

Numerical Optimization

Lecture Notes #4

Unconstrained Optimization; Line Search Methods

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Quick Recap: Last Time

Quick overview of optimization algorithms — two categories

1. **Line search** — Select a search direction, then optimize in that direction
2. **Trust region** — Build a local (simple) model of the objective, optimize the model in the local region where we trust it.

Convergence rates — linear / superlinear / quadratic.

More details on line search —

Search directions — Steepest descent (linear convergence)
Newton direction (quadratic convergence)

Enforcing sufficient decrease in the objective — **Wolfe conditions**.



Recall — Algorithm: Backtracking Linesearch

Algorithm: Backtracking Linesearch

- [0] Find a descent direction $\bar{\mathbf{p}}_k$
- [1] Set $\bar{\alpha} > 0$, $\rho \in (0, 1)$, $c \in (0, 1)$, set $\alpha = \bar{\alpha}$
- [2] While $f(\bar{\mathbf{x}}_k + \alpha \bar{\mathbf{p}}_k) > f(\bar{\mathbf{x}}_k) + c\alpha \bar{\mathbf{p}}_k^T \nabla f(\bar{\mathbf{x}}_k)$
- [3] $\alpha = \rho \alpha$
- [4] End-While
- [5] Set $\alpha_k = \alpha$

If an algorithm selects the step lengths appropriately (e.g. backtracking), we do not have to check the second inequality of the Wolfe conditions.

The algorithm above is especially well suited for use with Newton method ($\bar{\mathbf{p}}_k = \bar{\mathbf{p}}_k^N$), where $\bar{\alpha} = \mathbf{1}$.

The value of the **contraction factor** ρ can be allowed to vary at each iteration of the line search. (To be revisited)



Example: Minimizing $f(\bar{x}) = (x_1 + x_2^2)^2$

In the next few slides we illustrate our findings so far by minimizing $f(\bar{x}) = (x_1 + x_2^2)^2$ (with $\bar{x}_0 = [1, 1]$) using two algorithms:

- 1. Steepest Descent direction with Backtracking Linesearch.
- 2. Newton direction with Backtracking Linesearch.

One thing to notice is that the entire curve where $x_1 = -x_2^2$ gives $f(\bar{x}) = 0$ — the minimum is not isolated, nor unique.

Recall:

$$\bar{p}_k^{SD} = -\frac{\nabla f(\bar{x}_k)}{|\nabla f(\bar{x}_k)|}, \quad \bar{p}_k^N = -\left[\nabla^2 f(\bar{x}_k)\right]^{-1} \nabla f(\bar{x}_k).$$



Steepest Descent on $f(\bar{x}) = (x_1 + x_2^2)^2$, with $\bar{x}_0 = [1, 1]$

\bar{x}^T	$f(\bar{x})$	\bar{p}^{SD}	α
[1, 1]	4.000000	$[-4.472136 \cdot 10^{-1}, -8.944272 \cdot 10^{-1}]$	1
[0.552786, 0.105573]	$3.180193 \cdot 10^{-1}$	$[-9.784275 \cdot 10^{-1}, -2.065907 \cdot 10^{-1}]$	1
$[-0.425641, -0.101018]$	$1.725874 \cdot 10^{-1}$	$[9.801951 \cdot 10^{-1}, -1.980344 \cdot 10^{-1}]$	1/2
[0.064456, -0.200035]	$1.091409 \cdot 10^{-2}$	$[-9.284542 \cdot 10^{-1}, 3.714468 \cdot 10^{-1}]$	1/8
$[-0.051600, -0.153604]$	$7.843386 \cdot 10^{-4}$	$[9.559089 \cdot 10^{-1}, -2.936633 \cdot 10^{-1}]$	1/32
$[-0.021728, -0.162781]$	$2.274880 \cdot 10^{-5}$	$[-9.508768 \cdot 10^{-1}, 3.095697 \cdot 10^{-1}]$	1/128
$[-0.029157, -0.160363]$	$1.183829 \cdot 10^{-5}$	$[9.522234 \cdot 10^{-1}, -3.054022 \cdot 10^{-1}]$	1/256
$[-0.025437, -0.161556]$	$4.395456 \cdot 10^{-7}$	$[-9.515610 \cdot 10^{-1}, 3.074601 \cdot 10^{-1}]$	1/1024
$[-0.026367, -0.161255]$	$1.319155 \cdot 10^{-7}$	$[9.517280 \cdot 10^{-1}, -3.069426 \cdot 10^{-1}]$	1/2048
$[-0.025902, -0.161405]$	$2.246036 \cdot 10^{-8}$	$[-9.516447 \cdot 10^{-1}, 3.072010 \cdot 10^{-1}]$	1/4096
$[-0.026134, -0.161330]$	$1.137904 \cdot 10^{-8}$	$[9.516864 \cdot 10^{-1}, -3.070717 \cdot 10^{-1}]$	1/8192

Table: Steepest Descent with Backtracking line search applied to the problem $f(\bar{x}) = (x_1 + x_2^2)^2$, starting $\bar{x}_0 = [1, 1]$.



