Chapter 7

Line Search Methods

The strategy and the key objects

Problem. Let $f : D \subset \mathbb{R}^n \to \mathbb{R}$ be a $\mathbb{C}^1$ function. To solve

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

it is necessary to find out points (vectors) $x^\star$ such that $\nabla f(x^\star) = 0$.

Strategy (Line Search Methods). A possible strategy for doing so is to start at a given vector $x_0 \in D$ and construct a sequence

$$x_k = \min_{\alpha_k \in \mathbb{R}} f(x_{k-1} + \alpha_k p_k), \quad \text{with } p_k \in \mathbb{R}^n$$

such that $x_k \to x^\star$ with $\nabla f(x^\star) = 0$. We want to choose α_k (the step) and p_k (the line direction) at each step so that the convergence is optimal.

The direction

Theorem. Let $f : D \subset \mathbb{R}^n \longrightarrow \mathbb{R}$ be a differentiable function and let $a \in D$ and $\boldsymbol{u} \in \mathbb{R}^n$ be an unitary vector. Suppose that θ is the angle between $\boldsymbol{u}$ and $\nabla f(\boldsymbol{a})$. Then

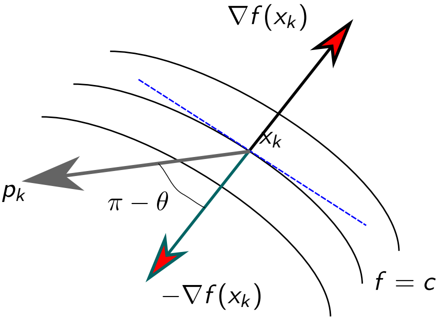
$$D_{\boldsymbol{u}} f(\boldsymbol{a}) =< (\nabla f(\boldsymbol{a})), \boldsymbol{u} >= \boldsymbol{u}^T \nabla f(\boldsymbol{a}) = \|\nabla f(\boldsymbol{a})\| \cos\theta.$$

In particular the vector $-\nabla f(\boldsymbol{a})$ gives the maximum descent direction of f at the point $\boldsymbol{a}$.

The direction p_k

Definition. We say that p_k is a descent direction if $p_k^T \nabla f(\boldsymbol{x}_k) < 0$.
More generically (in line search methods) we consider

$$p_k = -B_k^{-1} \nabla f(\boldsymbol{x}_k) \qquad \text{with } B_k \text{ positive definite.}$$



- $B_k = \mathrm{Id}$ (descent method)
- $B_k = Hf(\boldsymbol{x}_k)$ (Newton method)
- $B_k \approx Hf(\boldsymbol{x}_k)$ (quasi Newton method)

The step size α_k

Formally at each k-step we are finding a a solution of

$$\min_{\alpha \in \mathbb{R}^+} f\left(x_k + \alpha p_k\right).$$

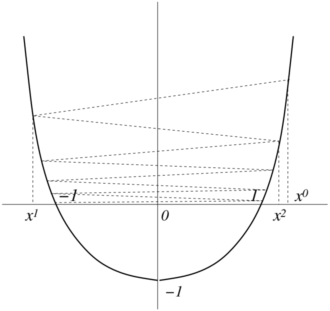
But we want to decide the value of α as fast as possible at each step. We are looking for a minimal cost to choose α. In other words we want to have a easy way to terminate our finding of α, and move forward to the next step.

A philosophical approach would be to (a) find an interval containing the desirable steps and (b) use a bisection method to conclude the desires α.

The step size α_k

First tentative. We want to terminate the process at each step k when we find α_k such that

$$f\left(x_k + \alpha_k p_k\right) < f\left(x_k\right).$$



The step size α_k: Sufficient decrease condition

Second tentative. We impose the following condition for α_k

$$\phi(\alpha_k) := f(x_k + \alpha_k p_k) < f(x_k) + c_1 \alpha_k (\nabla f(x_k))^T p_k, \; c_1 \in (0,1).$$

The condition is called (sufficient decrease condition).

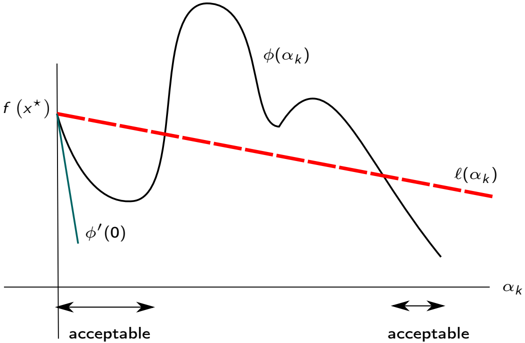
Remarks.

