A Tour on Optimization Methods Unconstrained Minimization - Line Search Methods

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Basic Terminology

Optimization Problem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be any cost function, and let $f_i : \mathbb{R}^n \to \mathbb{R}$ and $g_i : \mathbb{R}^n \to \mathbb{R}$ be the constraint functions.

$$egin{aligned} & \min_{x\in\mathcal{S}} & f(x) \ & ext{subject to} & f_i(x) = 0, \ i = 1, \cdots, m \ & g_i(x) \leq 0, \ i = 1, \cdots, n, \end{aligned}$$

where ${\mathcal S}$ is the intersection of domains of all the functions.

This talk will be focused on uncontrained optimization problems such as follows:

$$\min_{x\in\mathbb{R}^n}f(x),$$

where f satisfies some special conditions.

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Basic Terminology

Types of Minimizers

- A point x^{*} ∈ S is called the global minimizer if f(x^{*}) ≤ f(x) for all x ∈ S.
- A point x^{*} ∈ S is called the local minimizer if there is a neighborhood N ⊆ S of x^{*} such that f(x^{*}) ≤ f(x) ∀x ∈ N.
- A point x* ∈ S is called the strict local minimizer(also called as strong local minimizer) if there is a neighborhood N ⊆ S of x* such that f(x*) < f(x) ∀x ∈ N, x ≠ x*.

Q - Rate of Convergence

Let $\{x_k\}$ be a sequence in \mathbb{R}^n that converges to x^* .

• The convergence is said to be **Q-linear** if there is a constant $r \in (0, 1)$ such that

$$rac{\|x_{k+1}-x^*\|}{\|x_k-x^*\|} \leq r, ext{ for all } k ext{ sufficiently large}.$$

• The convergence is said to be **Q-superlinear** if

$$\lim_{k \to \infty} \frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|} = 0.$$

• The convergence is said to be **Q-quadratic** if there is a positive constant *M*, not necessarily less than 1, such that

$$\frac{\|x_{k+1} - x^*\|}{\|x_k - x^*\|^2} \le M, \text{ for all k sufficiently large.}$$

Example: $\{1 + (0.5)^k\}$, $\{1 + k^{-k}\}$, $\{1 + (0.5)^{2^k}\}$ respectively.

Identifying Minimizers

First-Order Necessary Condition

If x^* is a local minimizer and f is continuously differentiable in an open neighborhood of x^* , then $\nabla f(x^*) = 0$.

Remark: From the above condition notice that every local minimizer is a stationary point(i.e, point at which gradient of f vanishes).

Second-Order Necessary Condition

If x^* is a local minimizer and $\nabla^2 f$ is continuous in an open neighborhood of x^* , then $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive semi-definite.

Second-Order Sufficient Condition

Suppose that $\nabla^2 f$ is continuous in an open neighborhood of x^* and that $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive definite. Then x^* is a strict local minimizer of f.

Identifying Minimizers

Adding convexity to the picture yields the following results:

Optimality Conditions for convex problems

When f is convex, any local minimizer x^* is a global minimizer of f. If in addition f is differentiable, then any stationary point x^* is a global minimizer.

Goal of an Optimization Method

Given an initial point $x_0 \in \mathbb{R}^n$, iteratively find a sequence $\{x_n\}$ at each step such that as the limit tends to infinity, some of the above mentioned conditions of optimality are satisfied.

We now take a look at two broad classes of optimization methods.

Classification of Optimization Methods

- Line Search Methods
- Trust-Region Methods

Line Search Methods

Algorithm Prototype Line Search Methods

- 1: Pick an initial point x_0
- 2: repeat
- 3: Pick a direction p_k
- 4: Pick a step length $\alpha_k > 0$ in that direction
- 5: Update the solution. $x_{k+1} \leftarrow x_k + \alpha_k p_k$
- 6: **until** Convergence

Note: Steps 1,3,4 are non-trivial. Later we'll see why step 1 is non-trivial. Roughly speaking, we want to pick p_k and α_k such that $f(x_{k+1}) < f(x_k)$ except when x_k is optimal. Such methods are called **Descent Methods**. As $-\nabla f(x_k)$ is the steepest descent direction, we define p_k to be a **descent direction** if $\nabla f(x_k)^T p_k < 0$.

