Optimization Techniques

Numerical methods for unconstrained optimization

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$$\begin{aligned} g(x) &\equiv \nabla f(x) = \left(\frac{\partial f}{\partial x_i}\right)_{i=1}^{n} \\ H(x) &= \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)_{i,j=1}^{n} \end{aligned}$$

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Also, all vectors $x \in \mathbb{R}^n$ are column vectors, $x = (x_1, x_2, \ldots, x_n)^T$

Optimality conditions for unconstrained minimization

Theorem

Suppose that $f \in C^1$, *and that* x^* *is a local minimizer of* $f(x)$. *Then*

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Suppose that $f \in C^2$, *and that* x^* *is a local minimizer of* $f(x)$. *Then* $g(x^*) = 0$ *and* $H(x^*)$ *is positive semidefinite, that is*

$$y^T H(x^*) y \geq 0 \quad \forall y \in \mathbb{R}^n$$

Linesearch methods

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Definition

An **iteration** is a procedure in which a sequence of points $\{x_k\}_{k=1}^{\infty} \subset \mathbb{R}^n$ is generated, starting from some initial guess $x_0 \in \mathbb{R}^n$, with the overall aim of ensuring that sequence (a subsequence of) $\{x_k\}_{k=1}^{\infty}$ has favourable limiting properties.

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These might include that any limit generated satisfies 1-st order or, even better, second-order necessary optimality conditions.

Linesearch methods

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Linesearch methods

Theorem (Taylor for $\mathbb{R}^n$)

Let S be an open subset of $\mathbb{R}^n$, and suppose $f : S \to \mathbb{R}$ is twice continuously differentiable throughout S. Suppose further that $s \neq 0$, and that the interval $[x, x+s] \subset S$. Then

$$f(x+s) = f(x) + s^T g(x) + \frac{1}{2} s^T H(z) s$$

for some $z \in (x, x+s)$.

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Definition

A direction $p_k \in \mathbb{R}^n$ is called a descent direction if

$$p_k^T g_k < 0 \quad \textit{if} \quad g_k \neq 0$$

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So, small steps along p_k guarantees that the objective function may be reduced.

Second, a suitable steplength $\alpha_k > 0$ is calculated so that

$$f(x_k + \alpha_k p_k) < f_k$$

Linesearch methods

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Such a scheme sounds both natural and simple. But as with most simple ideas, it needs to be refined somewhat in order to become a viable technique.

Linesearch methods

What might go wrong?

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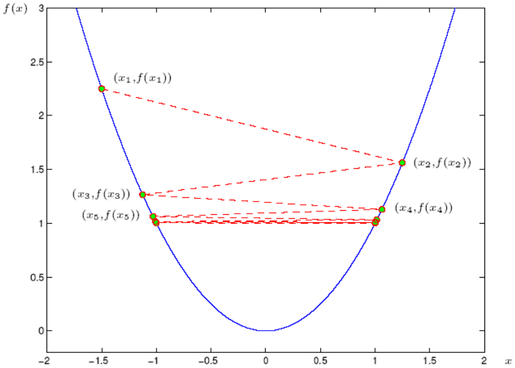

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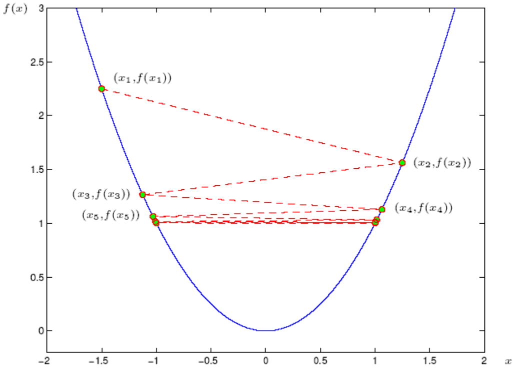

The objective function $f(x) = x^2$ and the iterates $x_{k+1} = x_k + \alpha_k p_k$ generated by the descent directions $p_k = (-1)^k$ and steps $\alpha_k = 2 + \frac{3}{2^{k+1}}$ from $x_0 = 2$.

