14. Newton’s method

- local convergence
- Kantorovich theorem
- inexact Newton method
Newton’s method for nonlinear equations

Newton iteration for solving a nonlinear equation \( f(x) = 0 \):

\[
x^{(k+1)} = x^{(k)} - f'(x^{(k)})^{-1} f(x^{(k)})
\]

- \( f : \mathbb{R}^n \to \mathbb{R}^n \) is a vector valued function \( f(x) = (f_1(x), \ldots, f_n(x)) \)
- \( f'(x) \) is the \( n \times n \) Jacobian matrix at \( x \):
  \[
  (f'(x))_{i,j} = \frac{\partial f_i}{\partial x_j}(x), \quad i, j = 1, \ldots, n
  \]
- \( x^{(k+1)} \) is the solution of the linearized equation at \( x^{(k)} \):
  \[
  f(x^{(k)}) + f'(x^{(k)})(x - x^{(k)}) = 0
  \]

we denote the iterates by the simpler notation \( x_k = x^{(k)} \) if the meaning is clear
Matrix norm

in this lecture, *operator norms* are used for square matrices:

\[ \|A\| = \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|} \]

the same (arbitrary) vector norm is used for \(\|Ax\|\) and \(\|x\|\)

**Properties** (*A, B are *n* × *n* matrices and *x* is an *n*-vector)

- *identity matrix*: \(\|I\| = 1\)
- *matrix–vector product*: \(\|Ax\| \leq \|A\|\|x\|\)
- *submultiplicative property*: \(\|AB\| \leq \|A\|\|B\|\)
- *perturbation lemma*: if *A* is invertible and \(\|A^{-1}B\| < 1\), then \(A + B\) is invertible,

\[ \|(A + B)^{-1}\| \leq \frac{\|A^{-1}\|}{1 - \|A^{-1}B\|} \]
Proof of perturbation lemma

• $A + B$ is invertible: if $(A + B)x = 0$, then

$$
\|x\| = \|A^{-1}Bx\| \leq \|A^{-1}B\|\|x\|
$$

if $\|A^{-1}B\| < 1$ this is only possible if $x = 0$

• $Y = (A + B)^{-1}$ satisfies $(I + A^{-1}B)Y = A^{-1}$; therefore

$$
\|Y\| = \|A^{-1} - A^{-1}BY\| \leq \|A^{-1}\| + \|A^{-1}BY\| \leq \|A^{-1}\| + \|A^{-1}B\|\|Y\|
$$

from which the inequality in the lemma follows

Newton’s method 14.4
**Lipschitz property**

**Lipschitz continuity of Jacobian**

\[ \| f'(x) - f'(y) \| \leq \beta \| x - y \| \quad \text{for all } x, y \in D \]

- $\beta$ is a positive constant, $D$ is an open convex set
- a common assumption in convergence theory of Newton's method

**Two consequences**

- deviation from linear approximation:
  \[ \| f(y) - f(x) - f'(x)(y - x) \| \leq \frac{\beta}{2} \| x - y \|^2 \quad \text{for all } x, y \in D \quad (1) \]

- distance between function values:
  \[ \| f(y) - f(x) \| \leq \| f'(x) \| \| y - x \| + \frac{\beta}{2} \| y - x \|^2 \quad \text{for all } x, y \in D \quad (2) \]

(proofs on next page)
Proof

• inequality (1):

\[ f(y) - f(x) - f'(x)(y - x) = \int_0^1 (f'(x + t(y - x)) - f'(x)) (y - x) \, dt \]

\[ \|f(y) - f(x) - f'(x)(y - x)\| \leq \int_0^1 \|f'(x + t(y - x)) - f(x)\| (y - x) \, dt \]

\[ \leq \|y - x\| \int_0^1 \|f'(x + t(y - x)) - f(x)\| \, dt \]

\[ \leq \beta \|y - x\|^2 \int_0^1 t \, dt \]

\[ = \frac{\beta}{2} \|y - x\|^2 \]

