NTNU

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TMA4125 Matematikk 4N

Numerical Solution of Nonlinear Equations

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Introduction.

We know that quadratic equations of the form

$$ax^2 + bx + c = 0$$

have the roots (or solutions) $r^{\pm} = \dfrac{-b \pm \sqrt{d^2 - 4ac}}{2a}$

More generally, for a given function f we want to consider the equation

$$f(x) = 0. \tag{1}$$

A solution x^* of (1) is called a root to the equation.

Challenge. In many applications, we encounter equations for which we do not have a simple solution formula as for quadratic functions.
In fact, an analytical solution might not even exist!
$\Rightarrow$ Develop numerical techniques to solve (1).

Scalar and systems of equations

We consider scalar equations first, i. e. $f : \mathbb{R} \to \mathbb{R}$, or with just one equation and variable, for example

$$x^3 + x^2 - 3x = 3.$$

Later we will also consider systems of equations, for example

$$\begin{aligned} x\mathrm{e}^y &= 1, \\ -x^2 + y &= 1. \end{aligned}$$

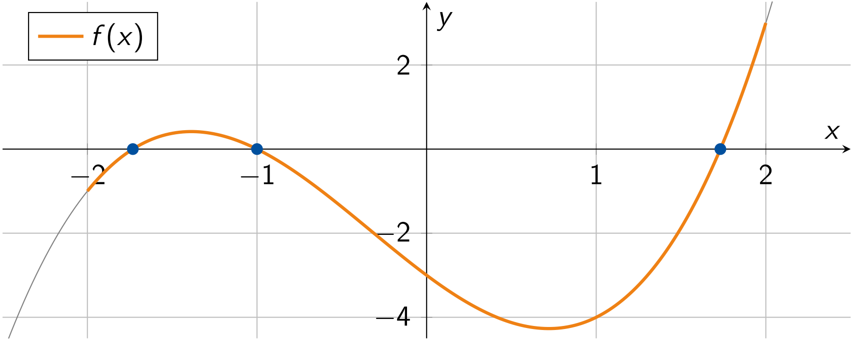
We can write this also as a functions $f : \mathbb{R}^n \to \mathbb{R}^n$, which in this example would be $n = 2$ and

$$f(x, y) = \begin{pmatrix} x\mathrm{e}^y - 1 \\ -x^2 + y - 1 \end{pmatrix} \quad \text{and we want to solve} \quad f(x, y) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Scalar equations

Let $f : [a, b] \to \mathbb{R}$ be a continuous function on some interval $[a, b]$.

Goal. Find a zero or root of f.
Let's get an intuition by plotting the function (try yourself in Python).
For example $f(x) = x^3 + x^2 - 3x - 3$ from last slide looks like



$\Rightarrow$ three real roots on $[-2, 2]$. Writing f as $f(x) = (x+1)(x^2-3)$
$\Rightarrow x_1^* = -1$, $x_{2,3}^* = \pm\sqrt{3}$.

Existence and uniqueness of solutions

Theorem. Let $f \in C[a,b]$ be given.

1. if $f(a)$ and $f(b)$ are of different sign, then there exists at lesat one $r \in (a,b)$ such that $f(r) = 0$
   Trick. the condition of different sign is $f(a)f(b) < 0$ in short.
2. The solution is unique if $f \in C^1[a,b]$ and $f'(x) < 0$ or $f'(x) > 0$ for all $x \in (a,b)$.

Bisection method

First part of the theorem already provides a very intuitive algorithm: Divide $[a, b]$ into two parts $[a, c], [c, b]$, check in which half the zero is and continue there.

Algorithm.

Input a function f and an interval, such that $f(a)f(b) < 0$

1. Set $a^{(0)} = a$, $b^{(0)} = b$
2. For $k = 0, 1, 2, \ldots$
   - $c^{(k)} = \dfrac{a^{(k)} + b^{(k)}}{2}$
   - Set the next interval to

$$[a^{(k+1)}, b^{(k+1)}] = \begin{cases} [a^{(k)}, c^{(k)}] & \text{if } f(a^{(k)})f(c^{(k)}) < 0 \\ [c^{(k)}, b^{(k)}] & \text{if } f(c^{(k)})f(b^{(k)}) < 0. \end{cases}$$

Idea. $c^{(k)}$ approximates the root r, note that $|c^{(k)} - r| \leq \frac{b^{(k)} - a^{(k)}}{2}$

We can stop if $\frac{b^{(k)} - a^{(k)}}{2}$ is small enough or if $f(c^{(k)})$ is zero.

