A SKETCH OF THE CONVERGENCE OF STEEPEST DESCENT METHOD FOR QUADRATIC OBJECTIVES

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We'll study the steepest descent method, also known as the gradient descent method, on a simple quadratic objective with exact line search. The point here is to show that, even in a simple case, this method converges slowly. (In this class, that means linear convergence.) Whether or not this slow convergence affects your problem is a judgement call that you'll have to make for yourself.

This material comes from Nocedal & Wright, page 42; Griva, Sofer & Nash, page 405; and some old notes from Juan Meza (former location: http://hpcrd.lbl.gov/-meza/papers/Steepest%20Descent.pdf) which seem to be in a Wiley paper http://dx.doi.org/10.1002/wics.117.

1 THE PROBLEM

We'll consider the optimization problem

minimize
$$\frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}$$

where Q is symmetric, positive definite.

The solution of this problem is $\mathbf{x} = 0$. We'll show that it takes us a while to find this solution using steepest descent!

2 THE METHOD

Steepest descent begins with some prescribed point \mathbf{x}_0 . At each step, it considers a linear approximation of $f(\mathbf{x})$ in the direction of the negative gradient. Formally,

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{g}_k$$

where $\mathbf{g}_k = \mathbf{g}(\mathbf{x}_k)$ is the gradient evaluated at \mathbf{x}_k .

The key decision in the method is how to choose α_k , what is called the step-length. An idealized choice of α_k is as the global solution of:

minimize
$$f(\mathbf{x}_k - \alpha \mathbf{g}_k)$$
 subject to $\alpha > 0$.

For reasons that we'll see soon, this is called *exact line search*. Usually, performing an exact line search is impossible, but for quadratic objectives of the form:

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \mathbf{Q}\mathbf{x} - \beta \mathbf{x}^T \mathbf{c}$$

we can derived a closed form solution for α .

3 EXACT LINE SEARCH FOR QUADRATICS

Let's do so for the simple objective $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T Q \mathbf{x}$. First, we need the gradient. For this function $\mathbf{g}(\mathbf{x}) = Q \mathbf{x}$ if \mathbf{Q} is symmetric, and $(\frac{1}{2}\mathbf{Q} + \frac{1}{2}\mathbf{Q}^T)\mathbf{x}$ if \mathbf{Q} is non-symmetric. We'll only consider the symmetric case where \mathbf{Q} is also positive definite.

At a point \mathbf{x}_k , then, our goal is to pick α_k to minimize

$$\ell(\alpha) = f(\mathbf{x}_k - \alpha \mathbf{g}_k) = \frac{1}{2} (\mathbf{x}_k - \alpha \mathbf{g}_k)^T \mathbf{Q} (\mathbf{x}_k - \alpha \mathbf{g}_k) = \frac{1}{2} \mathbf{x}_k^T \mathbf{Q} \mathbf{x}_k - \alpha \mathbf{g}_k^T \mathbf{Q} \mathbf{x}_k + \frac{1}{2} \alpha^2 \mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k.$$

The derivative with respect to α is:

$$\ell'(\alpha) = \alpha \mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k - \mathbf{g}_k^T \mathbf{Q} \mathbf{x}_k = \alpha \mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k - \mathbf{g}_k^T \mathbf{g}_k.$$

This is a strongly convex problem with a unique solution – just about as easy as things get

The negative gradient search direction is optimal for the model objective, $f(\mathbf{x}) \approx f(\mathbf{x}_k + \mathbf{p}) \approx f(\mathbf{x}_k) + \mathbf{p}^T \mathbf{g}(\mathbf{x}_k)$, in the sense that $-\mathbf{g}(\mathbf{x}_k)$ is the solution of

minimize $\frac{\mathbf{p}^T \mathbf{g}_k}{\|\mathbf{p}\| \|\mathbf{g}_k\|}$.

The only stationary point is where $\ell'(\alpha) = 0$, or

$$\alpha = \frac{\|\mathbf{g}_k\|^2}{\mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k}.$$

Because of the norms, this ratio must be positive (unless $\mathbf{g}_k = 0$, in which case we are already at a stationary point). Thus, the solution is feasible and hence, optimal.