• inequality (2):

\[ \|f(y) - f(x)\| \leq \|f'(x)(y - x)\| + \|f(y) - f(x) - f'(x)(y - x)\| \]

\[ \leq \|f'(x)\| \|y - x\| + \frac{\beta}{2} \|y - x\|^2 \]
Outline

- local convergence
- Kantorovich theorem
- inexact Newton method
Assumptions

- there exists a solution $x^*$

- $f'(x^*)$ is invertible with $\|f'(x^*)^{-1}\| \leq \alpha$

- $f'$ is Lipschitz continuous on $D = \{x \mid \|x - x^*\| < \rho\}$:
  $$\|f'(x) - f'(y)\| \leq \beta\|x - y\| \quad \text{for all } x, y \in D$$

- the starting point $x_0$ is in $D$ and sufficiently close to $x^*$:
  $$\alpha \beta\|x_0 - x^*\| \leq \frac{1}{2}$$
Local convergence

\[ x_{k+1} = x_k - f'(x_k)^{-1} f(x_k), \quad k = 0, 1, \ldots \]

under the assumptions on the previous page:

- the iteration is well defined, i.e., the Jacobian matrices \( f'(x_k) \) are invertible
- the iterates converge quadratically to \( x^* \):

\[ ||x_{k+1} - x^*|| \leq \alpha \beta ||x_k - x^*||^2 \]

hence,

\[ \alpha \beta ||x_k - x^*|| \leq (\alpha \beta ||x_0 - x^*||)^2 \leq \left( \frac{1}{2} \right)^{2^k} \]
Proof: suppose \( x_k \in D \) and \( \alpha \beta \| x_k - x^\star \| \leq 1/2 \)

1. \( f'(x_k) \) is invertible and \( \| f'(x_k)^{-1} \| \leq 2\alpha \)
   
   this follows from the perturbation lemma with \( A = f'(x^\star) \), \( B = f'(x_k) - f(x^\star) \):
   
   \[
   \| A^{-1}B \| \leq \| f'(x^\star)^{-1} \| \| f'(x_k) - f(x^\star) \| \leq \alpha \beta \| x_k - x^\star \| \leq 1/2
   \]
   
   and therefore
   
   \[
   \| f'(x_k)^{-1} \| = \| (A + B)^{-1} \| \leq \frac{\| A^{-1} \|}{1 - \| A^{-1}B \|} \leq 2\alpha
   \]

2. \( \| x_{k+1} - x^\star \| \leq \alpha \beta \| x_k - x^\star \|^2 \)
   
   this follows from the Lipschitz continuity of \( f' \) (inequality (1)) and part 1:
   
   \[
   \| x_{k+1} - x^\star \| = \| x_k - f'(x_k)^{-1} f(x_k) - x^\star \|
   \]
   
   \[
   = \| f'(x_k)^{-1} (f(x^\star) - f(x_k) - f'(x_k)(x^\star - x_k)) \| \leq \| f'(x_k)^{-1} \| \| f(x^\star) - f(x_k) - f'(x_k)(x^\star - x_k) \| \leq \alpha \beta \| x_k - x^\star \|^2
   \]

3. since \( \| x_{k+1} - x^\star \| \leq \| x_k - x^\star \| \), we have \( x_{k+1} \in D \) and \( \alpha \beta \| x_{k+1} - x^\star \| \leq 1/2 \)
Outline

- local convergence
- Kantorovich theorem
- inexact Newton method
Motivation

**Local convergence result:** convergence if $x_0$ is sufficiently close to a solution

$$
\|x_0 - x^*\| \leq \frac{1}{2\alpha \beta}
$$

- $x^*$ and $\alpha$ (upper bound on $\|f'(x^*)^{-1}\|$) are unknown
- assumes there exists a solution

**Kantorovich theorem:** a “semi-local” convergence result

- convergence conditions in terms of properties at the starting point
- existence of a solution is a consequence of the theorem, not an assumption
Assumptions in Kantorovich theorem

- the Jacobian is Lipschitz continuous on an open convex set $D$:

$$\|f'(x_0)^{-1}(f'(x) - f'(y))\| \leq \gamma \|x - y\| \quad \text{for all } x, y \in D$$