Bisection method – exercises and summary

Exercises.

- Choose appropriate intervals and find the other two roots of f
- Compute the solution(s) of $x^2 + sin(x) - 0.5 = 0$ using the bisection method
- Given the interval $[1.5, 2]$. How many iterations are required to guarantee that the error $|c^{(k)} - r|$ is less than 10^{-4}

Summary.
The bisection method is very robust but not particularly fast.

Fix point iterations

A major class of iteration schemes are the so-called fix point iterations.

General Idea. Given an equation $f(x) = 0$ with root r.
Rewrite the equation

$$f(x) = 0$$

to a a fix point form $x = g(x)$, i. e. construct a function g such that the root x^* of f is a fixed point of g, that is x^* satisfies

$$x^* = g(x^*).$$

Algorithm.

Input Given a function g and a starting value $x^{(0)}$

1. For $k = 0, 1, 2, \ldots$ compute

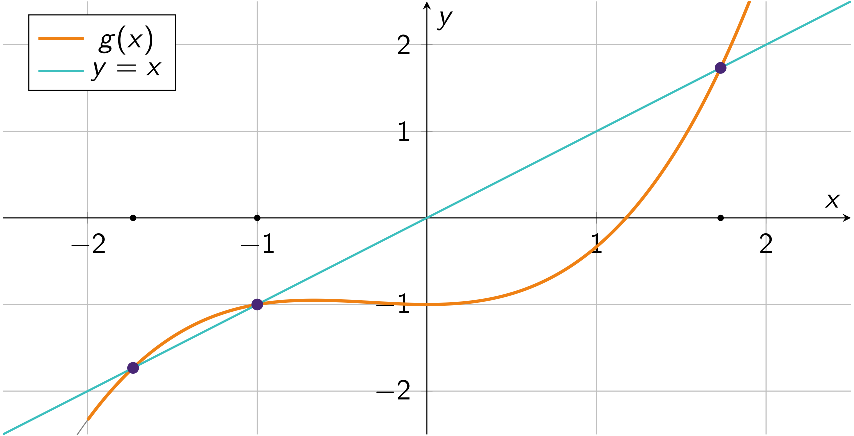
$$x^{(k+1)} = g(x^{(k)}).$$

Example. Fixed point equation

We rewrite

$$f(x) = x^3 + x^2 - 3x - 3 = 0 \quad \text{to} \quad x = \frac{x^3 + x^2 + 3}{3} = g(x).$$

Interpretation: Fixed points are intersections of $g(x)$ with $y = x$.

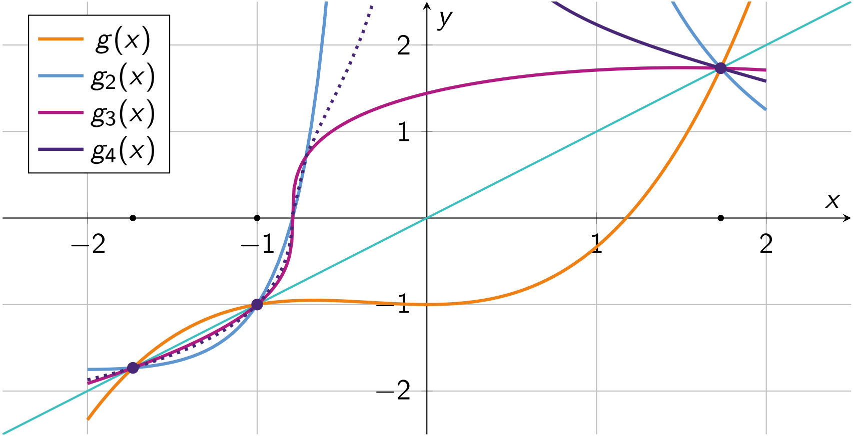


Example. Fixed point equation (cont.)

