Unconstrained minimization Lectures for PHD course on Non-linear equations and numerical optimization

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Unconstrained minimization

Outline

- General iterative scheme
 - Descent direction failure
- 2 Backtracking Armijo line-search
 - Global convergence of backtracking Armijo line-search
 - Global convergence of steepest descent
- 3 Wolfe–Zoutendijk global convergence
 - The Wolfe conditions
 - The Armijo-Goldstein conditions
- 4 Algorithms for line-search
 - Armijo Parabolic-Cubic search
 - Wolfe linesearch

Given $f : \mathbb{R}^n \mapsto \mathbb{R}$:

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

the following regularity about f(x) is assumed in the following:

Assumption (Regularity assumption)

We assume $f \in C^1(\mathbb{R}^n)$ with Lipschitz continuous gradient, i.e. there exists $\gamma > 0$ such that

$$\left\|
abla \mathsf{f}(oldsymbol{x})^T -
abla \mathsf{f}(oldsymbol{y})^T
ight\| \leq \gamma \left\|oldsymbol{x} - oldsymbol{y}
ight\|, \qquad orall oldsymbol{x}, oldsymbol{y} \in \mathbb{R}^n$$



Definition (Global minimum)

Given $\mathsf{f}:\mathbb{R}^n\mapsto\mathbb{R}$ a point $x_\star\in\mathbb{R}^n$ is a global minimum if

 $\mathsf{f}(oldsymbol{x}_{\star}) \leq \mathsf{f}(oldsymbol{x}), \qquad orall oldsymbol{x} \in \mathbb{R}^n.$

Definition (Local minimum)

Given $\mathsf{f}:\mathbb{R}^n\mapsto\mathbb{R}$ a point $x_\star\in\mathbb{R}^n$ is a local minimum if

$$\mathsf{f}({m{x}}_{\star}) \leq \mathsf{f}({m{x}}), \qquad orall {m{x}} \in B({m{x}}_{\star}; \delta).$$

Obviously a global minimum is a local minimum. Find a global minimum in general is not an easy task. The algorithms presented in the sequel will approximate local minima's.



Definition (Strict global minimum)

Given $\mathsf{f}:\mathbb{R}^n\mapsto\mathbb{R}$ a point $x_\star\in\mathbb{R}^n$ is a strict global minimum if

 $\mathsf{f}(oldsymbol{x}_{\star}) < \mathsf{f}(oldsymbol{x}), \qquad orall oldsymbol{x} \in \mathbb{R}^n \setminus \{oldsymbol{x}_{\star}\}.$

Definition (Strict local minimum)

Given $\mathsf{f}:\mathbb{R}^n\mapsto\mathbb{R}$ a point $x_\star\in\mathbb{R}^n$ is a strict local minimum if

 $\mathsf{f}(oldsymbol{x}_{\star}) < \mathsf{f}(oldsymbol{x}), \qquad orall oldsymbol{x} \in B(oldsymbol{x}_{\star};\delta) \setminus \{oldsymbol{x}_{\star}\}.$

Obviously a strict global minimum is a strict local minimum.

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Lemma (First order Necessary condition for local minimum)

Given $f : \mathbb{R}^n \mapsto \mathbb{R}$ satisfying the regularity assumption. If a point $x_* \in \mathbb{R}^n$ is a local minimum then

$$abla \mathbf{f}(\boldsymbol{x}_{\star})^T = \mathbf{0}.$$

Proof.

Consider a generic direction d, then for δ small enough we have

$$\lambda^{-1} ig(oldsymbol{x}_\star + \lambda oldsymbol{d} ig) - oldsymbol{\mathsf{f}} oldsymbol{x}_\star ig) ig) \leq 0, \qquad 0 < \lambda < \delta$$

so that

$$\lim_{\lambda \to 0} \lambda^{-1} \big(\mathsf{f}(\boldsymbol{x}_{\star} + \lambda \boldsymbol{d}) - \mathsf{f}(\boldsymbol{x}_{\star}) \big) = \nabla \mathsf{f}(\boldsymbol{x}_{\star}) \boldsymbol{d} \leq \mathsf{0},$$

because d is a generic direction we have $\nabla f(x_{\star})^T = \mathbf{0}$.



- The first order necessary condition do not discriminate maximum, minimum, or saddle points.
- To discriminate maximum and minimum we need more information, e.g. second order derivative of f(x).
- With second order derivative we can build necessary and sufficient condition for a minima.
- In general using only first and second order derivative at the point x_{*} it is not possible to deduce a necessary and sufficient condition for a minima.

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Lemma (Second order Necessary condition for local minimum)

Given $f \in C^2(\mathbb{R}^n)$ if a point $x_{\star} \in \mathbb{R}^n$ is a local minimum then $\nabla f(x_{\star})^T = \mathbf{0}$ and $\nabla^2 f(x_{\star})$ is semi-definite positive, i.e.

 $oldsymbol{d}^T
abla^2 \mathsf{f}(oldsymbol{x}_\star) oldsymbol{d} \geq 0, \qquad orall oldsymbol{d} \in \mathbb{R}^n$

Example

This condition is only, necessary, in fact consider $f(x) = x_1^2 - x_2^3$,

$$abla \mathsf{f}(\boldsymbol{x}) = ig(2x_1, -3x_2^2ig), \quad
abla^2\mathsf{f}(\boldsymbol{x}) = igg(egin{matrix} 2 & 0 \ 0 & -6x_2 \ \end{pmatrix}$$

for the point $x_{\star} = \mathbf{0}$ we have $\nabla f(\mathbf{0}) = \mathbf{0}$ and $\nabla^2 f(\mathbf{0})$ semi-definite positive, but **0** is a saddle point not a minimum.



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Proof.