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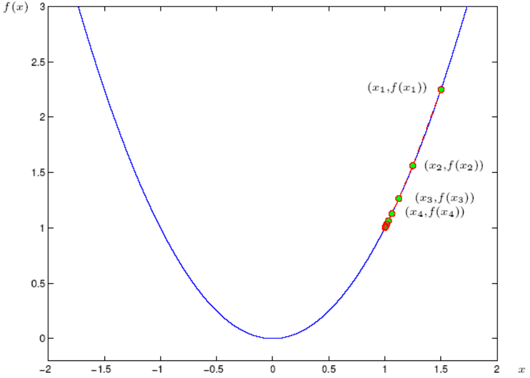

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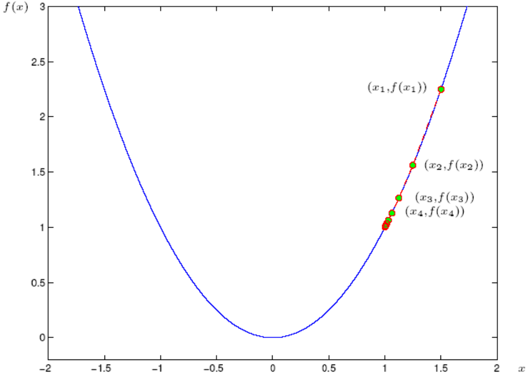

The iterates $x_{k+1} = x_k + \alpha_k p_k$ generated by the descent directions $p_k = -1$ and steps $\alpha_k = \frac{1}{2^{k+}}$ from $x_0 = 2$.

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The iterates approach the minimizer from one side, but the stepsizes are so small that each iterate falls short of the minimizer, and in the end converge to the non-critical value 1.

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Earlier, it was suggested that α_k should be chosen to minimize $f(x_k + \alpha p_k)$. This is known as an **exact** linesearch. In most cases, exact linesearches prove to be very expensive: they are essentially univariate minimizations and most definitely not cost effective, and are consequently rarely used nowadays.

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Modern linesearch methods prefer to use **inexact** linesearches, which are guaranteed to pick steps that are neither too long nor too short.

Linesearch methods with backtracking

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Here is a basic backtracking linesearch to find α_k:

1. Given $\alpha_{init} > 0$ (e.g., $\alpha_{init} = 1$), let $\alpha^{(0)} = \alpha_{init}$ and $l = 0$.
2. Until $f(x_k + \alpha^{(l)} p_k) < f_k$
   1. set $\alpha^{(l+1)} = \tau\alpha^{(l)}$, where $\tau \in (0; 1)$ (e.g.,$\tau = \frac{1}{2}$)
   2. and increase l by 1
3. Set $\alpha_k = \alpha^{(l)}$.

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Notice that the backtracking strategy prevents the step from getting too small, since the 1st allowable value stepsize of the form $\alpha_{init}\tau^i$, $i = 0; 1, \ldots$ is accepted.

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Such a role is played by the Armijo condition.

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The actual requirement is that

$$f(x_k + \alpha_k p_k) \leq f(x_k) + \alpha_k \beta p_k^T g_k$$

for some $\beta \in (0;1)$ (e.g., $\beta = 0.1$ or even $\beta = 0.0001$).

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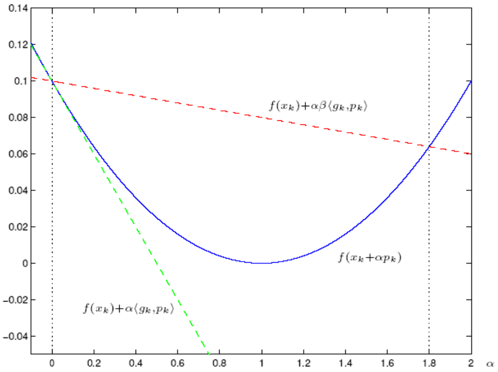
Observe that, since $p_k^T g_k < 0$, the longer the step, the larger the required decrease in f.

Linesearch methods with backtracking

The range of permitted values for the stepsize is illustrated below.



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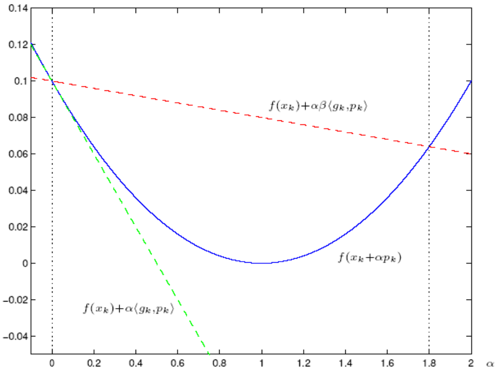

A steplength of anything up to 1.8 is permitted for this example, in the case where $\beta = 0.2$.

Linesearch methods with backtracking Armijo

The Armijo condition may then be inserted into our previous backtracking scheme to give the Backtracking-Armijo linesearch:

1. Given $\alpha_{init} > 0$ (e.g., $\alpha_{init} = 1$), let $\alpha^{(0)} = \alpha_{init}$ and $l = 0$.
2. Until $f(x_k + \alpha^{(l)} p_k) < f_k + \alpha^{(l)} \beta p_k^T g_k$
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Of course, it is one thing to provide likely-sounding rules to control stepsize selection, but another to be sure that they have the desired effect. Indeed, can we even be sure that there are points which satisfy the Armijo condition?