- the Jacobian matrix $f'(x_0)$ at the starting point $x_0 \in D$ is invertible

- the norm $\eta := \|f'(x_0)^{-1}f(x_0)\|$ of the first Newton step is bounded by

$$\eta \gamma \leq \frac{1}{2}$$

- $D$ contains the ball $B(x_0, r) = \{x \mid \|x - x_0\| \leq r\}$, where

$$r = \frac{1 - \sqrt{1 - 2\gamma \eta}}{\gamma}$$
Kantorovich theorem

\[ x_{k+1} = x_k - f'(x_k)^{-1} f(x_k), \quad k = 0, 1, \ldots \]

under the assumptions on the previous page:

- the iteration is well defined, i.e., the Jacobian matrices \( f'(x_k) \) are invertible
- the iterates remain in \( B(x_0, r) \)
- the iterates converge to a solution \( x^\ast \) of \( f(x) = 0 \)
- the following error bound holds:

\[ \|x_k - x^\ast\| \leq \frac{(2\gamma \eta)^{2^{k-1}}}{2^{k-1}} \eta \]
Comments

- this is the affine-invariant version of the theorem: invariant under transformation

\[ \tilde{f}(x) = Af(x), \quad A \text{ nonsingular} \]

- one can take \( \gamma = \beta \|f(x_0)^{-1}\| \), with \( \beta \) on page 14.5, but \( \beta \) is not affine-invariant

- the complete theorem includes uniqueness of solution in a larger region

- theorem explains very fast local convergence; for example, if \( \gamma \eta = 0.4 \)

<table>
<thead>
<tr>
<th>( k )</th>
<th>((2\gamma \eta)^{2^k-1}/2^{k-1})</th>
</tr>
</thead>
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<tr>
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<td>1</td>
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<td>2</td>
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<td>0.0000000245199287000000000000000</td>
</tr>
<tr>
<td>7</td>
<td>0.0000000000000077000000000000000</td>
</tr>
</tbody>
</table>
Newton method for quadratic scalar equation

we first examine the convergence of Newton’s method applied to $g(t) = 0$, where

$$g(t) = \frac{\gamma}{2} t^2 - t + \eta \quad \text{with } \gamma > 0, \ \eta > 0, \ h := \gamma \eta \leq \frac{1}{2}$$

- the roots will be denoted by $t^*$ and $t^{**}$

$$t^* = \frac{1 - \sqrt{1 - 2h}}{\gamma}, \quad t^{**} = \frac{1 + \sqrt{1 - 2h}}{\gamma}$$

- the Newton iteration started at $t_0 = 0$ is

$$t_{k+1} = \frac{(\gamma/2)t_k^2 - \eta}{\gamma t_k - 1}$$
Newton iteration can be written as \( t_{k+1} = \psi(t_k) \) where

\[
\psi(t) = \frac{(\gamma/2)t^2 - \eta}{\gamma t - 1}
\]

\[
\gamma = 1, \quad \eta = h = 3/8
\]

\[
\gamma = 1, \quad \eta = h = 1/2
\]
Recursions

to derive simple error bounds, we define $g_k(\tau)$ as $g(t)$ scaled and centered at $t_k$:

$$g_k(\tau) = \frac{g(\tau + t_k)}{-g'(t_k)} = \frac{\gamma_k}{2} \tau^2 - \tau + \eta_k, \quad k = 0, 1, \ldots$$

- coefficients $\gamma_k, \eta_k$, and $h_k = \gamma_k \eta_k$ satisfy the recursions (see next page)

$$\gamma_{k+1} = \frac{\gamma_k}{1 - h_k}, \quad \eta_{k+1} = \frac{h_k \eta_k}{2(1 - h_k)}, \quad h_{k+1} = \frac{h_k^2}{2(1 - h_k)^2}$$

with $\gamma_0 = \gamma, \eta_0 = \eta, h_0 = \gamma \eta$

- we denote the smallest root of $g_k$ by $r_k$:

$$r_k = t^* - t_k = \frac{1 - \sqrt{1 - 2h_k}}{\gamma_k} = \frac{2\eta_k}{1 + \sqrt{1 - 2h_k}}$$