Exercise. Repeat the experiment with $x^{(0)} = 1.5$ and

$$g_2(x) = \frac{-x^2+3x+3}{x^2}, \quad g_3(x) = \sqrt[3]{3+3x-x^2}, \quad g_4(x) = \sqrt{\frac{3+3x-x^2}{x}}$$

Interpretation: Fixed points are intersections of $g(x)$ with $y = x$.



Existence and uniqueness for fix point iteration

We can adapt the previous Theorem on the equation $f(x) = x - g(x) = 0$

Theorem. Let $g \in C[a, b]$

1. if $a < g(x) < b$ for all $x \in (a, b)$ then g has at least one fixed point x^*
2. if $g \in C^1[a, b]$ and $|g'(x)| < 1$ for all $x \in [a, b]$ then the fixed point x^* is unique.

We write the assumption $a < g(x) < b$ for all $x \in [a, b]$
as $g([a, b]) \subset (a, b)$.

Convergence of fix the point iteration

We denote the error after k iterations as $e^{(k)} = x^* - x^{(k)}$.

The iteration converges if $e^{(k)} \to 0$ as $k \to \infty$.
Under which conditions is this the case?

Here's a trick we will use: For any k we have

$$\begin{aligned} x^{(k+1)} &= g(x^{(k)}), && \text{the iterations} \\ x^* &= g(x^*) && \text{the fixed point.} \end{aligned}$$

Now use the last Theorem from the preliminaries (that generalised Rolle's theorem)

$$|e^{(k+1)}| = |x^* - x^{(k+1)}| = |g(x^*) - g(x^{(k)})| = |g'(\xi_k)| \cdot |x^* - x^{(k)}| = |g'(\xi_k)| \cdot |e_k|$$

where ξ_k is some unknown value between $x^{(k)}$ (known) and x^* (unknown).

The fix point theorem

Theorem. If there is an interval $[a, b]$ such that $g \in C^1[a, b]$, $g([a, b]) \subset (a, b)$ and there exist a positive constant $L < 1$ such that $|g'(x)| \leq L < 1$ for all $x \in [a, b]$, then

- g has a unique fixed point r in (a, b).
- The fixed point iterations $x^{(k+1)} = g(x^{(k)})$ converges towards x^* for all starting values $x^{(0)} \in [a, b]$.

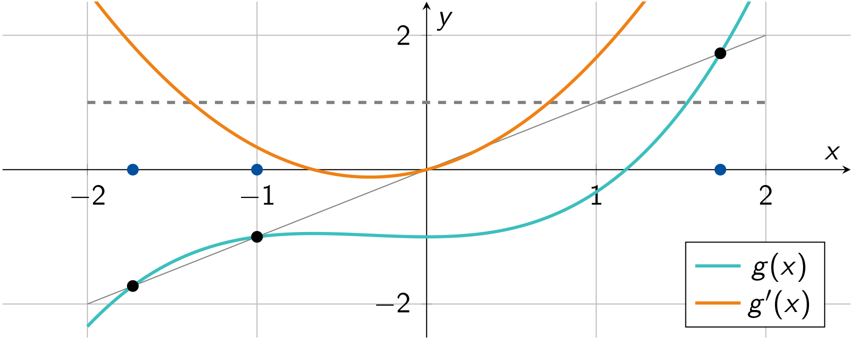
The property $g([a, b]) \subset (a, b)$ guarantees that if $x^{(0)} \in [a, b]$ then $x^{(k)} \in (a, b)$, for $k = 1, 2, \ldots$.
The condition $|g'(x)| \leq L < 1$ guarantees convergence towards the unique fixed point x^*, since

$$|e^{(k+1)}| \leq L|e^{(k)}| \quad \Rightarrow \quad |e^{(k)}| \leq L^k\, |e^{(0)}| \to 0 \quad \text{as } k \to \infty.$$

since $L^k \to 0$ as $k \to \infty$ due to $L < 1$ (also called linear convergence).

Example. The fix point interation (cont. II)

$$g(x) = \frac{x^3 + x^2 - 3}{3}, \qquad g'(x) = \frac{3x^2 + 2x}{3}$$



Exercise. How large can we make $[-0.7, 1.3]$ still having convergence? Check the same conditions for g_2, g_3, g_4.