- $\ell(\alpha_k) := f(x_k) + c_1 \alpha_k \nabla f^T(x_k) p_k$ is a linear function.
- For small values of $\alpha_k > 0$ we have $\phi(\alpha_k) < \ell(\alpha_k)$. This is so because $c_1 \in (0,1)$ and then

$$\phi'(0) = (\nabla f(x_k))^T p_k < c_1 (\nabla f(x_k))^T p_k = \ell'(0) < 0.$$

The step size α_k

Sufficient decrease. We ask for a decrease proportional to α and $\phi'(0) = \nabla f^T(x_k)\, p_k$. Usually $c_1 \approx 0.1$.

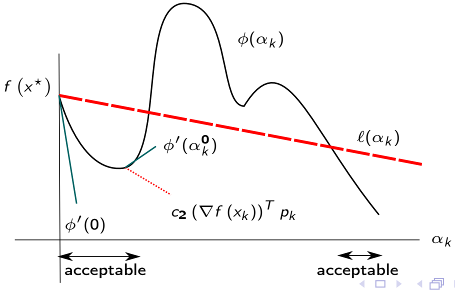


The step size α_k: curvature condition

Curvature condition. Since the previous condition is always satisfied for small values of α_k we need to add further conditions for termination. We use the so called curvature condition

$$\left(\nabla f\left(x_k+\alpha_k p_k\right)\right)^T p_k \geq c_2\left(\nabla f\left(x_k\right)\right)^T p_k, \;\; c_2 \in (c_1, 1)$$

In other words if $\phi'(\alpha_k)$ is not negative enough we terminate the k-step.



The step size α_k: (strong) Wolfe Conditions

Definition. The conditions (together) to terminate the k-step given by

$$f(x_k + \alpha_k p_k) < f(x_k) + c_1 \alpha_k (\nabla f(x_k))^T p_k,$$
$$(\nabla f(x_k + \alpha_k p_k))^T p_k \geq c_2 (\nabla f(x_k))^T p_k,$$

with $0 < c_1 < c_2 < 1$ are usually called Wolfe conditions.

Definition. The conditions (together) to terminate the k-step given by (we do not allow $\phi'(\alpha_k)$ to be too positive).

$$f(x_k + \alpha_k p_k) < f(x_k) + c_1 \alpha_k (\nabla f(x_k))^T p_k,$$
$$|(\nabla f(x_k + \alpha_k p_k))^T p_k| \leq |c_2 (\nabla f(x_k))^T p_k|,$$

with $0 < c_1 < c_2 < 1$ are usually called strong Wolfe conditions.

The step size α_k: Existence

Lemma. Suppose $f : D \subset \mathbb{R}^n \to \mathbb{R}$ be a $\mathcal{C}^1$ function. Let p_k a descent direction at the point $x_k \in D$ and assume $f|L_{p_k}$ is bounded below where $L_{p_k} = \{x \in \mathbb{R}^n \mid x = x_k + \alpha p_k,\ \alpha > 0\}$. Then if $0 < c_1 < c_2 < 1$ there exist intervals of step lengths satisfying the (strong) Wolfe conditions

Proof. Since $\ell'(\alpha_k) < 0$ (and constant) there exists a first intersection, $\hat{\alpha}_k > 0$, between $\ell(\alpha_k)$ and $\phi(\alpha_k)$:

$$f(x_k + \hat{\alpha}_k p_k) = f(x_k) + c_1 \hat{\alpha}_k (\nabla f(x_k))^T p_k. \tag{1}$$

The sufficient decrease condition it is satisfied for all $\alpha_k \in [0, \hat{\alpha}_k]$. By the Mean Value Theorem we have that there exists $\tilde{\alpha}_k \in [0, \hat{\alpha}_k]$ such that

$$f(x_k + \hat{\alpha}_k p_k) - f(x_k) = \hat{\alpha}_k (\nabla f(x_k + \tilde{\alpha}_k p_k))^T p_k$$

All together imply

$$(\nabla f(x_k + \tilde{\alpha}_k p_k))^T p_k = c_1 \hat{\alpha}_k (\nabla f(x_k))^T p_k > c_2 \hat{\alpha}_k (\nabla f(x_k))^T p_k.$$

Therefore $\tilde{\alpha}_k$ satisfies the Wolfe conditions and smoothness gives the desired interval.

Convergence of line search methods

Remark. Until this moment we just consider the definition of the process, that is the election of p_k and α_k. But we need to study if the process converge to somewhere.

