MAT 460 Numerical Differential Equations

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Lecture 7

Topics: Nonlinear Equations and Iterative Methods in $\mathbb{R}^n$

Example: Minimization problem in several variables

Problem: Find the minimum of the function

$$g : \mathbb{R}^2 \to \mathbb{R}^2, \qquad g(x) = e^{5\,x_1} + \sin^4(x_1 + 2\,x_2) + \cosh(x_2)$$

The position x where we find the minimum is a root of the gradient

$$f(x) := \nabla g(x) = \begin{bmatrix} 5\,e^{5\,x_1} + 4\sin^3(x_1 + 2\,x_2)\cos(x_1 + 2\,x_2) \\ 8\,\sin^3(x_1 + 2\,x_2)\cos(x_1 + 2\,x_2) + \sinh(x_2) \end{bmatrix}$$

We want to find a root x_* of the function $f : \mathbb{R}^2 \to \mathbb{R}^2$. And the root is a fix point of the function

$$\phi : \mathbb{R}^2 \to \mathbb{R}^2, \qquad \phi(x) = x + A(x)f(x),$$

where $A(x)$ is an invertible matrix. I. e. we can find x_*, by finding the fix points of ϕ.

Note: This is not the only method to find the position x_* where we find the minimum.

Fix point iteration in $\mathbb{R}^n$.

Let G be a subset of $\mathbb{R}^n$ and self-mapping $\phi : G \to G$.

Iteration sequence:

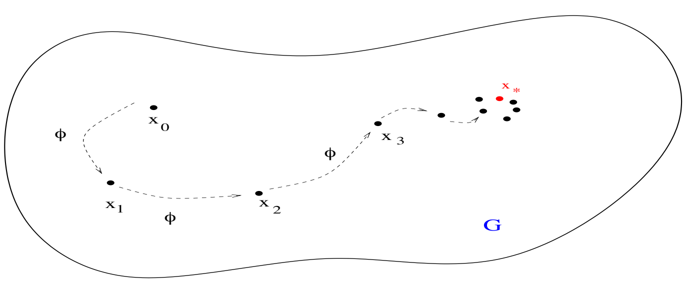
(1) Chose an initial value $x_0 \in G$.

(2) Set $x_{k+1} := \phi(x_k)$, $\quad k = 1, 2, \ldots$.

We have: If ϕ is continuous and the iteration sequence $x_0, x_1, x_2, \ldots$ converges, then the limit of the sequence is a fix point of ϕ.

Proof: Let $x_* = \lim_{k\to\infty} x_k$. Then

$$\phi(x_*) = \phi(\lim_{k\to\infty} x_k) = \lim_{k\to\infty} \phi(x_k) = \lim_{k\to\infty} x_{k+1} = \lim_{k\to\infty} x_k = x_*.$$



Attracting fix points for iterations in $\mathbb{R}^n$

Definition:

Let $G \subseteq \mathbb{R}^n$, $\phi : G \to G$ be a self-mapping and let x_* be a fix point of ϕ.
If a neighborhood $U_\epsilon = \{z \in \mathbb{R}^n \mid \|z - x_*\| < \epsilon\} \cap G$ of x_* and a constant $L < 1$ exist, such that

$$\|\phi(x) - x_*\| \le L\,\|x - x_*\| \qquad \text{for all } x \in U_\epsilon \qquad (*)$$

then x_* is called **attracting**.

Conclusion:

If a iteration sequence $x_{k+1} = \phi(x_k)$ starts in U_ϵ, then it converges to x_*, because from $(*)$ it follows that

$$\|x_k - x_*\| \le L^k\,\|x_0 - x_*\| \to 0.$$

We compute:

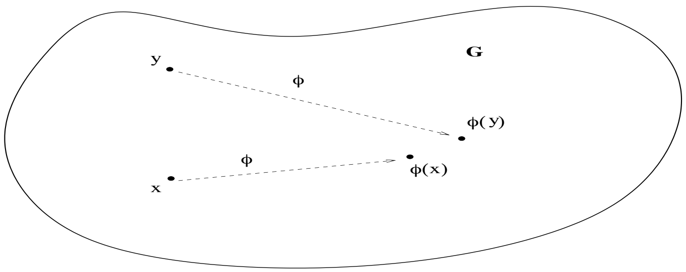
$$\begin{aligned} \|x_1 - x_*\| &= \|\phi(x_0) - x_*\| \le L\,\|x_0 - x_*\| \\ \|x_2 - x_*\| &= \|\phi(x_1) - x_*\| \le L\,\|x_1 - x_*\| \le L^2\,\|x_0 - x_*\| \\ \|x_3 - x_*\| &= \|\phi(x_2) - x_*\| \le L\,\|x_2 - x_*\| \le L^3\,\|x_0 - x_*\| \\ &\textit{etc.} \end{aligned}$$

Lipschitz-continuous maps and contractions

Let $G \subset \mathbb{R}^n$ and $\|\cdot\|$ be a norm on $\mathbb{R}^n$. A self-mapping $\phi : G \to G$ of the domain G is called **Lipschitz-continuous** (extension limited), if a constant L exist, such that

$$\|\phi(x) - \phi(y)\| \leq L\,\|x - y\| \qquad \text{for all } x, y \in G.$$

L is called **Lipschitz-Konstante**. If $L < 1$, then ϕ is called **contracting**. So that ϕ is contracting, means: The distance between the image points $\phi(x)$ and $\phi(y)$ is at least of the factor $L < 1$ smaller than the distance between the points x and y in the domain.



Banach's Fix point theorem (in $\mathbb{R}^n$)

Preliminary note: A set $G \subseteq \mathbb{R}^n$ is called **closed**, if every boundary point of G is contained in G.

Banach's Fix point theorem goes as follows:

Let G be a **closed** subset of $\mathbb{R}^n$, and let $\phi : G \to G$ be a **contracting** self-mapping with contraction constant $0 \leq L < 1$. Then

1. ϕ has exactly one fix point $x_* \in G$.

2. Every iteration sequence $x_{k+1} = \phi(x_k)$, $x_0 \in G$, converges to x_*

3. We have the following estimates

$$\|x_k - x_*\| \leq \frac{L}{1-L}\,\|x_k - x_{k-1}\| \qquad \text{(a posteriori)}$$

and

$$\|x_k - x_*\| \leq \frac{L^k}{1-L}\,\|x_1 - x_0\| \qquad \text{(a priori).}$$

Proof with geometric series (in the lecture).

Conclusion: The Iteration converges at least linearly to x_*.

Question: How can we find out if

- a map $\phi : G \to G$ is Lipschitz-continuous or even contracting?
- a fix point x_* of ϕ is attracting?

Answer: By computing the induced matrix norm of the Jacobi-matrix of ϕ.

Jacobi-matrix:

$$\phi'(x) = \begin{bmatrix} \frac{\partial \phi_1}{\partial x_1}(x) & \dots & \frac{\partial \phi_1}{\partial x_n}(x) \\ \vdots & & \vdots \\ \frac{\partial \phi_n}{\partial x_1}(x) & \dots & \frac{\partial \phi_n}{\partial x_n}(x) \end{bmatrix}$$

Norm:

$$\|\phi'(x)\| = \max_{v \neq 0} \frac{\|\phi'(x)v\|}{\|v\|} = \max_{\|v\|=1} \|\phi'(x)v\|.$$

To make meaningful statements such that ϕ is Lipschitz-continuous, etc. we need the **bound lemma** (see next slide).

Bound lemma

Note 1: The word 'lemma' is mathematics-slang for an auxiliary statement which is used in a theorem.

Note 2: The line $s_{x,y}$ which connects the points $x, y \in \mathbb{R}^n$ is the set of all $\xi \in \mathbb{R}^n$ satisfying

$$\xi = x + t\,(y - x) \qquad 0 \leq t \leq 1$$

The **bound lemma** says: Let $\phi : G \to \mathbb{R}^n$ be a continuous differentiable map. If G includes the line that connects the points $x, y \in G$, then

$$\|\phi(x) - \phi(y)\| \leq L\,\|x - y\|, \qquad \text{where} \qquad L = \max_{\xi \in s_{x,y}} \|\phi'(\xi)\|.$$

Proof of the bound lemma:

Let $g : [0,1] \to \mathbb{R}^n$ be defined as follows:

$$g(t) := \phi(x + t\,(y-x)).$$

Chain rule gives

$$g'(t) = \underbrace{\phi'(x + t\,(y-x))}_{Matrix}\,\underbrace{(y-x)}_{Vektor}.$$

From that it follows

$$\phi(y) - \phi(x) = g(1) - g(0) = \int_0^1 g'(t)\,dt = \int_0^1 \phi'(x + t\,(y-x))\,(y-x)\,dt.$$

And further

$$\begin{aligned}
\|\phi(y) - \phi(x)\| &= \left\| \int_0^1 \phi'(x + t\,(y-x))\,(y-x)\,dt \right\| \\
&\le \int_0^1 \|\phi'(x + t\,(y-x))\,(y-x)\|\,dt \qquad \text{(general: } \|\int f(t)\,dt\| \le \int \|f(t)\|\,dt) \\
&\le \int_0^1 \|\phi'(x + t\,(y-x))\|\,\|y-x\|\,dt \\
&= \int_0^1 \|\phi'(x + t\,(y-x))\|\,dt \quad \|y-x\| \\
&= \|\phi'(x + \theta\,(y-x))\| \quad \|y-x\| \qquad \theta \in [0,1] \qquad \text{(mean value theorem)} \\
&= \|\phi'(\xi)\| \quad \|y-x\|, \qquad \xi = x + \theta\,(y-x) \in s_{x,y}.
\end{aligned}$$

1. Conclusion from the bound lemma

Let $G \subset \mathbb{R}^n$ be a closed domain, which contains together each two points x, y also the line connecting these two points (such a region is called **convex**). Also let $\phi : G \to G$ be continuously differentiable. Assume $L > 0$ is an upper bound for the norm of the derivative ϕ', i. e.

$$\|\phi'(\xi)\| \le L \qquad \text{for all } \xi \in G$$

Then ϕ is Lipschitz-continuous with Lipschitz-constant L, i.e˙

$$\|\phi(x) - \phi(y)\| \le L\,\|x-y\| \qquad \text{for all } x, y \in G.$$

If $L < 1$, then ϕ is contracting. If in addition G is closed, then the prerequisites for Banach's fix point theorem are satisfied, and exactly one fix point x_* exist, to which each iteration converges.

2. Conclusion from the bound lemma

Let $\phi : G \to G$ be continuous differentiable with fix point x_* and

$$\|\phi'(x_*)\| < L.$$

ϕ' is continuous, so a neighborhood $U \subset G$ of x_* exist, such that

$$\|\phi'(x)\| < L \qquad \text{for all } x \in U.$$

If U contains the line connecting x and x_*, then it follows that

$$\|\phi(x) - x_*\| \le \|\phi(x) - \phi(x_*)\| \le L\,\|x - x_*\|.$$

If U is convex, i. e. contains all connecting lines, and we have $L < 1$, then the fix point is attracting.

Theorem on second order convergence

Let $\phi : G \to G$ be 2-times continuously differentiable with fix point x_* and

$$\phi'(x_*) = 0.$$

Then a neighborhood U of x_* exist which satisfies:
Every iteration sequence $x_{k+1} = \phi(x_k)$ with initial value $x_0 \in U$ converges to x_*, and a constant C exist, such that

$$\|x_{k+1} - x_*\| \le C\,\|x_k - x_*\|^2.$$

Root-finding problem in $\mathbb{R}^n$ and the Newton-method

Given: $G \subseteq \mathbb{R}^n$ and $f : G \to \mathbb{R}^n$ with root x_*.

Problem: Find x_*.

Equivalent equation:

$$x_* = \phi(x_*), \qquad \text{wobei} \qquad \phi(x) = x + B(x)\, f(x)$$

with a matrix $B(x) \in \mathbb{R}^{n\times n}$, $det(B(x)) \neq 0$.
For

$$B(x) = -f'(x)^{-1}$$

The corresponding iteration method converges with second order.
Because $\phi'(x_*) = 0$. The corresponding iteration step is

$$x_{k+1} = x_k - f'(x_k)^{-1}\, f(x_k).$$

This is the **Newton-method in** $\mathbb{R}^n$.