Newton's method

Since a small $g'(x^*)$ is preferable and we can choose g
$\Rightarrow$ can we choose g such that $g'(x^*) = 0$?

We use $x^{(k)} = x^* - e^{(k)}$ and a Taylor expansion (around x^*)

$$\begin{aligned} e^{(k+1)} &= x^* - x^{(k+1)} = g(x^*) - g(x^{(k)}) = g(x^*) - g(x^* - e^{(k)}) \\ &= -g'(x^*)e^{(k)} + \frac{1}{2}g''(\xi_k)\left(e^{(k)}\right)^2 \end{aligned}$$

Let's choose $g'(x^*) = 0$ and assume that we have a constant M such that $|g''(x)|/2 \leq M$. Then

$$|e^{(k+1)}| \leq M|e^{(k)}|^2$$

Also known as quadratic convergence.

How to find our favourite fix point equation.

Question. Given an equation

$$f(x) = 0$$

with an unknown solution x^*.
Can we find a g with fixed point x^* and $g'(x^*) = 0$?
Idea. Note that for any $h(x)$ we have due to $f(x^*) = 0$ that

$$g(x) = x - h(x)f(x)$$

has a fixed point x^*. The derivate reads

$$g(x) = 1 - h'(x)f(x) - h(x)f'(x)$$

and at the fixed point

$$g'(x^*) = 1 - h(x^*)f'(x^*).$$

Choose $h(x) = 1/f'(x)$ we achieve $g'(x^*) = 0$.

Newton's method. Algorithm

Algorithm.

Input a function f, its derivative f', and a start point $x^{(0)}$.

1. For $k = 0, 1, 2, \ldots$ compute

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

Error analysis

We constructed the method to give quadratic convergence

$$|e^{(k+1)}| \leq M\left|e^{(k)}\right|^2,$$

where $e^{(k)} = x^* - x^{(k)}$.
But under which conditions can we say something about the size of M?

Let's compare the Taylor series around x^* with Newton's method

$$0 = f(x^{(k)}) + f'(x^{(k)})(x^* - x^{(k)}) + \frac{1}{2}f''(\xi_k)(x^* - x^{(k)})^2 \quad \text{(Taylor series)}$$
$$0 = f(x^{(k)}) + f'(x^{(k)})(x^{(k+1)} - x^{(k)}), \quad \text{(Newton's method)}$$

where ξ_k is between x^* and $x^{(k)}$. Subtracting both yields

$$f'(x^{(k)})(x^* - x^{(k+1)}) + \frac{1}{2}f''(\xi_k)(x^* - x^{(k)})^2 = 0 \quad \Rightarrow \quad e^{(k+1)} = -\frac{1}{2}\frac{f''(\xi_k)}{f'(x^{(k)})}\left(e^{(k)}\right)^2$$

$\Rightarrow$ we need $f'(x^{(k)}) \neq 0$, $f \in C^2[a, b]$ and $x^{(0)}$ sufficiently close to x^*.

Convergence of Newton's method

Theorem. Assume that the function f has a root x^*, and let $I_\delta = [x^* - \delta, x^* + \delta]$ for some $\delta > 0$.
Assume further that

- $f \in C^2(I_\delta)$.
- There is a $M > 0$ such that $\left|\dfrac{f''(y)}{f'(x)}\right| \leq 2M, \quad$ for all $x, y \in I_\delta$.

In this case, Newton's method converges quadratically,

$$|e^{(k+1)}| \leq M|e^{(k)}|^2$$

for all starting values satisfying $|x^{(0)} - x^*| \leq \min\{1/M, \delta\}$.

Exercises.

- Repeat the example with different $x^{(0)}$ to find the two other roots.
- Verify quadratic convergence numerically (remember the EOC!).
- Solve $x(1 - \cos(x)) = 0$, both by the bisection and Newton's method, $x^{(0)} = 1$. What difference do you observe?