Let p_k be a descent direction, and let θ_k the angle of p_k and $-\nabla f(x^\star)$

$$\cos(\theta_k) = -\frac{1}{||\nabla f(x_k)||\,||p_k||} (\nabla f(x_k))^T p_k$$

Theorem. Assume notation above with p_k a descent direction and α_k satisfying Wolfe's conditions. Suppose f is $\mathcal{C}^2$ and bounded below in $\mathbb{R}^n$. Then

$$\sum_{k=0}^{\infty} \cos^2(\theta_k) ||\nabla f(x_k)|| < \infty. \tag{2}$$

Convergence of line search methods

Corollary. Under the above notation and assumptions we have

$$\cos^2(\theta_k)||\nabla f(x_k)|| \to 0$$

Moreover if there exists $\delta > 0$ such that $\cos(\theta) > \delta$ then

$$\lim_{k\to\infty} ||\nabla f(x_k)|| = 0 \quad \text{(globally convergent algorithms)}$$

Remark. The final δ-condition basically means that p_k do not get arbitrarily orthogonal to the gradient vector. This is, for instance, the case of the steepest descent method.

Convergence of line search methods: Newton's like methods

Assume that the matrices $B_k, \; k \geq 0$ which define the (Newton-like) direction $p_k = -B_k^{-1} \nabla f(\boldsymbol{x}_k)$ are uniformly positively definite

$$||B_k|| \; ||B_k^{-1}|| \leq M, \quad \forall k \geq 0.$$

Lemma. Under the assumptions we have that

$$\cos(\theta_k) \geq \frac{1}{M},$$

and so

$$\lim_{k \to \infty} ||\nabla f(x_k)|| = 0.$$

Convergence of line search methods: Final comments

Remark. We have shown that under the above hypothesis the line search method converge to an stationary point: $\nabla f(x^\star) = 0$. But this is not a guarantee that $x^\star$ is a minimizer. For this we need to add other conditions on the Hessian of f at $x = x^\star$.

Remark. Another consideration is about the speed or rate of convergence. The asymptotic behaviour (global convergence) is the desired one but what about the number of iterates?

Rate of convergence: Steepest descent method

The ideal case. Assume

$$f(x) = \frac{1}{2}x^T Qx - b^T x$$

where Q is symmetric and positive definite. The gradient is given by $\nabla f(x) = Qx - b$ and so the minimizer $x^\star$ is the (unique) solution of $Qx = b$. Algorithmically,

$$\min_{\alpha \in \mathbb{R}^+} f\left(x - \alpha_k \nabla f\left(x_k\right)\right) \quad \to \quad \hat{\alpha}_k = \frac{\left(\nabla f\left(x_k\right)\right)^T \nabla f\left(x_k\right)}{\left(\nabla f\left(x_k\right)\right)^T Q \nabla f\left(x_k\right)}$$

where notice that $\nabla f\left(x_k\right) = Qx_k - b$.

Rate of convergence: Steepest descent method

Definition. Accordingly we have that the steepest decent method with exact line searches writes as

$$x_{k+1} = x_k - \hat{\alpha}_k \, \nabla f\,(x_k)$$

To study the rate of convergence we introduce a weighted norm of a vector $x \in \mathbb{R}^n$ as follows

$$||x||_Q^2 = x^T Qx$$

Exercise. If $x^T = (x_1, x_2)$ and $Q = (a_{ij})$ with $i, j = 1, 2$ (symmetric) compute

$$||x||_Q^2.$$

Rate of convergence: Steepest descent method

Lemma. Assume above notation. We have

$$\frac{1}{2}||x - x^\star||_Q^2 = f(x) - f(x^\star).$$

Proof. The minimizer $x^\star$ satisfies $Qx^\star = b$. Then

$$f(x^\star) = \frac{1}{2}\left((x^\star)^T Q x^\star - 2b^T x^\star\right) = \frac{1}{2}\left((x^\star)^T b - 2b^T x^\star\right) =$$
$$= -\frac{1}{2} b^T x^\star = -\frac{1}{2}(x^\star)^T Q x^\star.$$

where the last equality uses that $Q^T = Q$. Then

$$f(x) - f(x^\star) = \frac{1}{2}\left(x^T Q x - 2b^T x + (x^\star)^T Q x^\star\right) = \frac{1}{2}||x - x^\star||_Q^2$$

since $b^T x = x^\star Q x$.

Rate of convergence: Steepest descent method

Theorem. When the steepest decent method with exact line searches $(\hat{\alpha}_k)$ is applied to the strongly convex quadratic function above then

$$||x_{k+1} - x^\star||_Q^2 \leq \left[\frac{\lambda^n - \lambda_1}{\lambda_n + \lambda_1}\right]^2 ||x_k - x^\star||_Q^2$$

where $0 < \lambda_1 \leq \cdots \lambda_n$ are the eigenvalues of Q.

