ETH Lecture 401-0663-00L Numerical Methods for CSE

Numerical Methods for Computational Science and Engineering

Prof. R. Hiptmair, SAM, ETH Zurich

(with contributions from Prof. P. Arbenz and Dr. V. Gradinaru)

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URL: http://www.sam.math.ethz.ch/~hiptmair/tmp/NumCSE/NumCSE16.pdf

VIII. Iterative Methods for non-linear Systems of Equations

$F: D \subset \mathbb{R}^n \longrightarrow \mathbb{R}^n$: $F(\underline{x}) = \underline{0}$

↳ vector of unknowns

same number of unknowns and equation

! No general theory

2.1. Iterative Methods

An iterative method for (approximately) solving the non-linear equation $F(\mathbf{x}) = 0$ is an algorithm generating an arbitrarily long sequence $\left(\mathbf{x}^{(k)}\right)_k$ of approximate solutions.

$\mathbf{x}^{(k)} \hat{=}$ k-th iterate

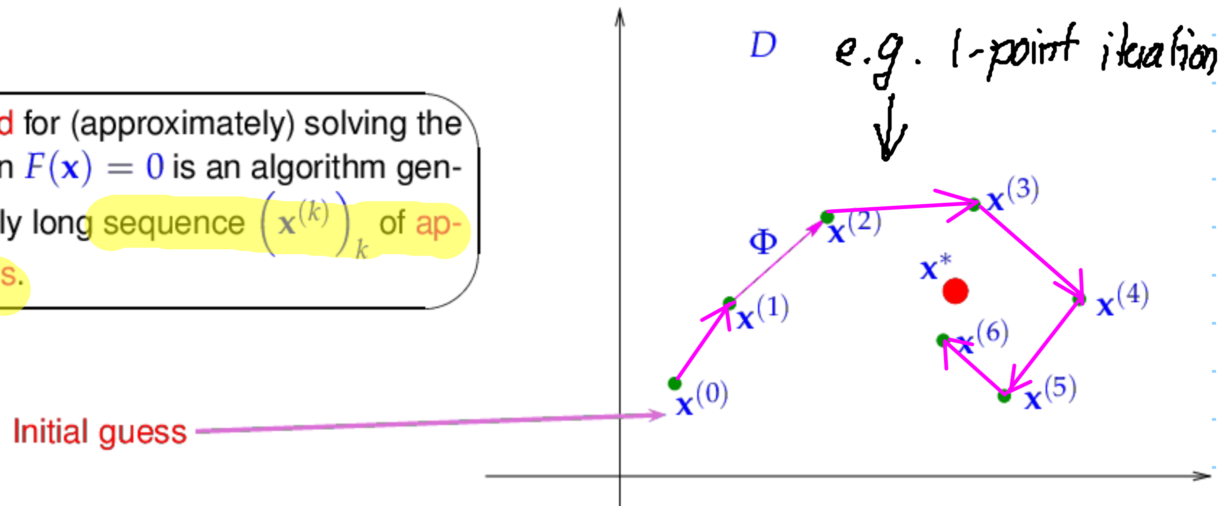

Fig. 282

Iteration error : $e^{(k)} := x^{(k)} - x^*$, $x^* \hat{=}$ solution

More concrete :

m-point iteration : $\underline{x}^{(k)} = \Phi_F(\underline{x}^{(k-1)}, \dots, x^{(k-m)})$

↳ iteration function

Needed initial guesses $x^{(0)}, \dots, \underline{x}^{(m-1)}$

Issues : • Convergence : $\underline{x}^{(k)} \longrightarrow \underline{x}^*$

• Consistency : $F(x^*) = 0 \overset{?}{\Longleftrightarrow} \Phi(\underline{x}^*, \dots, \underline{x}^*) = \underline{x}^*$

[Φ cont. & $x^{(k)}$ cvg. & consistent $\Longrightarrow$ limit is solution :

$\lim_{k\to\infty}$: | $\underline{x}^{(k)} = \Phi_F(\underline{x}^{(k-1)}, \dots, x^{(k-m)})$

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$$\underline{x}^* = \lim_{k\to\infty} \phi(\underline{x}^{(k-1)}, \dots, \underline{x}^{(k-m)}) \overset{\text{cont.}}{=} \phi_F(\underline{x}^*, \dots, \underline{x}^*)$$

- Speed of cvg.: How fast $\|\underline{x}^{(k)} - \underline{x}^*\| \to 0$ for some norm on $\mathbb{R}^n$

Much depends on initial guess:

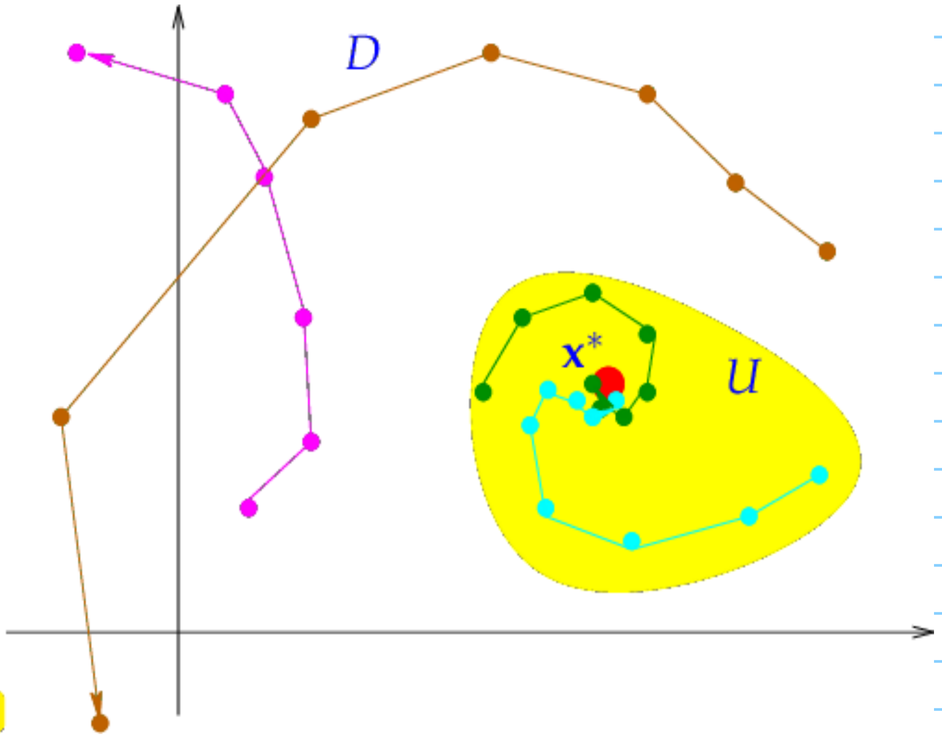


Fig. 283

Definition 8.1.8. Local and global convergence → [?, Def. 17.1]

As stationary m-point iterative method converges locally to $\mathbf{x}^* \in \mathbb{R}^n$, if there is a neighborhood $U \subset D$ of $\mathbf{x}^*$, such that

$$\mathbf{x}^{(0)}, \dots, \mathbf{x}^{(m-1)} \in U \quad \Rightarrow \quad \mathbf{x}^{(k)} \text{ well defined} \quad \wedge \quad \lim_{k\to\infty} \mathbf{x}^{(k)} = \mathbf{x}^*$$

where $(\mathbf{x}^{(k)})_{k\in\mathbb{N}_0}$ is the (infinite) sequence of iterates.
If $U = D$, the iterative method is globally convergent.

2.1.1. Speed of Convergence

Definition 8.1.9. Linear convergence

A sequence $\mathbf{x}^{(k)}$, $k = 0, 1, 2, \dots$, in $\mathbb{R}^n$ converges linearly to $\mathbf{x}^* \in \mathbb{R}^n$,

$$L \geq 0, \quad \exists L < 1: \quad \left\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\right\| \leq L \left\|\mathbf{x}^{(k)} - \mathbf{x}^*\right\| \quad \forall k \in \mathbb{N}_0 .$$

smallest L : rate

How to tell linear cvg. in an experiment?