Systems of equations

Instead of one function f with one variable x we now consider

Systems of nonlinear equations.

$$\begin{aligned} f_1(x_1, x_2, \dots, x_n) &= 0 \\ f_2(x_1, x_2, \dots, x_n) &= 0 \\ &\vdots \\ f_n(x_1, x_2, \dots, x_n) &= 0 \end{aligned}$$

We can write this in short as

$$\boldsymbol{f}(\boldsymbol{x}) = 0,$$

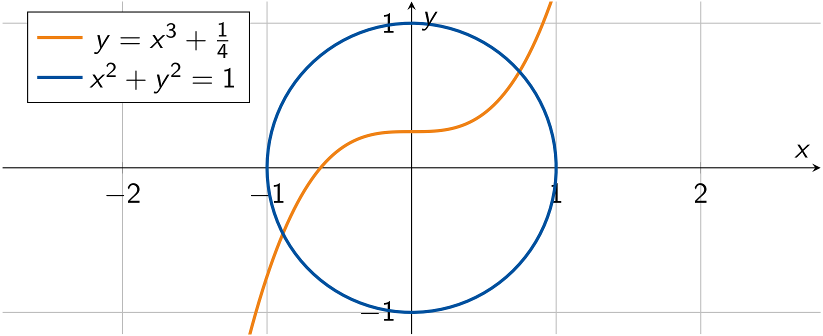
where $\boldsymbol{f} : \mathbb{R}^n \to \mathbb{R}^n$.

Example.

Example. Consider the two equations

$$x^3 - y + \frac{1}{4} = 0$$
$$x^2 + y^2 - 1 = 0$$

Interpretation.
Rewrite first equation to $y = x^3 + \frac{1}{4} \Rightarrow$ solutions lie on this graph.
Second equation means $1 = x^2 + y^2 \Rightarrow$ point with distance 1 from origin



Towards Newton's method for systems of equations I

Idea. Extend fixed point iterations to systems of equations.
We concentrate on Newton's method and the case $n = 2$:

$$f(x, y) = 0$$
$$g(x, y) = 0$$

to avoid getting lost in indices.

Notation. We denote a solution (root) to these by $\boldsymbol{r} = (x^*, y^*)^{\mathrm{T}}$.
Let $\hat{\boldsymbol{x}} = (\hat{x}, \hat{y})^{\mathrm{T}}$ that approximates $\boldsymbol{r}$.

$\Rightarrow$ Search for a better approximation by linearizing $\boldsymbol{f}(\boldsymbol{x}) = 0$.
In other words: use the multivariate Taylor expansion around $\hat{\boldsymbol{x}}$

$$f(x, y) = f(\hat{x}, \hat{y}) + \frac{\partial f}{\partial x}(\hat{x}, \hat{y})(x - \hat{x}) + \frac{\partial f}{\partial y}(\hat{x}, \hat{y})(y - \hat{y}) + \dots$$
$$g(x, y) = g(\hat{x}, \hat{y}) + \frac{\partial g}{\partial x}(\hat{x}, \hat{y})(x - \hat{x}) + \frac{\partial g}{\partial y}(\hat{x}, \hat{y})(y - \hat{y}) + \dots$$

where we omit higher order terms (in "..."), which are small for $\boldsymbol{x} \approx \hat{\boldsymbol{x}}$.

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Towards Newton's method for systems of equations II

Idea. Ignore the higher order terms and solve

$$\begin{aligned} f(\hat{x},\hat{y}) + \frac{\partial f}{\partial x}(\hat{x},\hat{y})(x-\hat{x}) + \frac{\partial f}{\partial y}(\hat{x},\hat{y})(y-\hat{y}) &= 0 \\ g(\hat{x},\hat{y}) + \frac{\partial g}{\partial x}(\hat{x},\hat{y})(x-\hat{x}) + \frac{\partial g}{\partial y}(\hat{x},\hat{y})(y-\hat{y}) &= 0 \end{aligned}$$

for x and y as a better approximation (or precise: next iterate).

More compact we can write

$$\mathrm{f}(\hat{\boldsymbol{x}}) + J(\hat{\boldsymbol{x}})(\boldsymbol{x}-\hat{\boldsymbol{x}}) = 0,$$

where $J(\boldsymbol{x})$ denotes the Jacobian of $\boldsymbol{f}$ given by

$$J(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial f}{\partial x}(x,y) & \frac{\partial f}{\partial y}(x,y) \\ \frac{\partial g}{\partial x}(x,y) & \frac{\partial g}{\partial y}(x,y) \end{pmatrix}$$

Newton's method for systems of equations

Algorithm.