- Newton step for $g_k$ at $\tau = 0$ is equal to Newton step for $g$ at $t = t_k$:

$$\eta_k = t_{k+1} - t_k$$
Proof of recursions

• since $g$ is quadratic,

\[
\frac{\gamma_k}{2} \tau^2 - \tau + \eta_k = \frac{g(t_k + \tau)}{-g'(t_k)} = \frac{(g''(t_k)/2)\tau^2 + g'(t_k)\tau + g(t_k)}{-g'(t_k)}
\]

• recursion for $\gamma_k$:

\[
\gamma_{k+1} = \frac{g''(t_{k+1})}{-g'(t_k + \eta_k)} = \frac{g''(t_k)}{-g'(t_k) - g''(t_k)\eta_k} = \frac{\gamma_k}{1 - \gamma_k \eta_k} = \frac{\gamma_k}{1 - h_k}
\]

• recursion for $\eta_k$:

\[
\eta_{k+1} = \frac{g(t_k + \eta_k)}{-g'(t_k + \eta_k)} = \frac{(g''(t_k)/2)\eta_k^2}{-g'(t_k) - g''(t_k)\eta_k} = \frac{\gamma_k \eta_k^2}{2(1 - \gamma_k \eta_k)} = \frac{h_k \eta_k}{2(1 - h_k)}
\]

• recursion for $h_k$ follows from $h_{k+1} = \gamma_{k+1} \eta_{k+1}$
Error bounds

- Newton step $\eta_k = t_{k+1} - t_k$:

\[
\eta_k \leq \frac{(2h)^{2^k-1}}{2^k} \eta
\]

(see next page)

- error $r_k = t^* - t_k$:

\[
r_k = \frac{2\eta_k}{1 + \sqrt{1 - 2h_k}} \leq 2\eta_k \leq \frac{(2h)^{2^k-1}}{2^{k-1}} \eta
\]
Proof of bound on $\eta_k$

- since $h_0 \leq 1/2$ the recursion for $h_k$ shows that
  \[
  2h_k = \frac{h_{k-1}^2}{(1 - h_{k-1})^2} \leq (2h_{k-1})^2
  \]

- applying this recursively we obtain $2h_k \leq (2h_0)^{2^k}$

- from the recursion for $\eta_k$ (and $h_k \leq 1/2$):
  \[
  \eta_k = \frac{h_{k-1} \eta_{k-1}}{2(1 - h_{k-1})} \leq h_{k-1} \eta_{k-1}
  \]

- applying this recursively and using the bound on $h_k$ we obtain the bound on $\eta_k$:
  \[
  \eta_k \leq h_{k-1} \cdots h_1 h_0 \eta_0 \\
  = 2^{-k} (2h_0)^{2^{k-1}} (2h_0)^{2^{k-2}} \cdots (2h_0)^2 (2h_0) \eta_0 \\
  = 2^{-k} (2h_0)^{2^{k-1}} \eta_0
  \]
Summary of proof of Kantorovich theorem

to prove the Kantorovich theorem (pp. 14.11–14.12), we show that

\[ \| x_{k+1} - x_k \| \leq t_{k+1} - t_k \]

where \( t_k \) are the iterates in Newton’s method, started at \( t_0 = 0 \), for

\[ \frac{\gamma}{2} t^2 - t + \eta = 0 \]

- \( t_k \) is called a majorizing sequence for the sequence \( x_k \)
- the bounds for \( t_k \) on page 14.18 provide bounds and convergence results for \( x_k \)
Consequences of majorization

\[ t_0 = 0, \quad \|x_{k+1} - x_k\| \leq t_{k+1} - t_k \quad \text{for } k \geq 0 \]

- by the triangle inequality, if \( k \geq j \),
  \[ \|x_k - x_j\| \leq \sum_{i=j}^{k-1} \|x_{i+1} - x_i\| \leq \sum_{i=j}^{k-1} (t_{i+1} - t_i) = t_k - t_j \]

- the inequality shows that \( x_k \) is a Cauchy sequence, so it converges
- taking \( j = 0 \) shows that \( x_k \) remains in the set \( B(x_0, r) \) (defined on page 14.11):
  \[ \|x_k - x_0\| \leq t_k - t_0 \leq t^* = r \]