The condition $\nabla f(x_{\star})^T = \mathbf{0}$ comes from first order necessary conditions. Consider now a generic direction d, and the finite difference:

$$rac{\mathsf{f}(oldsymbol{x}_{\star}+\lambdaoldsymbol{d})-2\mathsf{f}(oldsymbol{x}_{\star})+\mathsf{f}(oldsymbol{x}_{\star}-\lambdaoldsymbol{d})}{\lambda^2}\geq 0$$

by using Taylor expansion for f(x)

$$\mathsf{f}(\boldsymbol{x}_{\star} \pm \lambda \boldsymbol{d}) = \mathsf{f}(\boldsymbol{x}_{\star}) \pm \nabla \mathsf{f}(\boldsymbol{x}_{\star}) \lambda \boldsymbol{d} + \lambda^2 \boldsymbol{d}^T \nabla^2 \mathsf{f}(\boldsymbol{x}_{\star}) \boldsymbol{d} + o(\lambda^2)$$

and from the previous inequality

$$oldsymbol{d}^T
abla^2 \mathsf{f}(oldsymbol{x}_\star) oldsymbol{d} + oldsymbol{o}(\lambda^2)/\lambda^2 \geq 0$$

taking the limit $\lambda \to 0$ and form the arbitrariness of d we have that $\nabla^2 f(x_*)$ must be semi-definite positive.



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Second order sufficient condition

Lemma (Second order sufficient condition for local minimum)

Given
$$\mathsf{f} \in \mathsf{C}^2(\mathbb{R}^n)$$
 if a point $x_\star \in \mathbb{R}^n$ satisfy:

1
$$abla \mathsf{f}(x_{\star})^T = \mathbf{0};$$

2
$$abla^2 \mathsf{f}(x_\star)$$
 is definite positive; i.e.

$$oldsymbol{d}^T
abla^2 \mathsf{f}(oldsymbol{x}_{\star}) oldsymbol{d} > \mathsf{0}, \qquad orall oldsymbol{d} \in \mathbb{R}^n \setminus \{oldsymbol{x}_{\star}\}$$

then $x_{\star} \in \mathbb{R}^n$ is a strict local minimum.

Remark

Because $abla^2 \mathsf{f}(x_\star)$ is symmetric we can write

$$\lambda_{\min} \boldsymbol{d}^T \boldsymbol{d} \leq \boldsymbol{d}^T
abla^2 \mathbf{f}(\boldsymbol{x}_{\star}) \boldsymbol{d} \leq \lambda_{\max} \boldsymbol{d}^T \boldsymbol{d}$$

If $\nabla^2 f(x_{\star})$ is positive definite we have $\lambda_{\min} > 0$.

Proof.

Consider now a generic direction d, and the Taylor expansion for f(x)

$$egin{aligned} \mathsf{f}(m{x}_{\star}+m{d}) &= \mathsf{f}(m{x}_{\star}) +
abla \mathsf{f}(m{x}_{\star})m{d} + m{d}^T
abla^2 \mathsf{f}(m{x}_{\star})m{d} + o(\|m{d}\|^2) \ &\geq \mathsf{f}(m{x}_{\star}) + \lambda_{min} \, \|m{d}\|^2 + o(\|m{d}\|^2) \ &\geq \mathsf{f}(m{x}_{\star}) + \lambda_{min} \, \|m{d}\|^2 \left(1 + o(\|m{d}\|^2) / \,\|m{d}\|^2
ight) \end{aligned}$$

choosing d small enough we can write

$$\mathsf{f}(x_\star + d) \ge \mathsf{f}(x_\star) + rac{\lambda_{min}}{2} \|d\|^2 > \mathsf{f}(x_\star), \qquad d \neq \mathbf{0}, \ \|d\| \le \delta.$$

e. x_\star is a strict minimum.

Outline

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- 2 Backtracking Armijo line-search
 Global convergence of backtracking Armijo line-search
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- Wolfe–Zoutendijk global convergence
 The Wolfe conditions
 - The Armijo-Goldstein conditions
- Algorithms for line-search
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How to find a minimum

Given $f: \mathbb{R}^n \mapsto \mathbb{R}$: minimize_{$x \in \mathbb{R}^n$} f(x).

We can solve the problem by solving the necessary condition.
 i.e by solving the nonlinear systems

$$abla \mathsf{f}(oldsymbol{x})^T = oldsymbol{0}.$$

- **2** Using such an approach we looses the information about f(x).
- Moreover such an approach can find solution corresponding to a maximum or saddle points.
- A better approach is to use all the information and try to build minimizing procedure, i.e. procedures that, starting from a point x_0 build a sequence $\{x_k\}$ such that $f(x_{k+1}) \leq f(x_k)$. In this way, at least, we avoid to converge to a strict maximum.



Iterative Methods

- in practice very rare to be able to provide explicit minimizer.
- iterative method: given starting guess x_0 , generate the sequence,

$$\{\boldsymbol{x}_k\}, \qquad k=1,2,\ldots$$

- AIM: ensure that (a subsequence) has some favorable limiting properties:
 - satisfies first-order necessary conditions
 - satisfies second-order necessary conditions

Line-search Methods

A generic iterative minimization procedure can be sketched as follows:

- calculate a search direction $oldsymbol{p}_k$ from $oldsymbol{x}_k$
- ensure that this direction is a descent direction, i.e.

 $abla {\mathsf{f}}({m{x}}_k){m{p}}_k < {\mathsf{0}}, \qquad ext{whenever }
abla {\mathsf{f}}({m{x}}_k)^T
eq {\mathbf{0}}$

so that, at least for small steps along p_k , the objective function ${f f}(x)$ will be reduced

• use line-search to calculate a suitable step-length $\alpha_k > 0$ so that

$$f(\boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k) < f(\boldsymbol{x}_k).$$

• Update the point:

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k$$

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Generic minimization algorithm

Written with a pseudo-code the minimization procedure is the following algorithm:

Generic minimization algorithm

```
Given an initial guess x_0, let k = 0;

while not converged do

Find a descent direction p_k at x_k;

Compute a step size \alpha_k using a line-search along p_k.

Set x_{k+1} = x_k + \alpha_k p_k and increase k by 1.

end while
```

The crucial points which differentiate the algorithms are:

- The computation of the direction p_k ;
- 2 The computation of the step size α_k .