Steepest Descent with Backtracking Linesearch

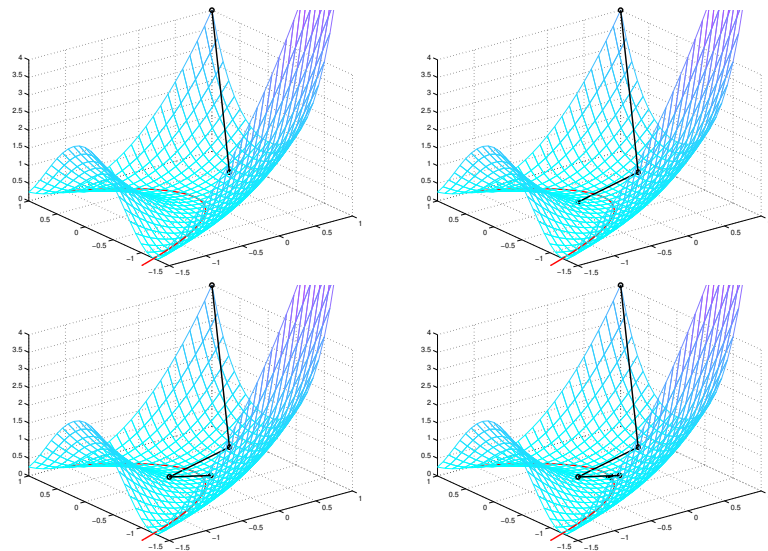


Figure: The iterations #1, #2, #3, and #9 (convergence to 10^{-8}).



Steepest Descent with Backtracking Linesearch

Linear Convergence

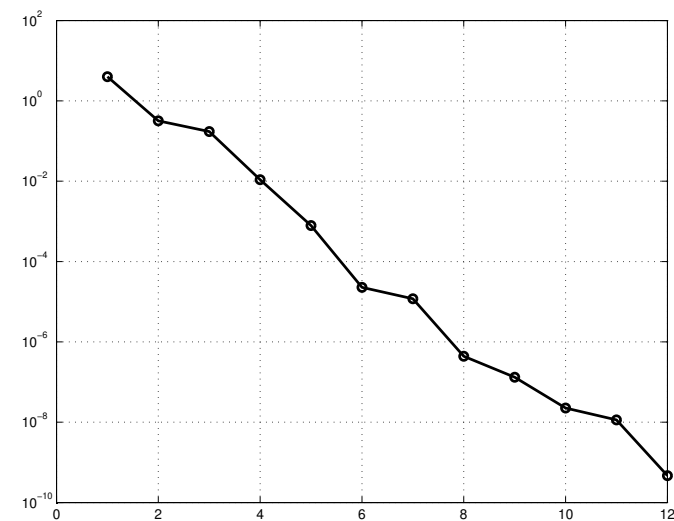


Figure: The size of the objective as a function of the iteration number.



Newton on $f(\bar{x}) = (x_1 + x_2)^2$, with $\bar{x}_0 = [1, 1]$

Oops! Non-local Minimum

\bar{x}^T	$f(\bar{x})$	p^N	α
[1, 1]	4.000000	[-2.000000, 0.000000]	1
[-1, 1]	0	—	—

Table: Newton direction with Backtracking line search applied to the problem $f(\bar{x}) = (x_1 + x_2)^2$, starting $\bar{x}_0 = [1, 1]$.

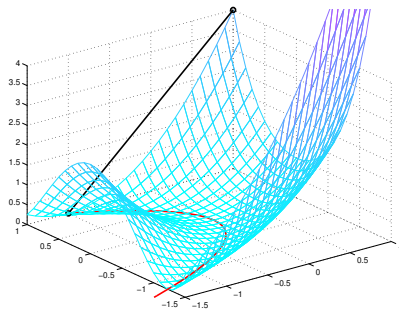


Figure: The only iteration; we achieve convergence right away. (\Rightarrow The problem is too easy...)



