1 Steepest Descent Convergence, Conjugate Directions (July 14)

1.1 Recap

Consider $f(x) = \frac{1}{2}x^TQx - b^Tx$, where Q is positive definite symmetric, and has eigenvalues $\lambda = \lambda_1 \leq \cdots \leq \lambda_n = \Lambda$. Since Q is positive definite, there is a unique minimizer x_* such that $Qx_* = b$. Let $g(x) = \nabla f(x) = Qx - b$. We may as well minimize $q(x) = \frac{1}{2}(x - x_*)^TQ(x - x_*) = f(x) + \text{const}$. Moreover, q is always positive except at $x = x_*$, so q is nicer to work with. Note that $\nabla q(x) = \nabla f(x) = g(x) = Qx - b$. Denote by g_k the point $g(x_k) = Qx_k - b$. Then, if x_k is generated by steepest descent, we derived the expression

$$q(x_{k+1}) = \left(1 - \frac{|g_k|^4}{(g_k^TQg_k)(g_k^TQ^{-1}g_k)}\right) q(x_k).$$

We may use this to study the rate of convergence of gradient descent.

1.2 Rate of Convergence of Steepest Descent

If $v = g_k$, then the term in the brackets may be written

$$1 - \frac{|v|^4}{(v^TQv)(v^TQ^{-1}v)}.$$

Kantorovich's inequality says that if Q is an $n \times n$ positive definite symmetric matrix with eigenvalues $\lambda = \lambda_1 \leq \cdots \leq \lambda_n = \Lambda$, then

$$\frac{|v|^4}{(v^TQv)(v^TQ^{-1}v)} \geq \frac{4\lambda\Lambda}{(\lambda + \Lambda)^2} \qquad \text{for all } v \in \mathbb{R}^n.$$

Thus

$$q(x_{k+1}) = \left(1 - \frac{|v|^4}{(v^TQv)(v^TQ^{-1}v)}\right) q(x_k) \leq \left(1 - \frac{4\lambda\Lambda}{(\lambda + \Lambda)^2}\right) q(x_k),$$

which simplifies to, after some work,

$$q(x_{k+1}) \leq \underbrace{\frac{(\lambda - \Lambda)^2}{(\lambda + \Lambda)^2}}_{r} q(x_k).$$

Then $0 \leq r < 1$. We shall call the constant r the *rate of convergence*. We state some properties of steepest descent in the quadratic case. The only thing we have to prove in the following theorem is that steepest descent converges.

Theorem 1.1. *(Steepest descent, quadratic case) For $x_0 \in \mathbb{R}^n$, the method of steepest descent starting at x_0 converges to the unique minimizer x_* of the function f, and we have $q(x_{k+1}) \leq rq(x_k)$.*

Proof. We know that $q(x_{k+1}) \leq r^k q(x_0)$. Since $0 \leq r < 1$, when $k \to \infty$, $r^k \to 0$. Note that

$$x_k \in \{x \in \mathbb{R}^n : q(x) \leq r^k q(x_0)\}.$$

This set is a sublevel set of q. The sublevel sets of q look like concentric filled-in ellipses centred at x_*, and as $k \to \infty$, they seem to "shrink" into x_*. Therefore steepest descent converges in the quadratic case. $\square$

Note that

$$r = \frac{(\Lambda - \lambda)^2}{(\Lambda - \lambda)^2} = \frac{(\Lambda/\lambda - 1)^2}{(\Lambda/\lambda - 1)^2},$$

so r depends only on the ratio Λ/λ. This number is called the *condition number of Q*. (The condition number may be defined as $\|Q\|\|Q^{-1}\|$ in the operator norm on matrices; it is not hard to see that these numbers agree in our case.)

If the condition number $\Lambda/\lambda \gg 1$ (large), then convergence is very slow. If $\Lambda/\lambda = 1$, then $r = 0$, and so convergence is achieved in one step.

1.3 Method of Conjugate Directions

We will develop a new method for finding the minimizers of quadratic functions $\frac{1}{2}x^T Qx - b^T x$.

Definition 1. *Let Q be symmetric. We say that d, d' are Q-conjugate or Q-orthogonal if $d^T Qd' = 0$. A finite set $d_0, \ldots, d_k$ of vectors is called Q-orthogonal if $d_i^T Qd_j = 0$ for all $i \geq j$.*

For example, if $Q = I$, then Q-orthogonality is equivalent to regular orthogonality. For another example, if Q has more than one distinct eigenvalue, let d and d' be eigenvectors corresponding to distinct eigenvalues. Then $d^T Qd' = \lambda' d^T d' = 0$, since the distinct eigenspaces of a symmetric matrix are orthogonal subspaces.

Recall that any symmetric matrix Q may the orthogonally diagonalized; there exists an orthonormal basis $d_0, \ldots, d_{n-1}$ of eigenvectors of Q. These eigenvectors are also Q-orthogonal. Hence to any symmetric matrix is a basis of orthonormal vectors that are also orthogonal with respect to the matrix, as just defined.