- taking limits for \( k \to \infty \) shows the error bound on page 14.12:
  \[ \|x^* - x_j\| \leq t^* - t_j = r_j \leq \frac{(2h)^{2^{j-1}}}{2j-1}\eta \]
Details of proof of Kantorovich theorem

we prove that the following inequalities hold for \( k = 0, 1, \ldots \)

\[
\| f'(x_{k+1})^{-1} f'(x_k) \| \leq \frac{1}{1 - h_k} \tag{3}
\]

\[
\| f'(x_k)^{-1} (f'(x) - f'(y)) \| \leq \gamma_k \| x - y \| \quad \text{for all } x, y \in D \tag{4}
\]

\[
\| f'(x_k)^{-1} f(x_k) \| \leq \eta_k \tag{5}
\]

\[
B(x_{k+1}, r_{k+1}) \subseteq B(x_k, r_k) \tag{6}
\]

- \( \gamma_k, \eta_k, h_k, r_k \) are the sequences defined on page 14.16
- for \( k = 0 \), inequalities (4) and (5) hold by assumption, since \( \gamma_0 = \gamma, \eta_0 = \eta \)
- (5) is the majorization inequality \( \| x_{k+1} - x_k \| \leq \eta_k = t_{k+1} - t_k \)
**Proof by induction:** suppose (4) and (5) hold at \( k = i \), and (6) holds for \( k < i \)

- \( x_{i+1} \in D \) because \( B(x_i, r_i) \subseteq \cdots \subseteq B(x_0, r_0) \subseteq D \) and \( \| x_{i+1} - x_i \| \leq \eta_i \leq r_i \)

- the inequality (4) at \( k = i \) implies that

\[
\| f'(x_i)^{-1} f'(x_{i+1}) - I \| = \| f'(x_i)^{-1} (f'(x_{i+1}) - f'(x_i)) \| \\
\leq \gamma_i \| x_{i+1} - x_i \| \\
\leq \gamma_i \eta_i \\
= h_i
\]

invertibility of \( f'(x_{i+1}) \) and (3) at \( k = i \) follow from the perturbation lemma

- inequality (4) at \( k = i + 1 \) follows from (3) and (4) at \( k = i \):

\[
\| f'(x_{i+1})^{-1} (f'(x) - f'(y)) \| \leq \| f'(x_{i+1})^{-1} f'(x_i) \| \| f'(x_i)^{-1} (f'(x) - f'(y)) \| \\
\leq \frac{\gamma_i}{1 - h_i} \| x - y \| \\
= \gamma_{i+1} \| x - y \|
\]
• Inequality (5) at \( k = i + 1 \) follows from (4) at \( k = i + 1 \): define \( v = x_{i+1} - x_i \),

\[
\left\| f'(x_{i+1})^{-1} f(x_{i+1}) \right\| = \left\| f'(x_{i+1})^{-1} \left( \int_0^1 f'(x + tv) v dt + f(x_i) \right) \right\| \\
= \left\| f'(x_{i+1})^{-1} \int_0^1 (f'(x + tv) - f'(x_i)) v dt \right\| \\
\leq ||v|| \int_0^1 \left\| f'(x_{i+1})^{-1} (f'(x + tv) - f'(x_i)) \right\| dt \\
\leq \frac{\gamma_{i+1}}{2} ||v||^2 \\
\leq \frac{\gamma_{i+1} \eta_i^2}{2} \\
= \eta_{i+1}
\]

• Inequality (6) at \( k = i \) follows from (5) at \( k = i + 1 \) and \( r_i = r_{i+1} + \eta_i \)

\[
\left\| x - x_{i+1} \right\| \leq r_{i+1} \implies \left\| x - x_i \right\| \leq \left\| x - x_{i+1} \right\| + \left\| x_{i+1} - x_i \right\| \leq r_{i+1} + \eta_i = r_i
\]
Limit

it remains to show that the limit $x^*$ solves the equation

- by the assumptions on page 14.11,

\[
\|f'(x_0)^{-1}f(x_k)\| = \|f'(x_0)^{-1}f'(x_k)(x_{k+1} - x_k)\| \\
= \|(f'(x_0)^{-1}(f'(x_k) - f'(x_0)) + I)(x_{k+1} - x_k)\| \\
\leq \left(\|f'(x_0)^{-1}(f'(x_k) - f'(x_0))\| + 1\right)\|x_{k+1} - x_k\| \\
\leq (\gamma r + 1)\|x_{k+1} - x_k\|
\]