Practical Line-search methods

• The first developed minimization algorithms try to solve

$$\alpha_k = \arg\min_{\alpha>0} f(\boldsymbol{x}_k + \alpha \boldsymbol{p}_k)$$

- performing exact line-search by univariate minimization;
- rather expensive and certainly not cost effective.
- Modern methods implements inexact line-search:
 - ensure steps are neither too long nor too short
 - try to pick useful initial step size for fast convergence

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- best methods are based on:
 - backtracking–Armijo search;
 - Armijo-Goldstein search;
 - Franke–Wolfe search;

backtracking line-search

To obtain a monotone decreasing sequence we can use the following algorithm:

Backtracking line-search

Given
$$\alpha_{init}$$
 (e.g., $\alpha_{init} = 1$);
Given $\tau \in (0, 1)$ typically $\tau = 0.5$;
Let $\alpha^{(0)} = \alpha_{init}$;
while not $f(x_k + \alpha^{(\ell)}p_k) < f(x_k)$ do
set $\alpha^{(\ell+1)} = \tau \alpha^{(\ell)}$;
increase ℓ by 1;
end while
Set $\alpha_k = \alpha^{(\ell)}$.

To be effective the previous algorithm should terminate in a finite number of steps. The next lemma assure that if p_k is a descent direction then the algorithm terminate.

Existence of a descent step

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Lemma (Descent Lemma)

Suppose that f(x) satisfy the standard assumptions and that p_k is a descent direction at x_k , i.e. $\nabla f(x_k)p_k < 0$. Then we have

$$\mathsf{f}(oldsymbol{x}_k+lphaoldsymbol{p}_k)\leq\mathsf{f}(oldsymbol{x}_k)+lpha
abla\mathsf{f}(oldsymbol{x}_k)oldsymbol{p}_k+rac{\gamma}{2}lpha^2\,\|oldsymbol{p}_k\|^2$$

for all
$$\alpha \in [0, \alpha_k^{\star}]$$
 where $\alpha_k^{\star} = \frac{-2\nabla f(\boldsymbol{x}_k)\boldsymbol{p}_k}{\gamma \|\boldsymbol{p}_k\|^2} > 0$

Assumption (Regularity assumption)

We assume $f \in C^1(\mathbb{R}^n)$ with Lipschitz continuous gradient, i.e. there exists $\gamma > 0$ such that

$$\left\|
abla \mathsf{f}(oldsymbol{x}) -
abla \mathsf{f}(oldsymbol{y})
ight\| \leq \gamma \left\|oldsymbol{x} - oldsymbol{y}
ight\|, \qquad orall oldsymbol{x}, oldsymbol{y} \in \mathbb{R}^n$$



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Existence of a descent step

Proof.

Let be $g(\alpha) = f(\boldsymbol{x}_k + \alpha \boldsymbol{p}_k)$ then we can write:

$$g(\alpha) - g(0) = \int_0^\alpha g'(\xi) d\xi = \alpha g'(0) + \int_0^\alpha \left(g'(\xi) - g'(0) \right) d\xi$$

$$= \alpha \nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k + \int_0^\alpha \left(\nabla f(\boldsymbol{x}_k + \xi \boldsymbol{p}_k) - \nabla f(\boldsymbol{x}_k) \right) \boldsymbol{p}_k \, d\xi$$

$$\leq lpha
abla \mathsf{f}(oldsymbol{x}_k)oldsymbol{p}_k + \int_0^lpha \|
abla \mathsf{f}(oldsymbol{x}_k + \xioldsymbol{p}_k) -
abla \mathsf{f}(oldsymbol{x}_k)\| \, \|oldsymbol{p}_k\| \, \, d\xi$$

$$\leq lpha
abla \mathsf{f}(oldsymbol{x}_k)oldsymbol{p}_k + \|oldsymbol{p}_k\|^2 \int_0^lpha \gamma \xi \, d\xi$$

$$\leq \alpha \nabla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k + \frac{\gamma \alpha^2}{2} \|\boldsymbol{p}_k\|^2 = \alpha \left[\nabla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k + \frac{\gamma \alpha}{2} \|\boldsymbol{p}_k\|^2 \right]$$

now the lemma follows trivially.



Existence of a descent step

- The descent lemma means that there is a parabola that is entirely over the function f(x) in the direction p_k if this is a descent direction.
- The second part of the lemma permits to ensure a minimal reduction if the step length is chosen to be $\alpha_k = \alpha_k^*/2$.

$$\int_{\mathbf{f}(\boldsymbol{x}_k) + \alpha \nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k + \frac{\gamma}{2} \alpha^2 \|\boldsymbol{p}_k\|^2}{f(\boldsymbol{x}_k + \alpha \boldsymbol{p}_k)}$$

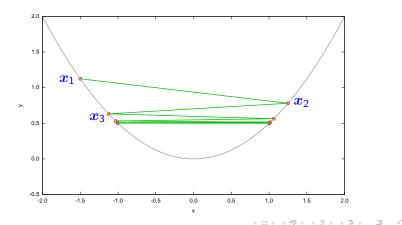
Descent direction failure

- The simple request to have a descent direction may be not enough.
- In fact, step length may be asymptotically too short
- Or step length may be asymptotically too long

Steps may be too long

The objective function is $f(x) = x^2$ and the iterates are generated by the descent directions $p_k = (-1)^{k+1}$ from $x_0 = 2$ with:

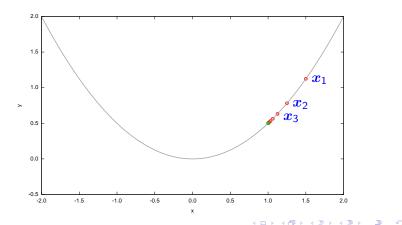
$$x_{k+1} = x_k + \alpha_k p_k, \qquad \alpha_k = 2 + 3 \cdot 2^{-(k+1)}$$



Steps may be too short

The objective function is $f(x) = x^2$ and the iterates are generated by the descent directions $p_k = -1$ from $x_0 = 2$ with:

$$x_{k+1} = x_k + \alpha_k p_k, \qquad \alpha_k = 2^{-(k+1)}$$



Outline

General iterative schemeDescent direction failure

2 Backtracking Armijo line-search

- Global convergence of backtracking Armijo line-search
- Global convergence of steepest descent

Wolfe–Zoutendijk global convergence The Wolfe conditions The Armite Coldstein conditions

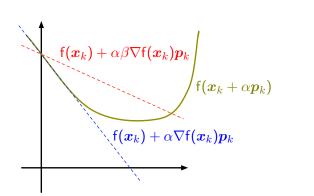
- The Armijo-Goldstein conditions
- Algorithms for line-search
 Armijo Parabolic-Cubic search
 Walfe lineseerch
 - Wolfe linesearch

Armijo condition

To prevent large steps relative to the decreasing of f(x) we require that

$$\mathsf{f}(\boldsymbol{x}_k + lpha_k \boldsymbol{p}_k) \leq \mathsf{f}(\boldsymbol{x}_k) + lpha_k eta
abla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k$$

for some $\beta \in (0,1)$. Typical values of β ranges form 10^{-4} to 0.1.