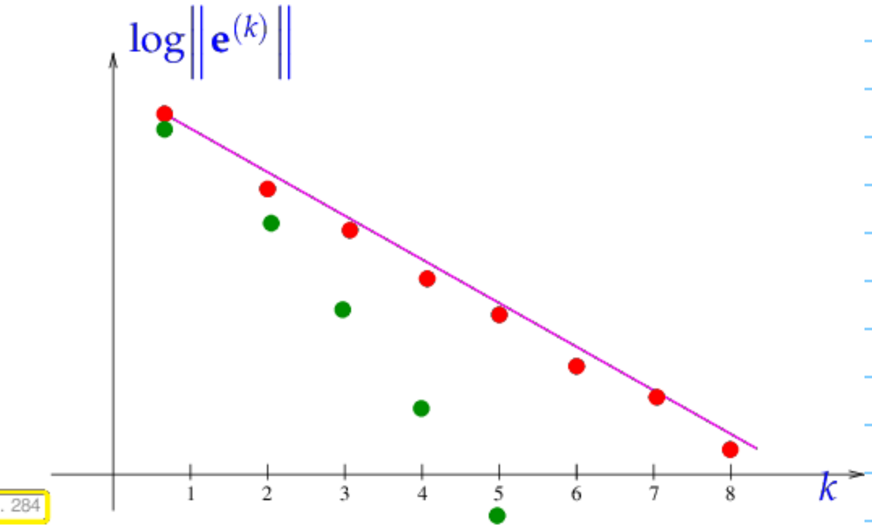
Assume sharpness $\varepsilon_k := \|\underline{x}^{(k)} - \underline{x}^*\| \approx L \|\underline{x}^{(k-1)} - \underline{x}^*\| = \varepsilon_{k-1}$

Visual evidence of linear cvg:

$$\varepsilon_k \approx L\, \varepsilon_{k-1}$$

$$\log \cdot \,| \quad \varepsilon_k \approx L^k \varepsilon_0 \Rightarrow \log \varepsilon_k \approx k \log L + \log \varepsilon_0$$

log | $\epsilon_k \approx L^k \epsilon_0 \Rightarrow \underbrace{\log \epsilon_k \approx k \log L + \log \epsilon_0}$



Data points on straight line* in k vs. $\log \epsilon_k$ plot.

* slope ~ rate

! Different notions & and terminology for

Approximation error
quadrature errors
↓
alg. cvg. / exp. cvg.

iteration errors
↓
linear cvg.
cvg. of order p

"Faster" than linear cvg:

Definition 8.1.17. Order of convergence → [?, Sect. 17.2], [?, Def. 5.14], [?, Def. 6.1]

A **convergent** sequence $\mathbf{x}^{(k)}$, $k = 0, 1, 2, \ldots$, in $\mathbb{R}^n$ with limit $\mathbf{x}^* \in \mathbb{R}^n$ converges with order p, if

$$\exists C > 0: \quad \left\| \mathbf{x}^{(k+1)} - \mathbf{x}^* \right\| \leq C \left\| \mathbf{x}^{(k)} - \mathbf{x}^* \right\|^p \quad \forall k \in \mathbb{N}_0 , \tag{8.1.18}$$

and, in addition, $C < 1$ in the case $p = 1$ (linear convergence → Def. 8.1.9).

How to tell cvg of order $p > 1$?
[assuming sharpness of estimate]

log | $\epsilon_k \approx C \epsilon_{k-1}^p$

$$\log \epsilon_k \approx \log C + p \log \epsilon_{k-1}$$
$$- \quad \log \epsilon_{k-1} \approx \log C + p \log \epsilon_{k-2}$$

$$p \approx \underbrace{\frac{\log \epsilon_k - \log \epsilon_{k-1}}{\log \epsilon_{k-1} - \log \epsilon_{k-2}}}_{\text{study these quotients}}$$

NLSE : $F(\underline{x}) = 0$, $F : \mathbb{R}^n \to \mathbb{R}^n$

Iteration produces sequence $(x^{(k)})_{k \in \mathbb{N}_0}$

Linear cvg : $\|x^{(k+1)} - x^*\| \leq L \|x^{(k)} - x^*\|$ for $0 \leq L < 1$

order-p cvg. : $\|x^{(k+1)} - x^*\| \leq C \|x^{(k)} - x^*\|^p$, $C > 0$
$(p > 1)$

Example : $\sqrt{}$-iteration $(n = 1)$

$$\underbrace{x^{(k+1)} = \frac{1}{2}\left(x^{(k)} + \frac{a}{x^{(k)}}\right)} \Rightarrow |x^{(k+1)} - \sqrt{a}| = \frac{1}{2x^{(k)}}|x^{(k)} - \sqrt{a}|^2 . \qquad (8.1.21)$$

$a > 0$

1-point iteration : $\Phi(t) = \frac{1}{2}\left(t + \frac{a}{t}\right)$

Convergence to $\sqrt{a}$ with order 2

$\|\underline{x}^{(k+1)} - x^*\| \leq C \|\underline{x}^{(k)} - \underline{x}^*\|^2$

Note: Convergence of order $p > 1$ guarantees local convergence

$\|\underline{x}^{(k+1)} - x^*\| \leq C \|x^{(k)} - x^*\|^{p-1} \|x^{(k)} - x^*\|$