- since $\|x_{k+1} - x_k\| \to 0$ and $f$ is continuous,

\[
\|f'(x_0)^{-1}f(x^*)\| = \lim_{k \to \infty} \|f'(x_0)^{-1}f(x_k)\| = 0
\]
Outline

- local convergence
- Kantorovich theorem
- inexact Newton method
Inexact Newton method

inexact Newton method for solving nonlinear equation \( f(x) = 0 \):

\[
x_{k+1} = x_k + s_k \quad \text{where} \quad s_k \approx -f'(x_k)^{-1}f(x_k)
\]

- \( s_k \) is an approximate solution of the Newton equation

\[
f'(x_k)s = -f(x_k)
\]

- goal is to reduce cost per iteration while retaining fast convergence

- in *Newton-iterative methods*, Newton equation is solved by iterative method

- an example is the *Newton-CG method* if \( f'(x) \) is symmetric positive definite
Forcing condition

accept the inexact Newton step $s_k$ if

$$\| f'(x_k)s_k + f(x_k) \| \leq \omega_k \| f(x_k) \|$$

- coefficient $\omega_k$ is called the forcing term
- $\omega_k$ limits relative error in the Newton equation
- provides a stopping condition in iterative method for solving Newton equation
- $\omega_k$ is constant or adjusted adaptively
Effect on local convergence

Assumptions

• the equation has a solution $x^*$ and $f'(x^*)$ is invertible with $\|f'(x^*)^{-1}\| \leq \alpha$

• $f'$ is $\beta$-Lipschitz continuous in a neighborhood of $x^*$

Local convergence result

• if $x_0$ is sufficiently close to $x^*$, the iterates $x_k$ converge to $x^*$

• the following bound holds (see next page):

$$\|x_{k+1} - x^*\| \leq \alpha \beta (1 + \omega_k) \|x_k - x^*\|^2 + \alpha \omega_k \|f'(x^*)\| \|x_k - x^*\|$$

• this shows how the forcing term determines the rate of convergence

<table>
<thead>
<tr>
<th>$\omega_k$</th>
<th>$\omega_k = 0$</th>
<th>$\omega_k$ a small constant</th>
<th>$\omega_k \downarrow 0$</th>
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<tbody>
<tr>
<td>convergence:</td>
<td>quadratic</td>
<td>linear</td>
<td>superlinear</td>
</tr>
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</table>
Proof.

\[
\|x_{k+1} - x^*\| = \|x_k + s_k - x^*\| \\
\leq \|x_k - f'(x_k)^{-1} f(x_k) - x^*\| + \|f'(x_k)^{-1} (f'(x_k) s_k + f(x_k))\| \\
\leq \alpha \beta \|x_k - x^*\|^2 + \omega_k \|f(x_k)^{-1}\| \|f(x_k)\| \\
\leq \alpha \beta \|x_k - x^*\|^2 + 2 \omega_k \alpha \|f(x_k)\| \\
\leq \alpha \beta \|x_k - x^*\|^2 + 2 \omega_k \alpha \left( \|f'(x^*)\| \|x_k - x^*\| + \frac{\beta}{2} \|x_k - x^*\|^2 \right) \\
= \alpha \beta (1 + \omega_k) \|x_k - x^*\|^2 + 2 \omega_k \alpha \|f'(x^*)\| \|x_k - x^*\|
\]

- line 3 follows from page 14.8 and the definition of $\omega_k$
- on line 4 we use the first result on page 14.9
- on line 5 we apply (2) with $y = x_k$ and $x = x^*$
References

Newton method


Kantorovich theorem: the statement and proof of the theorem in the lecture follow


Inexact Newton method