Backtracking Armijo line-search

```
Given \alpha_{init} (e.g., \alpha_{init} = 1);

Given \tau \in (0, 1) typically \tau = 0.5;

Let \alpha^{(0)} = \alpha_{init};

while not f(x_k + \alpha^{(\ell)}p_k) \le f(x_k) + \alpha^{(\ell)}\beta\nabla f(x_k)p_k do

set \alpha^{(\ell+1)} = \tau \alpha^{(\ell)};

increase \ell by 1;

end while

Set \alpha_k = \alpha^{(\ell)}.
```

- Backtracking Armijo line-search prevents the step from getting too large.
- Now the question is: will the backtracking Armijo line-search terminate in a finite number of steps ?



Finite termination of Armijo line-search

Theorem (Finite termination of Armijo linesearch)

Suppose that f(x) satisfy the standard assumptions and $\beta \in (0, 1)$ and that p_k is a descent direction at x_k . Then the Armijo condition

$$\mathsf{f}(\boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k) \leq \mathsf{f}(\boldsymbol{x}_k) + \alpha_k \beta \nabla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k$$

is satisfied for all
$$\alpha_k \in [0, \omega_k]$$
 where $\omega_k = \frac{2(\beta - 1) \nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k}{\gamma \|\boldsymbol{p}_k\|^2}$

Assumption (Regularity assumption)

We assume $f \in C^1(\mathbb{R}^n)$ with Lipschitz continuous gradient, i.e. there exists $\gamma > 0$ such that

$$\|
abla \mathsf{f}(\boldsymbol{x}) -
abla \mathsf{f}(\boldsymbol{y})\| \leq \gamma \|\boldsymbol{x} - \boldsymbol{y}\|, \qquad \forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$$

Backtracking Armijo line-search

Finite termination of Armijo line-search

To prove finite termination we need the following Taylor expansion due to the regularity assumption:

$$\mathsf{f}(oldsymbol{x}+lphaoldsymbol{p})=\mathsf{f}(oldsymbol{x})+lpha
abla\mathsf{f}(oldsymbol{x})oldsymbol{p}+E \quad ext{where} \quad |E|\leq rac{\gamma}{2}lpha^2\left\|oldsymbol{p}
ight\|^2$$

Proof.

If $\alpha \le \omega_k$ we have $\alpha \gamma \|p_k\|^2 \le 2(\beta - 1)\nabla f(x_k)p_k$ and by using Taylor expansion

$$egin{aligned} \mathsf{f}(oldsymbol{x}_k + lpha oldsymbol{p}_k) &\leq \mathsf{f}(oldsymbol{x}_k) + lpha
abla \mathsf{f}(oldsymbol{x}_k) oldsymbol{p}_k + lpha (eta - 1)
abla \mathsf{f}(oldsymbol{x}_k) oldsymbol{p}_k + lpha (eta - 1)
abla \mathsf{f}(oldsymbol{x}_k) oldsymbol{p}_k &\leq \mathsf{f}(oldsymbol{x}_k) + lpha eta
abla
abla \mathsf{f}(oldsymbol{x}_k) + lpha eta
abla \mathsf{f}(oldsymbol{x}_k) oldsymbol{p}_k & \end{aligned}$$

Finite termination of Armijo line-search

Corollary (Finite termination of Armijo linesearch)

Suppose that f(x) satisfy the standard assumptions and $\beta \in (0, 1)$ and that p_k is a descent direction at x_k . Then the step-size generated by then backtracking-Armijo line-search terminates with

 $\alpha_k \geq \min \left\{ \alpha_{\textit{init}}, \tau \omega_k
ight\}, \qquad \omega_k = 2(\beta - 1) \nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k / (\gamma \| \boldsymbol{p}_k \|^2)$

Proof.

Line-search will terminate as soon as $\alpha^{(\ell)} \leq \omega_k$:

- **(**) May be that α_{init} satisfies the Armijo condition $\Rightarrow \alpha_k = \alpha_{\text{init}}$.
- ② Otherwise in the last line-search iteration we have

$$\alpha^{(\ell-1)} > \omega_k, \qquad \alpha_k = \alpha^{(\ell)} = \tau \alpha^{(\ell-1)} > \tau \omega_k.$$

Combining these 2 cases gives the required result.

Backtracking-Armijo line-search

- The previous analysis permit to say that Backtracking-Armijo line-search ends in a finite number of steps.
- The line-search produce a step length not too long due to the condition

$$f(\boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k) \leq f(\boldsymbol{x}_k) + \alpha_k \beta \nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k$$

- The line-search produce a step length not too short due to the finite termination theorem.
- Armijo line-search can be improved by adding some further requirements on the step length acceptance criteria.

Global convergence

Theorem (Global convergence)

Suppose that f(x) satisfy the standard assumptions, then, for the iterates generated by the Generic minimization algorithm with backtracking Armijo line-search either:

$${f 0} \ \,
abla {f f}({m x}_k)^T = {f 0}$$
 for some $k \geq {f 0}$;

② or
$$\lim_{k o\infty} \mathsf{f}(oldsymbol{x}_k) = -\infty$$
;

$$\textbf{3} \ \, \textit{or} \lim_{k \to \infty} |\nabla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k| \min \left\{ 1, \|\boldsymbol{p}_k\|^{-1} \right\} = 0.$$

Remark

If the theorem, point 1 means that we found a stationary point in a finite number of steps. Point 2 means that function f(x) is unbounded below, so that a minimum does not exists. Point 3 alone do not imply convergence, but if $\nabla f(x_k)$ and p_k do not become orthogonal and $||p_k|| \neq 0$ then $||\nabla f(x_k)|| \rightarrow 0$.

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Proof.