Remark. The convergence of the steepest decent method under the best conditions, is linear.

(Local) Rate of convergence: Newton's method

Definition. Let f twice differentiable. The Newton's method is the line search method defined by

$$p_k = -\left(Hf\left(x_k\right)\right)^{-1} \nabla f\left(x_k\right).$$

Remark. Since $\left(Hf\left(x_k\right)\right)^{-1}$ might not always be positive definite then Newton's method does not always define a descent method. However near the solutions (minimizers) the convergence is quadratic.

(Local) Rate of convergence: Newton's method

Theorem. Assume f is regular (class $\mathcal{C}^3$ is enough) in a neighbourhood of a solution $x^\star$ (minimum of f) where the sufficient optimality conditions hold.
Consider the iteration

$$x_{k+1} = x_k + p_k$$

where p_k is the Newton direction expressed above. Then

(a) $x_k \to x^\star$, if x_0 is close enough to $x^\star$.

(b) The rate of convergence of $\{x_k\}_{k \geq 0}$ is quadratic.

(c) $||\nabla f(x_k)|| \to 0$ quadratically.

(Local) Rate of convergence: Newton's method

proof. Observe that $\nabla f(x^\star) = 0$ (optimality condition). So,

$$\begin{aligned} x_k + p_k - x^\star &= x_k - x^\star - (Hf(x_k))^{-1} \nabla f(x_k) = \\ &= (Hf(x_k))^{-1} \left[Hf(x_k)(x_k - x^\star) - \nabla f(x_k) + \nabla f(x^\star)\right] \end{aligned}$$

Observe also that

$$\begin{aligned} \nabla f(x^\star) - \nabla f(x_k) &= \int_0^1 \frac{d}{dt} \nabla f(x_k - t(x_k - x^\star))\ dt = \\ &= \int_0^1 Hf(x_k - t(x_k - x^\star))(x_k - x^\star)\ dt \end{aligned}$$

All together implies (L is the Lipschitz constant for $Hf(x)$)

$$\begin{aligned} &||Hf(x_k)(x_k - x^\star) - (\nabla f(x_k) - \nabla f(x^\star))|| \leq \\ &\leq \int_0^1 ||Hf(x_k) - Hf(x_k - t(x_k - x^\star))||\ ||x_k - x^\star||\ dt \leq \\ &\leq ||x_k - x^\star||^2 \int_0^1 Lt\ dt = \frac{1}{2} L ||x_k - x^\star||^2 \end{aligned}$$

(Local) Rate of convergence: Newton's method

proof. We go back to

$$||x_k + p_k - x^\star|| = ||\left(Hf\left(x_k\right)\right)^{-1}|| \; ||\left[Hf\left(x_k\right)\left(x_k - x^\star\right) - \nabla f\left(x_k\right) + \nabla f\left(x^\star\right)\right]||.$$

We bounded red. Using the regularity of f and th fact that $Hf(x^\star)$ is non singular we have

$$||\left(Hf\left(x_k\right)\right)^{-1}|| \leq 2\,||\left(Hf\left(x^\star\right)\right)^{-1}|| \quad \text{if } ||x_k - x^\star|| < r$$

for some $r > 0$. Finally

$$||x_{k+1} - x^\star|| = ||x_k + p_k - x^\star|| = L||\left(Hf\left(x_k\right)\right)^{-1}|| \; ||x_k - x^\star||^2 \leq \hat{L}||x_k - x^\star||^2.$$

Choosing x_0 such that $||x_0 - x^\star|| < r$ we can use the inequality inductively to prove (a) and (b). Statement (c) can be proved using similar arguments.

(Local) Rate of convergence: General result

Theorem. Suppose f is regular (class $\mathcal{C}^2$ is enough) Consider the iteration $x_{k+1} = x_k + \alpha_k p_k$, where p_k is a descent direction and α_k satisfying the Wolfe conditions with $c_1 \leq 1$. Assume that the sequence $\{x_k\}_{k\geq 0}$ converges to a point $x^\star$ such that $\nabla f(x^\star) = 0$, $Hf(x^\star)$ is positive definite, and

$$\lim_{k\to\infty} \frac{||\nabla f(x^\star) + Hf(x^\star)(p_k)||}{||p_k||} = 0.$$

Then, the step length $\alpha_k = 1$ is admissible for k large enough and the convergence is linear.