Example #2: Minimizing $f(\bar{x}) = (x_1 + x_2)^2 + 0.5(x_1^2 + x_2^2)$

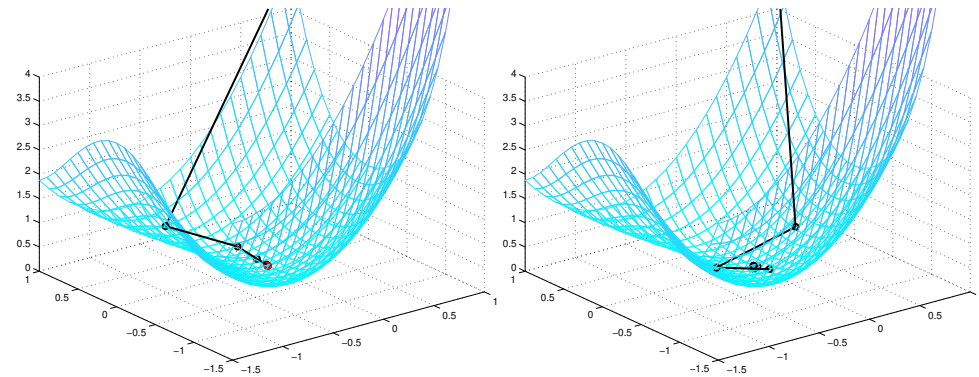


Figure: Comparison of Newton direction (left) and Steepest Descent direction (right) with backtracking line search applied to the objective $f(\bar{x}) = (x_1 + x_2)^2 + 0.5(x_1^2 + x_2^2)$ with $\bar{x}_0^T = [1, 1]$. In this case, the minimum is unique $\bar{x}^* = [0, 0]$. The Newton algorithm requires 6 iterations to reach the minimum up to desired accuracy, and the Steepest Descent algorithm requires 16 iterations.



Example: Minimizing $f(\bar{x}) = (x_1 + x_2)^2 + 0.5(x_1^2 + x_2^2)$

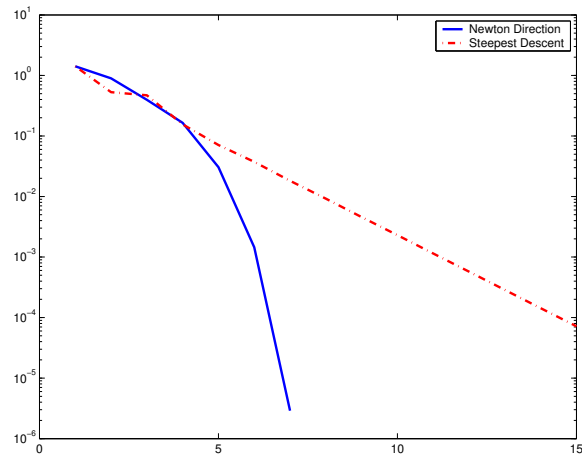


Figure: Convergence comparison of Newton direction (blue/solid) and Steepest Descent direction (red/dash-dotted) with backtracking line search applied to the objective $f(\bar{x}) = (x_1 + x_2)^2 + 0.5(x_1^2 + x_2^2)$ with $\bar{x}_0^T = [1, 1]$. We see that the Steepest Descent algorithm is linearly convergent and that the Newton algorithm is significantly faster (quadratically convergent).



Convergence of Line Search Methods

$\cos \theta_k$

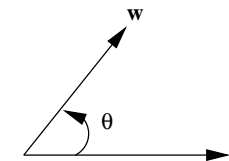


Figure: $\bar{v}^T \bar{w} = \cos \theta \|\bar{v}\| \cdot \|\bar{w}\|$.

All our algorithms rely on the directional derivative $\bar{p}_k^T \nabla f(\bar{x}_k)$.

One of the key properties in expressing requirements on the search direction is the **angle** θ_k .