Assume points 1 and 2 are not satisfied, then we prove point 3. Consider

$$\mathsf{f}(\boldsymbol{x}_{k+1}) \leq \mathsf{f}(\boldsymbol{x}_k) + lpha_k eta
abla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k \leq \mathsf{f}(\boldsymbol{x}_0) + \sum_{j=0}^k lpha_j eta
abla \mathsf{f}(\boldsymbol{x}_j) \boldsymbol{p}_j$$

by the fact that $oldsymbol{p}_k$ is a descent direction we have that the series:

$$\sum_{j=0}^{\infty} \alpha_j \left| \nabla f(\boldsymbol{x}_j) \boldsymbol{p}_j \right| \leq \beta^{-1} \lim_{k \to \infty} \left[f(\boldsymbol{x}_0) - f(\boldsymbol{x}_{k+1}) \right] < \infty$$

and then

$$\lim_{j\to\infty}\alpha_j |\nabla f(\boldsymbol{x}_j)\boldsymbol{p}_j| = \boldsymbol{0}$$

(2/3).

Proof.

Recall that

$$lpha_k \geq \min\left\{lpha_{ ext{init}}, au \omega_k
ight\}, \qquad \omega_k = 2(eta-1)
abla \mathsf{f}(oldsymbol{x}_k)oldsymbol{p}_k/(\gamma \left\|oldsymbol{p}_k
ight\|^2)$$

and consider the two index set:

$$\mathcal{K}_1 = \big\{ k \mid \alpha_k = \alpha_{\mathsf{init}} \big\}, \qquad \mathcal{K}_2 = \big\{ k \mid \alpha_k < \alpha_{\mathsf{init}} \big\},$$

Obviously $\mathbb{N} = \mathcal{K}_1 \cup \mathcal{K}_2$ and from $\lim_{k \to \infty} \alpha_k |\nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k| = 0$ we have

$$\lim_{k \in \mathcal{K}_1 \to \infty} \alpha_k |\nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k| = 0, \tag{A}$$
$$\lim_{k \in \mathcal{K}_2 \to \infty} \alpha_k |\nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k| = 0, \tag{B}$$

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(3/3)

Proof.

For $k \in \mathcal{K}_1$ we have $\alpha_k = \alpha_{\text{init}}$ and $\alpha_k |\nabla f(\boldsymbol{x}_k)\boldsymbol{p}_k| = \alpha_{\text{init}} |\nabla f(\boldsymbol{x}_k)\boldsymbol{p}_k|$ and from (A) we have

$$\lim_{k\in\mathcal{K}_{1} o\infty}|
abla {\mathsf{f}}({m{x}}_{k}){m{p}}_{k}|=0$$
 (*)

For $k \in \mathcal{K}_2$ we have $\tau \omega_k \leq \alpha_k \leq \omega_k$ so

$$lpha_k |
abla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k| \ge au \omega_k |
abla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k| \ge 2 au (1 - eta) rac{|
abla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k|^2}{\gamma \|\boldsymbol{p}_k\|^2}$$

and from (B) we have

$$\lim_{k \in \mathcal{K}_1 o \infty} rac{|
abla \mathsf{f}(oldsymbol{x}_k)oldsymbol{p}_k|}{\|oldsymbol{p}_k\|} = \mathsf{0}$$

Combining (\star) and $(\star\star)$ gives the required result.

 $(\star\star)$

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Steepest descent algorithm

Steepest descent algorithm

```
Given an initial guess x_0, let k = 0;
while not converged do
```

Compute a step-size α_k using a line-search along $-\nabla f(\boldsymbol{x}_k)^T$. Set $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \alpha_k \nabla f(\boldsymbol{x}_k)^T$ and increase k by 1. end while

- The steepest descent algorithm is simply the generic minimization algorithm with search direction the opposite of the gradient in x_k .
- The search direction $-\nabla f(x_k)^T$ is always a descent direction unless the point x_k is a stationary point.



Global convergence of steepest descent

Corollary (Global convergence of steepest descent)

Suppose that f(x) satisfy the standard assumptions, then, for the iterates generated by the steepest descent algorithm with backtracking Armijo line-search either:

1
$$abla \mathsf{f}({m x}_k)^T = {m 0}$$
 for some $k \ge {m 0}$;

② or
$$\lim_{k
ightarrow\infty} \mathsf{f}(oldsymbol{x}_k) = -\infty$$
;

3) or
$$\lim_{k o\infty}
abla \mathsf{f}(oldsymbol{x}_k)^T = oldsymbol{0}.$$

Backtracking Armijo line-search

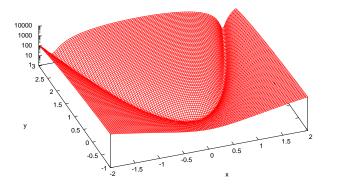
The Rosenbrock example

Global convergence of steepest descent

(1/3)

- Although the steepest descent scheme is globally convergent it can be very slow!
- A classical example is the Rosenbrock function:

$$f(x,y) = 100 (y - x^2)^2 + (x - 1)^2$$

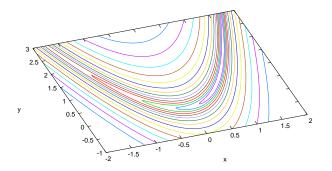




The Rosenbrock example

(2/3)

• This function has a unique minimum at $(1,1)^T$ inside a banana shaped valley.

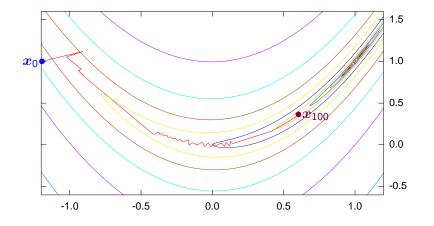


Backtracking Armijo line-search

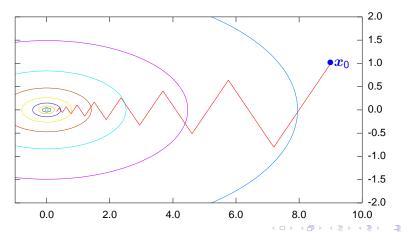
Global convergence of steepest descent

The Rosenbrock example

- (3/3)
- After 100 iteration starting from $(-1.2, 1)^T$ the approximate minimum is far from the solution.



- The steepest descent is a slow method, not only on a difficult test case like the Rosenbrock example.
- Given the function $f(x, y) = \frac{1}{2}x^2 + \frac{9}{2}y^2$ starting from $x_0 = (9, 1)^T$ we have the zig-zag pattern toward $(0, 0)^T$.