Backtracking Armijo linesearch

Theorem

Suppose that $f \in C^2$, and that p is a descent direction at x. Then the Armijo condition

$$f(x+\alpha p) < f(x) + \alpha\beta p^T g(x)$$

is satisfied for all $\beta \in [0, \alpha_{\max(x,p)}]$, where

$$\alpha_{\max(x,p)} = \frac{2(\beta-1)p^T g(x)}{C_g \|p\|_2^2}$$

and C_g is the Lipschitz constant of gradient $g(x)$

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The numerator in $\alpha_{\max(x,p)}$ corresponds to the slope and the denominator to the curvature term. It can be interpreted as follows: If the curvature term is large, then the admissible range of α is small. Similarly, if the projected gradient along the search direction is large, then the range of admissible is larger.

Backtracking Armijo linesearch

Theorem

Suppose that $f \in C^2$, $\beta \in (0;1)$ and that p_k is a descent direction at x_k. Then the stepsize generated by the backtracking-Armijo linesearch terminates with

$$\alpha_k \geq \min\left(\alpha_{init}, \frac{2\tau(\beta - 1)p_k^T g_k}{C_g \left\| p_k \right\|_2^2}\right)$$

In order to tie all of the above together, we first need to state our **Generic Linesearch Method**:

Convergence of generic linesearch methods

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1. Given an initial guess x_0, let $k = 0$
2. Until convergence:
    1. Find a descent direction p_k at x_k.
    2. Compute a stepsize α_k using a backtracking-Armijo linesearch along p_k.
    3. Set $x_{k+1} = x_k + \alpha_k p_k$, and increase k by 1.

Convergence of generic linesearch methods

Theorem

Suppose that $f \in C^2$. Then, for the iterates generated by the Generic Linesearch Method, either

$$g_l = 0 \quad \text{for} \quad \text{some} \quad l > 0$$

or

$$\lim_{k \to \infty} f_k = -\infty$$

or

$$\lim_{k \to \infty} \min \left(\left| p_k^T g_k \right|, \frac{\left| p_k^T g_k \right|}{\| p_k \|_2^2} \right) = 0$$

Convergence of generic linesearch methods

In words, either we find a 1st-order critical point in a finite number of iterations, or we encounter a sequence of iterates for which the objective function is unbounded from below, or the slope (or a normalized slope) along the search direction converges to zero.

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For one thing, it certainly does not say that the gradient converges to zero, that is the iterates may not ultimately be first-order critical, since it might equally occur if the search direction and gradient tend to be mutually orthogonal.

Thus we see that simply requiring that p_k be a descent directionis not a sufficiently demanding requirement.

Method of steepest descent

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The so-called **steepest descent direction**.

Convergence of steepest descent method

Theorem

Suppose that $f \in C^2$. Then, for the iterates generated by the Steepest Descent Method, either

$$g_l = 0 \quad \textit{for} \quad \textit{some} \quad l > 0$$

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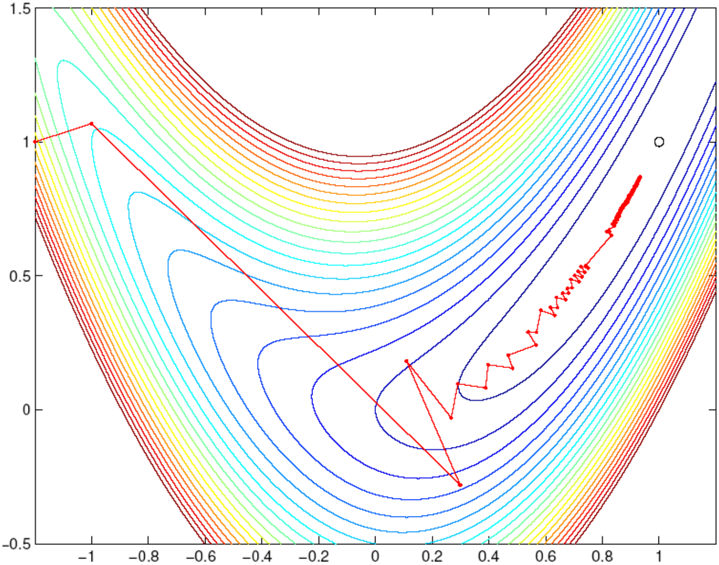
Convergence of steepest descent method



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In next lecture we will consider methods that try to avoid this defect.