Step Length Selection

Given a descent direction p_k , the ideal step length would be

$$\alpha^* = \underset{\alpha > 0}{\operatorname{argmin}} f(x_k + \alpha_k p_k).$$

Generally, we prefer inexact methods, where we try out a sequence of step lengths until certain conditions are satisfied which guarantee optimality.

Wolfe Conditions on step length α_k

Define $\phi(\alpha_k) = f(x_k + \alpha_k p_k)$ and $l(\alpha_k) = f(x_k) + (c_1 \nabla f(x_k)^T p_k) \alpha_k$, which is a linear function in α_k with negative slope $(c_1 \nabla f(x_k)^T p_k)$.

• Armijo condition or sufficient decrease condition

$$f(x_k + \alpha_k p_k) \le f(x_k) + c_1 \alpha_k \nabla f(x_k)^T p_k$$
 (or) $\phi(\alpha_k) \le l(\alpha_k)$

Curvature condition

 $abla f(x_k + \alpha_k p_k)^T p_k \ge c_2 \nabla f(x_k)^T p_k \text{ (or) } \phi'(\alpha_k) \ge c_2 \phi'(0)$ where $0 < c_1 < c_2 < 1$.

Wolfe Conditions on step length α_k

Theorem

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is continuously differentiable. Let p_k be a descent direction at x_k , and assume that f is bounded below along the ray $\{x_k + \alpha p_k : \alpha > 0\}$. Then if $0 < c_1 < c_2 < 1$, there exists intervals of step lengths satisfying the Wolfe conditions.

Descent Direction Selection

Let the angle between the steepest descent direction $-\nabla f(x_k)$ and p_k be θ_k , then $\cos \theta_k = \frac{-\nabla f(x_k)^T p_k}{\|\nabla f(x_k)\| \|p_k\|}$.

Theorem

Consider any iteration of the form $x_k + \alpha_k p_k$, where p_k is a descent direction and α_k satisfies the Wolfe conditions. Suppose that f is bounded below in \mathbb{R}^n and that f is continuously differentiable in an open set \mathcal{N} containing the level set $\mathcal{L} \equiv \{x : f(x) \leq f(x_0)\}$, where x_0 is the initial point. Assume also that the gradient ∇f is Lipschitz continuous on \mathcal{N} , i.e, there exists a constant L > 0 such that $\|\nabla f(x) - \nabla f(\tilde{x})\| \leq L \|x - \tilde{x}\|$, for all $x, \tilde{x} \in \mathcal{N}$. Then,

$$\sum_{k\geq 0}\cos^2\theta_k\|\nabla f(x_k)\|^2 < \infty \text{ (or) } \lim_{k\to\infty}\cos^2\theta_k\|\nabla f(x_k)\|^2 = 0.$$

Steepest Descent Method

Theorem

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable, and that the iterates generated by steepest descent method (where $p_k = -\nabla f(x_k)$) with the exact line searches converges Q-linearly to a point x^* where the Hessian matrix $\nabla^2 f(x^*)$ is positive definite. Then

$$f(x_{k+1}) - f(x^*) \leq \left(\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1}\right)^2 [f(x_k) - f(x^*)],$$

where $\lambda_1 \leq \cdots \leq \lambda_n$ are the eigenvalues of $\nabla^2 f(x^*)$.

Newton's Method

The descent direction
$$p_k^N \equiv -\nabla^2 f(x_k)^{-1} \nabla f(x_k)$$
.

Theorem

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable, and that the Hessian $\nabla^2 f(x)$ is Lipschitz continuous in a neighborhood of a solution x^* at which the second-order sufficient conditions hold. Consider the iteration $x_{k+1} = x_k + p_k^N$. Then

- if the starting point x₀ is sufficiently close to x^{*}, the sequence of iterates converges to x^{*}.
- the rate of convergence of $\{x_k\}$ is Q-quadratic; and
- the sequence of gradient norms {∇f(x_k)} converges Q-quadratically to zero.

References I

J. Nocedal and S. Wright. *Numerical Optimization*.