Outline

- General iterative schemeDescent direction failure
- Backtracking Armijo line-search
 Global convergence of backtracking Armijo line-search
 Global convergence of steepest descent
- 3 Wolfe–Zoutendijk global convergence
 - The Wolfe conditions
 - The Armijo-Goldstein conditions
 - Algorithms for line-search
 Armijo Parabolic-Cubic search
 - Wolfe linesearch

The Wolfe and Armijo Goldstein conditions

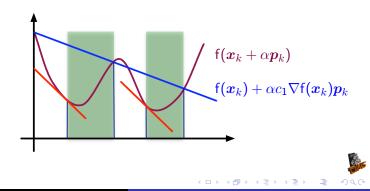
- The simple condition of descent step is in general not enough for the convergence of a iterative minimization scheme.
- The condition of sufficient decrease of backtracking Armijo line-search may be insufficient on general inexact line-search algorithm.
- Adding another condition to the sufficient decrease condition such that we avoid too short step length we obtain globally convergent numerical procedure.
- Oppending on which additional condition is added we obtain the:
 - Wolfe conditions;
 - Armijo Goldstein conditions.

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The Wolfe conditions

Let c_1 and c_2 two constant such that $0 < c_1 < c_2 < 1$. We say that the step length α_k satisfy the Wolfe conditions if α_k satisfy:

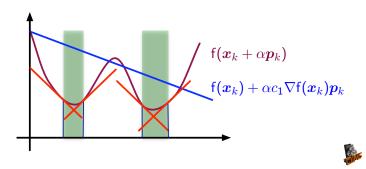
- sufficient decrease: $f(x_k + \alpha_k p_k) \le f(x_k) + c_1 \alpha_k \nabla f(x_k) p_k$;
- **2** curvature condition: $\nabla f(\boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k) \boldsymbol{p}_k \geq c_2 \nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k$.



The strong Wolfe conditions

Let c_1 and c_2 two constant such that $0 < c_1 < c_2 < 1$. We say that the step length α_k satisfy the strong Wolfe conditions if α_k satisfy:

- sufficient decrease: $f(x_k + \alpha_k p_k) \le f(x_k) + c_1 \alpha_k \nabla f(x_k) p_k$;
- 2 curvature condition: $|\nabla f(\boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k) \boldsymbol{p}_k| \leq c_2 |\nabla f(\boldsymbol{x}_k) \boldsymbol{p}_k|.$



Existence of "Wolfe" step length

- The Wolfe condition seems quite restrictive.
- The next lemma answer to the question if a step length satisfying Wolfe conditions does exists.

Lemma (strong Wolfe step length)

Let $f : \mathbb{R}^n \mapsto \mathbb{R}$ satisfying the regularity assumption. If the following condition are satisfied:

$$oldsymbol{0}$$
 $oldsymbol{p}_k$ is a descent direction for the point $oldsymbol{x}_k$, i.e. $abla {\sf f}(oldsymbol{x}_k)oldsymbol{p}_k < {\sf 0};$

 Is f(x_k + αp_k) is bounded from below, i.e. lim_{α→∞} f(x_k + αp_k) > -∞.

then for any $0 < c_1 < c_2 < 1$ there exists an interval [a, b] such that all $\alpha_k \in [a, b]$ satisfy the strong Wolfe conditions.



Proof.

Define $\ell(\alpha) = f(x_k) + \alpha c_1 \nabla f(x_k) p_k$ and $g(\alpha) = f(x_k + \alpha p_k)$. From $\lim_{\alpha \to \infty} \ell(\alpha) = -\infty$ and from condition 1 it follows that there exists $\alpha_* > 0$ such that

$$\ell(lpha_{\star}) = g(lpha_{\star})$$
 and $\ell(lpha) > g(lpha), \quad orall lpha \in (0, lpha_{\star})$

so that all step length $\alpha \in (0, \alpha_{\star})$ satisfy strong Wolfe condition 1. Because $\ell(0) = g(0)$ form Cauchy-Rolle theorem there exists $\alpha_{\star\star} \in (0, \alpha_{\star})$ such that

$$g'(\alpha_{\star\star}) = \ell'(\alpha_{\star\star}) \qquad \Rightarrow$$

 $0 >
abla \mathsf{f}(oldsymbol{x}_k + lpha_{\star\star}oldsymbol{p}_k) oldsymbol{p}_k = c_1
abla \mathsf{f}(oldsymbol{x}_k) oldsymbol{p}_k > c_2
abla \mathsf{f}(oldsymbol{x}_k) oldsymbol{p}_k$

by continuity we find an interval around $\alpha_{\star\star}$ with step lengths satisfying strong Wolfe conditions.

The Zoutendijk condition

Theorem (Zoutendijk)

Let $f : \mathbb{R}^n \mapsto \mathbb{R}$ satisfying the regularity assumption and bounded from below, i.e.

$$\inf_{oldsymbol{x}\in\mathbb{R}^n} \mathsf{f}(oldsymbol{x}) > -\infty$$

Let $\{x_k\}$, $k = 0, 1, ..., \infty$ generated by a generic minimization algorithm where line-search satisfy Wolfe conditions, then

$$\sum_{k=1}^{\infty}(\cos heta_k)^2\left\|
abla {\mathsf{f}}(oldsymbol{x}_k)^T
ight\|^2<+\infty$$

where

$$\cos \theta_k = \frac{-\nabla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k}{\|\nabla \mathsf{f}(\boldsymbol{x}_k)^T\| \, \|\boldsymbol{p}_k\|}$$

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Proof.

Using the second condition of Wolfe

$$abla extsf{f}(oldsymbol{x}_k+lpha_koldsymbol{p}_k)oldsymbol{p}_k\geq c_2
abla extsf{f}(oldsymbol{x}_k)oldsymbol{p}_k\geq (c_2-1)
abla extsf{f}(oldsymbol{x}_k)oldsymbol{p}_k\geq (c_2-1)
abla extsf{f}(oldsymbol{x}_k)oldsymbol{p}_k$$

by using Lipschitz regularity

$$ig\|
abla \mathsf{f}(oldsymbol{x}_k+lpha_koldsymbol{p}_kig\|\leq\gamma\,\|oldsymbol{x}_{k+1}-oldsymbol{x}_k\|\,\|oldsymbol{p}_k\|\ =lpha_k\gamma\,\|oldsymbol{p}_k\|^2$$

and using both inequality we obtain the estimate for α_k :

$$lpha_k \geq rac{c_2 - 1}{\gamma \left\| \boldsymbol{p}_k
ight\|^2}
abla \mathsf{f}(\boldsymbol{x}_k) \boldsymbol{p}_k$$

Proof.