4 DECREASE IN THE FUNCTION

Our goal is to understand the convergence properties of the steepest descent method. Now that we have fully specified the method by deriving the form of α at each step, we can study the decrease in the objective function from $f(\mathbf{x}_k)$ to $f(\mathbf{x}_{k+1})$. Substituting $\alpha_k = \frac{\|\mathbf{g}_k\|^2}{\mathbf{g}_k^T Q \mathbf{g}_k}$ into $f(\mathbf{x}_k - \alpha \mathbf{g}_k)$ we have:

$$f(\mathbf{x}_{k+1}) = f(\mathbf{x}_k) - \alpha \|\mathbf{g}\|^2 + \frac{1}{2}\alpha^2 \mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k = f(\mathbf{x}_k) - \frac{1}{2} \|\mathbf{g}_k\|^4 / (\mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k).$$

From this form, it seems like we might have algebraic convergence! However, note that

$$f(\mathbf{x}_k) = \frac{1}{2}\mathbf{x}_k^T \mathbf{Q} \mathbf{x}_k = \frac{1}{2}\mathbf{g}_k^T \mathbf{Q}^{-1} \mathbf{g}_k.$$

Thus, we can rewrite the decrease as follows:

$$f(\mathbf{x}_{k+1}) = f(\mathbf{x}_k) \left[1 - \frac{\|\mathbf{g}_k\|^4}{(\mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k)(\mathbf{g}_k^T \mathbf{Q}^{-1} \mathbf{g}_k)} \right].$$

If we can bound $\frac{\|\mathbf{g}_k\|^4}{(\mathbf{g}_k^TQ\mathbf{g}_k)(\mathbf{g}_k^TQ^{-1}\mathbf{g}_k)}$ by a constant, then we will have proved linear convergence.

5 THE KANTOROVICH INEQUALITY

There is indeed such a bound, known as the Kantorovich inequality.

LEMMA 1 Let **A** be a symmetric, positive definite matrix. Let **x** be a vector with $\mathbf{x}^T\mathbf{x} = 1$. Then

$$(\mathbf{x}^T A \mathbf{x}) (\mathbf{x}^T A^{-1} \mathbf{x}) \leq \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1 \lambda_n}$$

where λ_1 and λ_n are the smallest and largest eigenvalues of **A**.

Proof First, we transform the problem into eigenvalue space with $A = V \Lambda V^T$. This results in

$$(\mathbf{x}^T A \mathbf{x})(\mathbf{x}^T A^{-1} \mathbf{x}) = (\mathbf{y}^T \Lambda \mathbf{y})(\mathbf{y}^T \Lambda^{-1} \mathbf{y}) = \left(\sum_{i=1}^n y_i^2 \lambda_i\right) \left(\sum_{i=1}^n y_i^2 \lambda_i^{-1}\right).$$

Note that $\sum_i y_i^2 = 1$. The key idea is to write $\lambda_i = p_i \lambda_1 + q_i \lambda_n$ and $\lambda_i^{-1} = p_i \lambda_1^{-1} + q_i \lambda_n^{-1}$. Thus, $p_i \ge 0$ and $q_i \ge 0$, and

$$\lambda_i\lambda_i^{-1}=1=(p_i+q_i)^2+p_iq_i(\lambda_1-\lambda_n)^2/(\lambda_1\lambda_n).$$

Let $p = \sum_i y_i^2 p_i$ and $q = \sum_i y_i^2 q_i$, then $p + q \le 1$.

$$(\mathbf{x}^T A \mathbf{x}) (\mathbf{x}^T A^{-1} \mathbf{x}) = (\lambda_1 p + \lambda_n q) (\lambda_1^{-1} p + \lambda_n^{-1} q) \le (p + q)^2 \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1 \lambda_n} \le \frac{(\lambda_1 + \lambda_n)^2}{4\lambda_1 \lambda_n}$$

after a few more steps of algebra involving geometry mean inequalities.

6 TYING UP LOOSE ENDS

We are basically done. We use the Kantorovich inequality to bound the decrease. A bit more algebra yields the identity:

$$\frac{f(\mathbf{x}_{k+1})}{f(\mathbf{x}_k)} \le \left(\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}\right)^2 = \left(\frac{\kappa(\mathbf{Q}) - 1}{\kappa(\mathbf{Q}) + 1}\right)^2.$$

This proof due to P. Henrici, Mathematical Notes, 1961.