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

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February 9, 2026

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

$$\text{minimize} \quad \tfrac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}$$

where $\mathbf{Q}$ is symmetric, positive definite.

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

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:

$$\begin{array}{ll} \underset{\alpha}{\text{minimize}} & f(\mathbf{x}_k - \alpha\mathbf{g}_k) \\ \text{subject to} & \alpha > 0 \end{array}.$$

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

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

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 $f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{Q}\mathbf{x}$. First, we need the gradient. For this function $\mathbf{g}(\mathbf{x}) = \mathbf{Q}\mathbf{x}$ 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

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

The derivative with respect to α is:

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

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 $\alpha_k = \frac{\|\mathbf{g}_k\|^2}{\mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k}$ into $f(\mathbf{x}_k - \alpha \mathbf{g}_k)$ we have:

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

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

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

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 $\frac{\|\mathbf{g}_k\|^4}{(\mathbf{g}_k^T \mathbf{Q} \mathbf{g}_k)(\mathbf{g}_k^T \mathbf{Q}^{-1} \mathbf{g}_k)}$ 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 $\boldsymbol{A}$ be a symmetric, positive definite matrix. Let $\mathbf{x}$ be a vector with $\mathbf{x}^T \mathbf{x} = 1$. Then*

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

where λ_1 and λ_n are the smallest and largest eigenvalues of $\boldsymbol{A}$.

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

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

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

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

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

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

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

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:

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