Using the first condition of Wolfe and estimate of α_k

$$egin{aligned} & (oldsymbol{x}_k+lpha_koldsymbol{p}_k) \leq \mathsf{f}(oldsymbol{x}_k)+lpha_kc_1
abla\mathsf{f}(oldsymbol{x}_k)oldsymbol{p}_k \ & \leq \mathsf{f}(oldsymbol{x}_k)-rac{c_1(1-c_2)}{\gamma\left\|oldsymbol{p}_k
ight\|^2}ig(
abla\mathsf{f}(oldsymbol{x}_k)oldsymbol{p}_kig)^2 \end{aligned}$$

setting $A=c_1(1-c_2)/\gamma$ and using the definition of $\cos\theta_k$

$$\mathsf{f}(\boldsymbol{x}_{k+1}) = \mathsf{f}(\boldsymbol{x}_k + \alpha_k \boldsymbol{p}_k) \le \mathsf{f}(\boldsymbol{x}_k) - A(\cos \theta_k)^2 \left\| \nabla \mathsf{f}(\boldsymbol{x}_k)^T \right\|^2$$

and by induction

$$\mathsf{f}(oldsymbol{x}_{k+1}) \leq \mathsf{f}(oldsymbol{x}_1) - A \sum_{j=1}^k (\cos heta_j)^2 \left\|
abla \mathsf{f}(oldsymbol{x}_j)^T
ight\|^2$$



Proof.

The function f(x) is bounded from below, i.e.

$$\inf_{oldsymbol{x}\in\mathbb{R}^n} \mathsf{f}(oldsymbol{x}) > -\infty$$

so that

$$A\sum_{j=1}^{k}(\cos\theta_{j})^{2}\left\|\nabla\mathsf{f}(\boldsymbol{x}_{j})^{T}\right\|^{2}\leq\mathsf{f}(\boldsymbol{x}_{1})-\mathsf{f}(\boldsymbol{x}_{k+1})$$

and

$$A\sum_{j=1}^{\infty}(\cos\theta_j)^2\left\|\nabla\mathsf{f}(\boldsymbol{x}_j)^T\right\|^2\leq\mathsf{f}(\boldsymbol{x}_1)-\lim_{k\to\infty}\mathsf{f}(\boldsymbol{x}_{k+1})<+\infty$$

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(3/3).

Corollary (Zoutendijk condition)

Let $f : \mathbb{R}^n \mapsto \mathbb{R}$ satisfying the regularity assumption and bounded from below. Let $\{x_k\}$, $k = 0, 1, ..., \infty$ generated by a generic minimization algorithm where line-search satisfy Wolfe conditions, then

$$\cos heta_k \left\|
abla \mathsf{f}(oldsymbol{x}_k)^T
ight\| o \mathsf{0} \qquad \textit{where} \qquad \cos heta_k = rac{-
abla \mathsf{f}(oldsymbol{x}_k) oldsymbol{p}_k}{\|
abla \mathsf{f}(oldsymbol{x}_k)^T \| \, \| oldsymbol{p}_k \|}$$

Remark

If $\cos \theta_k \ge \delta > 0$ for all k from the Zoutendijk condition we have:

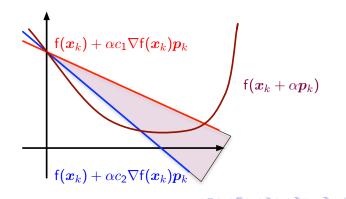
$$\left\|
abla \mathsf{f}(oldsymbol{x}_k)^T
ight\|
ightarrow \mathsf{0}$$

i.e. the generic minimization algorithm where line-search satisfy Wolfe conditions converge to a stationary point.



The Armijo-Goldstein conditions

Let c_1 and c_2 two constant such that $0 < c_1 < c_2 < 1$. We say that the step length α_k satisfy the Wolfe conditions if α_k satisfy:



The Armijo-Goldstein conditions

- Armijo-Goldstein conditions has very similar theoretical properties like the Wolfe conditions.
- Iconvergence theorems can be established.
- The weakness of Armijo-Goldstein conditions respect to Wolfe conditions is that the former can exclude local minima's from the step length as you can see in the figure below.

$$f(\boldsymbol{x}_{k}) + \alpha c_{1} \nabla f(\boldsymbol{x}_{k}) \boldsymbol{p}_{k}$$
$$f(\boldsymbol{x}_{k} + \alpha \boldsymbol{p}_{k})$$
$$f(\boldsymbol{x}_{k}) + \alpha c_{2} \nabla f(\boldsymbol{x}_{k}) \boldsymbol{p}_{k}$$



Outline

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Armijo Parabolic-Cubic search

- Backtracking-Armijo line-search can be slow if a large number of reduction must be performed to satisfy Armijo condition.
- A better performance is obtained if instead of reducing by a fixed factor we use polynomial interpolation to estimate the location of the minimum.
- Solution Assuming that that $f(x_k)$ and $\nabla f(x_k)p_k$ are known at the first step we know also $f(x_k + \lambda p_k)$ if λ is the first trial step.
- In this case a parabolic interpolation can be used to estimate the minimum.
- If we store the last trial step length, in the successive iteration we can use cubic interpolation to estimate the minima's.
- The resulting algorithm is in the following slides.