However, **prerequisite for second order convergence** is $det(f'(x_*)) \neq 0$.
Note that even without this the sequence can converge fast to x_*.

Disadvantage of the method: We have to compute or approximage $f'(x)$.
Often the method converges only if the initial value is close to the root.

In the literature many variants and improvements of the Newton-method are proposed, e. g. the damped: $x_{k+1} = x_k - \lambda(x_k)\, f'(x_k)^{-1}\, f(x_k), \qquad \lambda(x_k) \in (0, 1).$

Iterative solution methods for linear equation systems

Given: $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$.

Problem: Find x_*, such that $Ax_* = b$.

Equivalent equation:

$$x_* = \phi(x_*), \qquad \text{where} \qquad \phi(x) = x + B^{-1}(b - Ax)$$

with an invertible matrix $B \in \mathbb{R}^{n\times n}$. We have

$$x = \phi(x) \qquad \Leftrightarrow \qquad b - Ax = 0 \qquad x = x_*$$

The problem: How do we choose B, such that the iteration sequence

$$x_{k+1} = \phi(x_x) = x_k + B^{-1}(b - Ax_k)$$

converges (fast) for every initial value x_0?
A good choice of B depends on A.

Another criteria for the choice of B:
Equation systems with a matrix B should be easier to solve than equation systems with A, otherwise it would not be worthwhile, since we have to compute $B^{-1}(b - Ax)$.
In particular the choice $B = A$ does not make sense.

When does an iterative method converge to the solution of a linear equation system?

Iterative methods for the solution of $Ax = b$: $\quad x_{k+1} = \phi(x_k)$, where

$$\phi(x) = x + B^{-1}(b - Ax) = \underbrace{(I - B^{-1}A)}_{C}x + B^{-1}b$$

Whe have

$$\phi(x) - \phi(y) = (Cx + B^{-1}b) - (Cy + B^{-1}b) = C(x - y) \qquad (*)$$

In particular fo x_*:

$$\phi(x) - x_* = \phi(x) - \phi(x_*) = C(x - x_*) \qquad (**)$$

From $(*)$ and $(**)$ follows for every vector norm and its corresponding matrix norm:

$$\|\phi(x) - \phi(y)\| \leq \|C\|\,\|y - x\|, \qquad \|\phi(x) - x_*\| \leq \|C\|\,\|(x - x_*)\|$$

Conclusion: Convergence of the method is guaranteed, when the induced matrix norm satisfies the inequality $\|C\| < 1$.

We also have a criteria which does not depend on a norm.

Theorem The method converges if and only if for every initial value x_0 and every right side b to x_*, if all eigenvalues of C have an absolute value of smaller than 1.

Proof idea: From $(**)$ follows $x_{k+1} - x_* = C^k(x_0 - x_*)$.
When all eigenvalues of C are absolute smaller than 1,
then the matrix sequence C^k converges to the zero matrix.

Implementation and the main important examples:

Iteration step: $x_{k+1} = x_k + B^{-1}(b - Ax_k)$

Practically, we compute x_{k+1} in 2 steps:

$$\begin{aligned} \text{Solve } B\,d &= Ax_k - b \\ \text{Set } x_{k+1} &= x_k - d, \end{aligned}$$

We can choose the matrix B as:

- $B = \text{diag}(a_{11}, \ldots, a_{nn}) \to$ Jacobi-Verfahren
- $B = \begin{bmatrix} \frac{a_{11}}{\omega} & & & 0 \\ a_{21} & \frac{a_{22}}{\omega} & & \\ \vdots & \ddots & \ddots & \\ a_{n1} & \cdots & a_{n,n-1} & \frac{a_{nn}}{\omega} \end{bmatrix} \to$ relaxed Gauss-Seidel-method

The Jacobi-method converges for strictly diagonal dominant matrices, i. e. for matrices A, which satisfy

$$|a_{jj}| > \sum_{k \neq j} |a_{k,j}| \qquad \text{for all } j.$$

The relaxed Gauss-Seidel-method converges for symmetric and positiv definite matrices, when the relaxation parameter satisfies: $0 < \omega < 2$.