Proposition 1. *If Q is symmetric and positive definite, then any set of non-zero Q-orthogonal vectors $\{d_i\}$ is linearly independent.*

Proof. If $\sum \alpha_i d_i = 0$, then left-multiplying by $d_j^T Q$ gives $\alpha_j d_j^T Qd_j = 0$. Positive definiteness implies $\alpha_j = 0$. $\square$

Let Q be an $n \times n$ symmetric positive definite matrix. Recall that $f(x) = \frac{1}{2}x^T Qx - b^T x$ has the unique global minimizer $x_* = Q^{-1}b$. Let $d_0, \ldots, d_{n-1}$ be non-zero Q-orthogonal vectors. Then $d_0, \ldots, d_{n-1}$ form a basis of $\mathbb{R}^n$. Thus there are scalars $\alpha_0, \ldots, \alpha_{n-1}$ such that $x_* = \sum \alpha_i d_i$. We would like a formula for the α_i's.

Multiplying both sides of the sum $x_* = \sum \alpha_i d_i$ by $d_j^T Q$ implies that $d_j^T Q x_* = \alpha_j d_j^T Q d_j$, implying that

$$\alpha_j = \frac{d_j^T b}{d_j^T Q d_j}.$$

Therefore

$$x_* = \sum_{i=1}^{n-1} \frac{d_i^T b}{d_i^T Q d_i} d_i.$$

This implies that we can actually solve for x_* by computing the $d_0, \ldots, d_{n-1}$ and the coefficients above. Computationally, computing inner products is very easy. The disadvantage is that we do not know how to find the vectors $d_0, \ldots, d_{n-1}$.

Theorem 1.2. *(Method of Conjugate Directions) Let $d_0, \ldots, d_{n-1}$ be a set of non-zero Q-orthogonal vectors. For a starting point $x_0 \in \mathbb{R}^n$, consider the sequence $\{x_l\}$ defined by*

$$x_{k+1} = x_k + \alpha_k d_k,$$

where

$$\alpha_k = -\frac{g_k^T d_k}{d_k^T Q d_k} \qquad \text{where } g_k = Qx_k - b.$$

The sequence $\{x_k\}$ converges to the minimizer x_* it at most n steps; $x_n = x_*$.

Proof. Write $x_* - x_0 = \alpha_0' d_0 + \cdots + \alpha_{n-1}' d_{n-1}$. Multiply both sides by $d_i^T Q$ to get

$$d_i^T Q(x_* - x_0) = \alpha_i d_i^T Q d_i,$$

giving us the expression

$$\alpha_i' = \frac{d_i^T Q(x_* - x_0)}{d_i^T Q d_i}. \qquad (*)$$

Note that

$$\begin{aligned}
x_1 &= x_0 + \alpha_0 d_0 \\
x_2 &= x_0 + \alpha_0 d_0 + \alpha_1 d_1 \\
&\vdots \\
x_k &= x_0 + \alpha_0 d_0 + \cdots + \alpha_{k-1} d_{k-1},
\end{aligned}$$

implying that

$$x_k - x_0 = \alpha_0 d_0 + \cdots + \alpha_{k-1} d_{k-1}.$$

Multiplying both sides by $d_k^T Q$ gives $d_k^T Q(x_k - x_0) = 0$. By (*) we have

$$\alpha_k' = \frac{d_k^T Q(x_* - x_0) - d_k^T Q(x_k - x_0)}{d_k^T Q d_k} = \frac{d_k^T Q(x_* - x_k)}{d_k^T Q d_k} = -\frac{(Qx_k - Qx_*)^T d_k}{d_k^T Q d_k}$$

simplifying to

$$\alpha_k' = -\frac{g_k^T d_k}{d_k^T Q d_k} = \alpha_k.$$

So

$$x_* = x_0 + \alpha_0 d_0 + \cdots + \alpha_{n-1} d_{n-1} = x_n.$$

So after n steps, we reach the minimizer. □

(There may be an error in the above calculations. The professor will send a note on this.)

1.4 Geometric Interpretation of Conjugate Directions

Let $d_0, \ldots, d_{n-1}$ be a set of non-zero Q-orthogonal vectors in $\mathbb{R}^n$. Let B_k be the span of the first k of these vectors. Note that B_k has dimension k and contains $B_1, \ldots, B_{k-1}$, so $B_1, \ldots, B_n$ is a sequence of expanding subspaces of $\mathbb{R}^n$. Let us agree that $B_0 = \{0\}$.

Fix $x_0 \in \mathbb{R}^n$ and consider the affine subspaces $x_0 + B_k$ each with "origin" x_0. We now have a sequence of expanding affine subspaces of $\mathbb{R}^n$.

Theorem 1.3. *The sequence $\{x_k\}$ generated from x_0 by the method of conjugate directions has the property that x_k is the minimizer of $f(x) = \frac{1}{2}x^T Q x - b^T x$ on the affine subspace $x_0 + B_k$.*