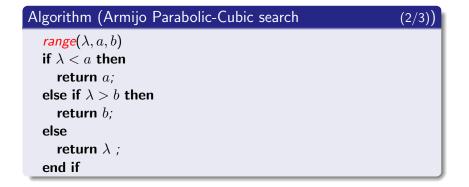


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Algorithm (Armijo Parabolic-Cubic search

armijo_linesearch(f, x, p, τ) $f_0 \leftarrow f(x)$; $\nabla f_0 \leftarrow \nabla f(x)p$; $\lambda \leftarrow 1$; while $\lambda > \lambda_{\min}$ do $f_{\lambda} \leftarrow f(x + \lambda p)$: if $f_{\lambda} \leq f_0 + \lambda \tau \nabla f_0$ then return λ ; successful search else if $\lambda = 1$ then $\lambda_{tmp} \leftarrow \nabla f_0 / [2(f_0 + \nabla f_0 - f_\lambda)];$ else $\lambda_{tmp} \leftarrow cubic(f_0, \nabla f_0, f_\lambda, \lambda, f_n, \lambda_n);$ end if $\lambda_n \leftarrow \lambda$; $f_n \leftarrow f_{\lambda}$; $\lambda \leftarrow range(\lambda_{tmn}, \lambda/10, \lambda/2)$; end if end while return λ_{\min} ; failed search







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Algorithm (Armijo Parabolic-Cubic search

 $\frac{cubic}{f_0} (f_0, \nabla f_0, f_\lambda, \lambda, f_p, \lambda_p)$ Evaluate:

$$\begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\lambda^2 \lambda_p^2 (\lambda - \lambda_p)} \begin{pmatrix} \lambda_p^2 & -\lambda^2 \\ -\lambda_p^3 & \lambda^3 \end{pmatrix} \begin{pmatrix} \mathsf{f}_\lambda - \mathsf{f}_0 - \lambda \nabla \mathsf{f}_0 \\ \mathsf{f}_p - \mathsf{f}_0 - \lambda_p \nabla \mathsf{f}_0 \end{pmatrix}$$

if a = 0 then

return $-\nabla f_0/(2b)$;

else

 $d \leftarrow b^2 - 3 a \nabla f_0;$ return $(-b + \sqrt{d})/(3a);$ end if cubic is a quadratic

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discriminant legitimate cubic



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Wolfe linesearch

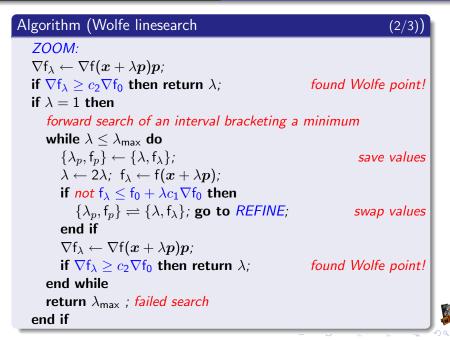
- Wolfe linesearch is identical to the Armijo Parabolic-Cubic search, until a point satisfying the first condition is found.
- At this point the Armijo algorithm stop while Wolfe search try to refine the search until the second condition is satisfied.
- If the step estimated is too short then is is enlarged until it contains a minimum.
- If the step estimated is too long it is reduced until the second condition is satisfied.

(1/3)

Algorithm (Wolfe linesearch

wolfe_linesearch(f, x, p, c_1, c_2) $f_0 \leftarrow f(x)$; $\nabla f_0 \leftarrow \nabla f(x)p$; $\lambda \leftarrow 1$; while $\lambda > \lambda_{\min}$ do $f_{\lambda} \leftarrow f(x + \lambda p)$: if $f_{\lambda} < f_0 + \lambda c_1 \nabla f_0$ then go to ZOOM; found a λ satisfying condition 1 else if $\lambda = 1$ then $\lambda_{tmp} \leftarrow \nabla f_0 / [2(f_0 + \nabla f_0 - f_\lambda)];$ else $\lambda_{tmp} \leftarrow cubic(f_0, \nabla f_0, f_\lambda, \lambda, f_n, \lambda_n);$ end if $\lambda_n \leftarrow \lambda$; $f_n \leftarrow f_{\lambda}$; $\lambda \leftarrow range(\lambda_{tmp}, \lambda/10, \lambda/2)$; end if end while return λ_{\min} ; failed search





Wolfe linesearch

(3/3)

Algorithm (Wolfe linesearch

$$\begin{array}{l} \textit{REFINE:} \\ \{\lambda_{lo}, \mathsf{f}_{lo}, \nabla \mathsf{f}_{lo}\} \leftarrow \{\lambda, \mathsf{f}_{\lambda}, \nabla \mathsf{f}_{\lambda}\}; \ \Delta \leftarrow \lambda_p - \lambda_{lo}; \\ \textit{while } \Delta > \epsilon \textit{ do} \\ \delta \lambda \leftarrow \Delta^2 \nabla \mathsf{f}_{lo} / \big[2(\mathsf{f}_{lo} + \nabla \mathsf{f}_{lo} \Delta - \mathsf{f}_p) \big]; \\ \delta \lambda \leftarrow range(\delta \lambda, 0.2 \Delta, 0.8 \Delta); \\ \lambda \leftarrow \lambda_{lo} + \delta \lambda; \ \mathsf{f}_{\lambda} \leftarrow \mathsf{f}(x + \lambda p); \\ \textit{if } \mathsf{f}_{\lambda} \leq \mathsf{f}_0 + \lambda c_1 \nabla \mathsf{f}_0 \textit{ then} \\ \nabla \mathsf{f}_{\lambda} \leftarrow \nabla \mathsf{f}(x + \lambda p)p; \\ \textit{if } \nabla \mathsf{f}_{\lambda} \geq c_2 \nabla \mathsf{f}_0 \textit{ then return } \lambda; \qquad \textit{found Wolfe point!} \\ \{\lambda_{lo}, \mathsf{f}_{lo}, \nabla \mathsf{f}_{lo}\} \leftarrow \{\lambda, \mathsf{f}_{\lambda}, \nabla \mathsf{f}_{\lambda}\}; \ \Delta \leftarrow \Delta - \delta \lambda; \\ \textit{else} \\ \{\lambda_p, \mathsf{f}_p\} \leftarrow \{\lambda, \mathsf{f}_{\lambda}\}; \ \Delta \leftarrow \delta \lambda; \\ \textit{end if} \\ \textit{end while} \\ \textit{return } \lambda; \textit{ failed search} \end{array}$$



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J. Stoer and R. Bulirsch Introduction to numerical analysis Springer-Verlag, Texts in Applied Mathematics, **12**, 2002.

J. E. Dennis, Jr. and Robert B. Schnabel Numerical Methods for Unconstrained Optimization and Nonlinear Equations SIAM, Classics in Applied Mathematics, 16, 1996.