Input A function $\boldsymbol{f}(\boldsymbol{x})$, its Jacobian $J(\boldsymbol{x})$ and a starting value $\boldsymbol{x}^{(0)}$.

1. For $k = 0, 1, 2, \dots$
   - **1.1** Solve the linear system $J(\boldsymbol{x}^{(k)})\Delta^{(k)} = -\boldsymbol{f}(\boldsymbol{x}^{(k)})$
   - **1.2** Set $\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \Delta^{(k)}$

Note. This can be generalized to n equations with n unknowns, where the Jacobian reads

$$J(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(\boldsymbol{x}) & \frac{\partial f_1}{\partial x_2}(\boldsymbol{x}) & \cdots & \frac{\partial f_1}{\partial x_n}(\boldsymbol{x}) \\ \frac{\partial f_2}{\partial x_1}(\boldsymbol{x}) & \frac{\partial f_2}{\partial x_2}(\boldsymbol{x}) & \cdots & \frac{\partial f_2}{\partial x_n}(\boldsymbol{x}) \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n}{\partial x_1}(\boldsymbol{x}) & \frac{\partial f_n}{\partial x_2}(\boldsymbol{x}) & \cdots & \frac{\partial f_n}{\partial x_n}(\boldsymbol{x}) \end{pmatrix}$$

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Example.

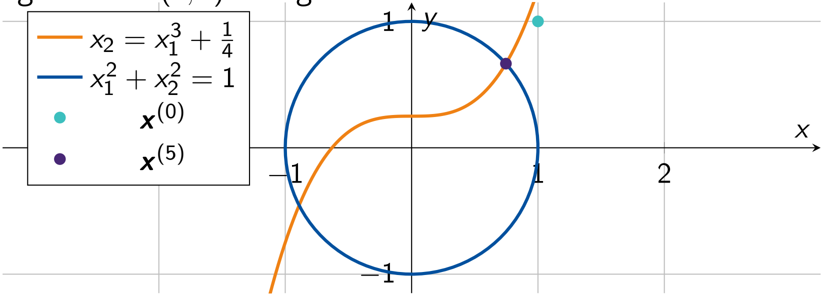
To solve our example from before

$$f(x,y) = x^3 - y + \frac{1}{4} = 0$$
$$g(x,y) = x^2 + y^2 - 1 = 0$$

we need its Jacobian

$$J(x,y) = \begin{pmatrix} 3x^2 & -1 \\ 2x & 2y \end{pmatrix}$$

Starting in $\boldsymbol{x}^{(0)} = (1,1)^{\mathrm{T}}$ we get



Further exercises for you to try

- Search for the solution of the Example in the third quadrant by changing the initial value $\boldsymbol{x}^{(0)}$.
- Apply Newton's method to the system

$$\begin{aligned} xe^{y} &= 1 \\ -x^2 + y &= 1 \end{aligned}$$

using $x^{(0)} = y^{(0)} = 0$.

Error analysis for multivariate Newton's method

Error and convergence analysis for the multivariate case is beyond the scope of this lecture.

Summary. If $\boldsymbol{f}$ is sufficiently differentiable, and there is a solution $\boldsymbol{x}^*$ of the system $\boldsymbol{f}(\boldsymbol{x}) = 0$ with $J(\boldsymbol{x}^*)$ nonsingular, then the Newton iterations will converge quadratically towards $\boldsymbol{x}^*$ for all $\boldsymbol{x}^{(0)}$ sufficiently close to $\boldsymbol{x}^*$.

Outlook. Multivariate Newton's method

- finding solutions in the multivariate case is hard
- especially choosing a good starting point $\boldsymbol{x}^{(0)}$ is
- systems of equations usually have multiple solutions
- how do you find the one you want?
- for large n: Evaluating the Jacobian $J(\boldsymbol{x}^{(k)})$ is expensive
- there exist efficient versions – including slow, but robust algorithms to find $\boldsymbol{x}^{(0)}$.