 f(\theta)}{\partial \theta_2^2} & \cdots & \frac{\partial^2 f(\theta)}{\partial \theta_2 \partial \theta_d} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^2 f(\theta)}{\partial \theta_d \partial \theta_1} & \frac{\partial^2 f(\theta)}{\partial \theta_d \partial \theta_2} & \cdots & \frac{\partial^2 f(\theta)}{\partial \theta_d^2}
\end{bmatrix}
$$
In offline learning, we have a batch of data $x_{1:n} = \{x_1, x_2, \ldots, x_n\}$. We typically optimize cost functions of the form

$$f(\theta) = f(\theta, x_{1:n}) = \frac{1}{n} \sum_{i=1}^{n} f(\theta, x_i)$$

The corresponding gradient is

$$g(\theta) = \nabla_{\theta} f(\theta) = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\theta} f(\theta, x_i)$$

For linear regression with training data $\{x_i, y_i\}_{i=1}^{n}$, we have have the quadratic cost

$$f(\theta) = f(\theta, X, y) = (y - X\theta)^T(y - X\theta) = \sum_{i=1}^{n} (y_i - x_i\theta)^2$$
Gradient vector and Hessian matrix

\[ f(\theta) = f(\theta, X, y) = (y - X\theta)^T(y - X\theta) = \sum_{i=1}^{n}(y_i - x_i^T\theta)^2 \]

\[ \nabla f(\theta) = 2X^TX\theta - 2X^Ty \quad \equiv \quad \nabla^2 f(\theta) = -2\sum_{i=1}^{n}x_i(x_i^T\theta) \]

\[ H = \nabla^2 f(\theta) = 2X^TX \]
**Steepest gradient descent algorithm**

One of the simplest optimization algorithms is called gradient descent or steepest descent. This can be written as follows:

\[
\theta_{k+1} = \theta_k - \eta_k g_k = \theta_k - \eta_k \nabla f(\theta_k)
\]

where \( k \) indexes steps of the algorithm, \( g_k = g(\theta_k) \) is the gradient at step \( k \), and \( \eta_k > 0 \) is called the learning rate or step size.
Steepest gradient descent algorithm for least squares

\[ f(\theta) = f(\theta, X, y) = (y - X\theta)^T (y - X\theta) = \sum_{i=1}^{n} (y_i - x_i \theta)^2 \]

\[ \nabla f(\theta) = 2 X^T X \theta \rightarrow 2X^T y = -2 \sum_{i=1}^{n} x_i^T (y_i - x_i \theta) \]

\[ \theta_{k+1} = \theta_k - 2 \eta \left[ X^T X \theta_k - X^T y \right] \]

\[ \theta_{k+1} = \theta_k + 2 \eta \sum_{i=1}^{n} x_i^T (y_i - x_i \theta) \]
How to choose the step size?

\[ \eta = 0.1 \]

\[ \Theta_{k+1} = \Theta_k - (0.1) \nabla f(\Theta_k) \]
Newton’s algorithm

The most basic second-order optimization algorithm is Newton’s algorithm, which consists of updates of the form

$$\theta_{k+1} = \theta_k - H_K^{-1} g_k$$

This algorithm is derived by making a second-order Taylor series approximation of $f(\theta)$ around $\theta_k$:

$$f_{quad}(\theta) = f(\theta_k) + g_k^T (\theta - \theta_k) + \frac{1}{2} (\theta - \theta_k)^T H_k (\theta - \theta_k)$$

differentiating and equating to zero to solve for $\theta_{k+1}$.

$$\frac{\partial f_{quad}(\theta)}{\partial \theta} = 0 + g_k + H_k (\theta - \theta_k) = 0$$

$$-g_k = H_k \theta - H_k \theta_k$$

$$-H_k^{-1} g_k = \theta - \theta_k$$
Newton’s as bound optimization
Newton’s algorithm for linear regression

\[ f(\theta) = f(\theta, X, y) = (y - X\theta)^T(y - X\theta) = \sum_{i=1}^{n}(y_i - x_i\theta)^2 \]

\[ g = \nabla f(\theta) = 2X^T X \theta - 2X^T y \]

\[ H = 2x^T x \]

\[ \Theta_{k+1} = \Theta_k - \frac{\lambda}{2} (X^T X)^{-1} \left[ X^T \Theta_k - x^T y \right] \]

\[ = \Theta_k - (X^T X)^{-1} (X^T X)\Theta_k + \left( X^T X \right)^{-1} \right) \hat{y} \]

\[ = (X^T X)^{-1} \hat{x}^T y \]

Exercise: Show this is (\hat{x}^T X^{-1} X)^{-1} \hat{x}^T y
Advanced: Newton CG algorithm

Rather than computing \( d_k = -H_k^{-1}g_k \) directly, we can solve the linear system of equations \( H_k d_k = -g_k \) for \( d_k \).

One efficient and popular way to do this, especially if \( H \) is sparse, is to use a conjugate gradient method to solve the linear system.

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1. Initialize \( \theta_0 \)
2. for \( k = 1, 2, \ldots \) until convergence do
3. Evaluate \( g_k = \nabla f(\theta_k) \)
4. Evaluate \( H_k = \nabla^2 f(\theta_k) \)
5. Solve \( H_k d_k = -g_k \) for \( d_k \)
6. Use line search to find stepsize \( \eta_k \) along \( d_k \)
7. \( \theta_{k+1} = \theta_k + \eta_k d_k \)
Online learning
aka stochastic gradient descent

**Batch**

$$\Theta_{k+1} = \Theta_k + \eta \sum_{i=1}^{n} x_i (y_i - x_i \Theta_k)$$

**Online**

$$\Theta_{k+1} = \Theta_k + \eta x_k^{\top} (y_k - x_k \Theta_k)$$

**Mini-batch**

$$\Theta_{k+1} = \Theta_k + \eta \sum_{j=1}^{20} x_j^{\top} (y_j - x_j \Theta_k)$$
The online learning algorithm
Stochastic gradient descent

SGD can also be used for offline learning, by repeatedly cycling through the data; each such pass over the whole dataset is called an epoch. This is useful if we have massive datasets that will not fit in main memory. In this offline case, it is often better to compute the gradient of a mini-batch of $B$ data cases. If $B = 1$, this is standard SGD, and if $B = N$, this is standard steepest descent. Typically $B \sim 100$ is used.

Intuitively, one can get a fairly good estimate of the gradient by looking at just a few examples. Carefully evaluating precise gradients using large datasets is often a waste of time, since the algorithm will have to recompute the gradient again anyway at the next step. It is often a better use of computer time to have a noisy estimate and to move rapidly through parameter space.

SGD is often less prone to getting stuck in shallow local minima, because it adds a certain amount of “noise”. Consequently it is quite popular in the machine learning community for fitting models such as neural networks and deep belief networks with non-convex objectives.
Next lecture

In the next lecture, we apply these ideas to learn a neural network with a single neuron (logistic regression).