The expression for the cos of this angle is given by

$$\cos \theta_k = \frac{\bar{p}_k^T \nabla f(\bar{x}_k)}{\|\bar{p}_k^T\| \|\nabla f(\bar{x}_k)\|}$$



Convergence of Line Search Methods

the Zoutendijk condition

Theorem (Zoutendijk's Theorem)

Consider any iteration of the form $\bar{\mathbf{x}}_{k+1} = \bar{\mathbf{x}}_k + \alpha_k \bar{\mathbf{p}}_k$, where $\bar{\mathbf{p}}_k$ is a descent direction and α_k satisfies the Wolfe conditions

$$\begin{aligned} f(\bar{\mathbf{x}}_k + \alpha \bar{\mathbf{p}}_k) &\leq f(\bar{\mathbf{x}}_k) + c_1 \alpha \bar{\mathbf{p}}_k^T \nabla f(\bar{\mathbf{x}}), & c_1 &\in (0, 1) \\ \bar{\mathbf{p}}_k^T \nabla f(\bar{\mathbf{x}}_k + \alpha \bar{\mathbf{p}}_k) &\geq c_2 \bar{\mathbf{p}}_k^T \nabla f(\bar{\mathbf{x}}_k), & c_2 &\in (c_1, 1). \end{aligned}$$

Suppose that f is bounded from below in \mathbb{R}^n and that f is continuously differentiable in an open set N containing the level set $\mathcal{L} = \{x \in \mathbb{R}^n : f(\bar{\mathbf{x}}) \leq f(\bar{\mathbf{x}}_0)\}$ where $\bar{\mathbf{x}}_0$ is the starting point of the iteration. Assume also that the gradient ∇f is Lipschitz continuous on N , i.e. there exists a constant L such that

$$\|\nabla f(\bar{\mathbf{x}}) - \nabla f(\bar{\mathbf{y}})\| \leq L \|\bar{\mathbf{x}} - \bar{\mathbf{y}}\|, \quad \forall \bar{\mathbf{x}}, \bar{\mathbf{y}} \in \mathcal{L}$$

Then

$$\sum_{k=0}^{\infty} \cos^2 \theta_k \|\nabla f(\bar{\mathbf{x}}_k)\|^2 < \infty.$$



Convergence of Line Search Methods

the Zoutendijk Condition

This result seems, at first (and probably second too!) glance, to be quite technical and obscure...

However, the **Zoutendijk condition**

$$\sum_{k=0}^{\infty} \cos^2 \theta_k \|\nabla f(\bar{\mathbf{x}}_k)\|^2 < \infty$$

implies that

$$\lim_{k \rightarrow \infty} \cos^2 \theta_k \|\nabla f(\bar{\mathbf{x}}_k)\|^2 \rightarrow 0$$

Now, **if** we have a method for choosing the search directions $\bar{\mathbf{p}}_k$ so that $\cos \theta_k \geq \delta > 0$ for all k , **then** this shows that $\|\nabla f(\bar{\mathbf{x}}_k)\| \rightarrow 0$.



The Zoutendijk Condition: Steepest Descent

For the steepest descent direction we have $\cos \theta_k = -1$. Hence, if we use a line search algorithm which satisfies the Wolfe conditions, it will always converge to a stationary point (under the conditions of the theorem — f bounded below, and ∇f Lipschitz continuous).

This means that steepest descent is **globally convergent** in the sense

$$\lim_{k \rightarrow \infty} \|\nabla f(\bar{\mathbf{x}}_k)\| = 0.$$

We cannot guarantee convergence to a minimum, only to a stationary point.

In order to guarantee convergence to a minimum, more conditions (for example on the Hessian) are required.



The Zoutendijk Condition: Newton Direction

It can be shown that Newton methods are also globally convergent in this sense, under these additional conditions:

The Hessian must be **positive definite**, and the **condition numbers** must be uniformly bounded, i.e.

$$\left\| [\nabla^2 f(\bar{\mathbf{x}}_k)] \right\| \cdot \left\| [\nabla^2 f(\bar{\mathbf{x}}_k)]^{-1} \right\| \leq M, \quad \text{for some positive } M.$$

That is, the ratio of the largest and smallest eigenvalues, $\lambda_k^{\max} / \lambda_k^{\min}$ must remain bounded. (Think of λ_k^j as the curvature in the eigen-directions.)

The proof for the steepest descent direction is given in (NW^{1st} pp.43–44, NW^{2nd} pp.38–39) and the key part to the proof for the Newton direction is exercise #3.5 (NW^{1st} p.62, NW^{2nd} p.63)



Notes & Looking Forward

We note that the Zoutendijk condition gives us global convergence, *i.e.* a guarantee that we will arrive at a stationary point.

It does, however, not say anything about the **rate of convergence**.

Next we will look (in a less hand-waving way) at the **local convergence rates** (*i.e.* the convergence “speed”) of Steepest descent, Newton, and Quasi-Newton methods.



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