If $x^{(0)} \in \mathcal{U} := \{ \underline{z} : C\|z - x^*\|^{p-1} < 1 \}$

$\Rightarrow x^{(k)} \to x^*$ for $k \to \infty$

k	$x^{(k)}$	$e^{(k)} := x^{(k)} - \sqrt{2}$	$\log \frac{\lvert e^{(k)} \rvert}{\lvert e^{(k-1)} \rvert} : \log \frac{\lvert e^{(k-1)} \rvert}{\lvert e^{(k-2)} \rvert}$
0	2.00000000000000000	0.58578643762690485	
1	1.50000000000000000	0.08578643762690485	
2	1.41666666666666652	0.00245310429357137	1.850
3	1.41421568627450966	0.00000212390141452	1.984
4	1.41421356237468987	0.00000000000159472	2.000
5	1.41421356237309492	0.00000000000000022	$\boxed{0.630}$

Note the doubling of the number of significant digits in each step ! [impact of roundoff !]

Relative errors : $x^{(k)} = x^*(1 + \delta_k)$

order-2 cvg : $\|x^{(k+1)} - x^*\| \leq C \|x^{(k)} - x^*\|^2$

$\delta_{k+1} \|x^*\| \leq C \delta_k^2 \|x^*\|^2$

"sharpness" $\delta_{k+1} \approx C\|x^*\| \delta_k^2$

If $C\|x^*\| \approx 1$, $\delta_k \approx 10^{-\ell} \Rightarrow \delta_{k+1} \approx 10^{-2\ell}$

2.1.2 Termination

↳ Stopping rules

Ideal:

STOP, if $\|x^{(k)} - x^*\| \leq \tau_{rel} \|x^*\|$: relative error

$\|x^{(k)} - x^*\| \leq \tau_{abs}$: absolute error

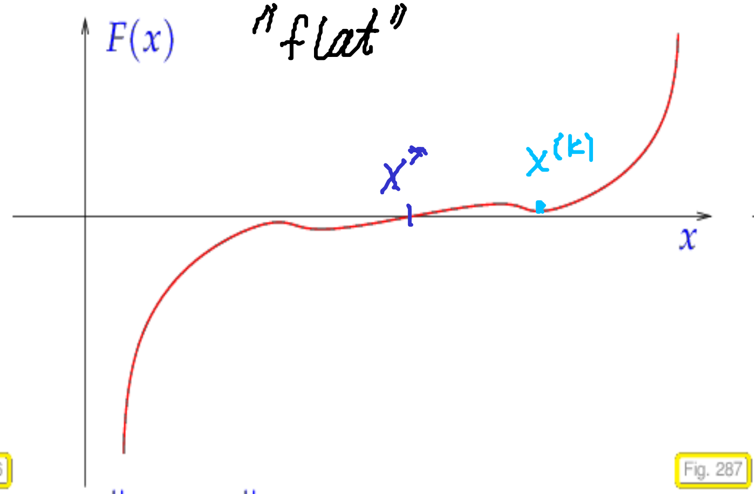
↑ not accessible

Practical:

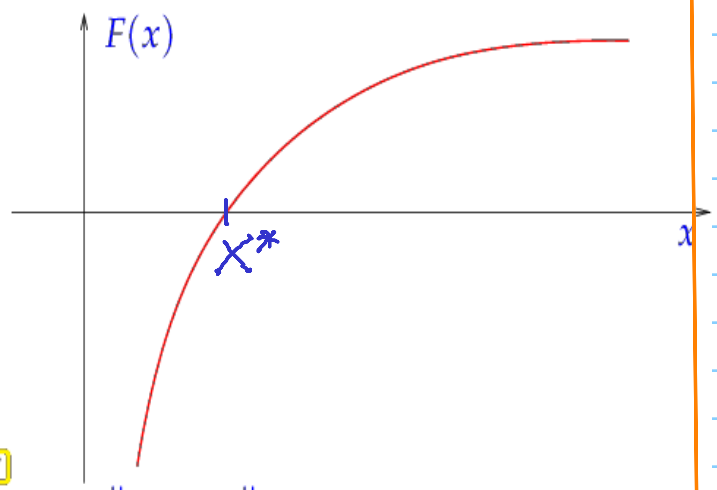
① Residual based termination

STOP, if $\underbrace{\|F(x^{(k)})\| \leq \tau}_{\text{tells little about error}}$

"flat"



$\|F(\mathbf{x}^{(k)})\|$ small $\not\Rightarrow |x - x^*|$ small



$\|F(\mathbf{x}^{(k)})\|$ small $\Rightarrow |x - x^*|$ small

② Correction based termination:

STOP, if $\|x^{(k+1)} - x^{(k)}\| \leq \begin{cases} \tau_{rel} \|x^{(k+1)}\| \\ \tau_{abs} \end{cases}$

→ Still no guarantee, except for linearly cvg. iterations with known rate L

$\|x^{(k+1)} - x^*\| \leq L \|x^{(k)} - x^*\|$

$\|x^{(k)} - x^*\| = \|x^{(k)} - x^{(k+1)} + x^{(k+1)} - x^*\|$

$$\left\|\mathbf{x}^{(k)} - \mathbf{x}^*\right\| \overset{\triangle\text{-inequ.}}{\leq} \left\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right\| + \left\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\right\| \leq \left\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right\| + L\left\|\mathbf{x}^{(k)} - \mathbf{x}^*\right\| .$$

$\frac{1-L}{L} \|x^{(k+1)} - x^*\| \leq (1-L) \|x^{(k)} - x^*\| \leq \|x^{(k+1)} - x^{(k)}\|$

▶ Iterates satisfy: $$\boxed{\left\|\mathbf{x}^{(k+1)} - \mathbf{x}^*\right\| \leq \frac{L}{1-L}\left\|\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}\right\|} . \qquad (8.1.29)$$

! Upper bound $\tilde{L} < 1$ for L sufficient to obtain reliable bound!

$\|x^{(k)} - x^*\| \leq L^{k-1} \|x^{(1)} - x^*\|$

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$$\left\|\mathbf{x}^*-\mathbf{x}^{(k)}\right\| \leq \frac{L^{k-l}}{1-L}\left\|\mathbf{x}^{(l+1)}-\mathbf{x}^{(l)}\right\| . \qquad (8.2.21)$$

Set $l=0$ in (8.2.21)	Set $l=k-1$ in (8.2.21)
a priori termination criterion	a posteriori termination criterion
$\boxed{\left\|\mathbf{x}^*-\mathbf{x}^{(k)}\right\| \leq \frac{L^{k}}{1-L}\left\|\mathbf{x}^{(1)}-\mathbf{x}^{(0)}\right\|}$ (8.2.22)	$\left\|\mathbf{x}^*-\mathbf{x}^{(k)}\right\| \leq \frac{L}{1-L}\left\|\mathbf{x}^{(k)}-\mathbf{x}^{(k-1)}\right\|$ (8.2.23)

- $\Phi_2(x) = x \Leftrightarrow 1+x = (1+e^x)x \Leftrightarrow 1 = xe^x$
  $\Leftrightarrow F(x) = 0$
-

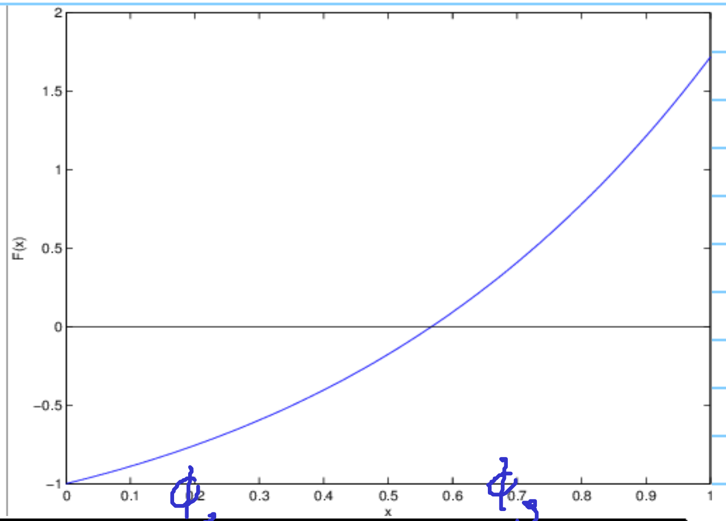
2.2. Fixed Point Iterations

$$x^{(k+1)} = \Phi_F(x^{(k)})$$

$\Phi : U \subset \mathbb{R}^n \to \mathbb{R}^n$ iteration function

consistent : $\Phi_F(x^*) = x^* \Leftrightarrow F(x^*) = 0$
with $F(x)=0$

$$F(x) = xe^x - 1\,, \quad x \in [0,1]\,.$$



Different fixed point forms:

$$\Phi_1(x) = e^{-x}\,,$$
$$\Phi_2(x) = \frac{1+x}{1+e^x}\,,$$
$$\Phi_3(x) = x + 1 - xe^x\,.$$

[all consistent]

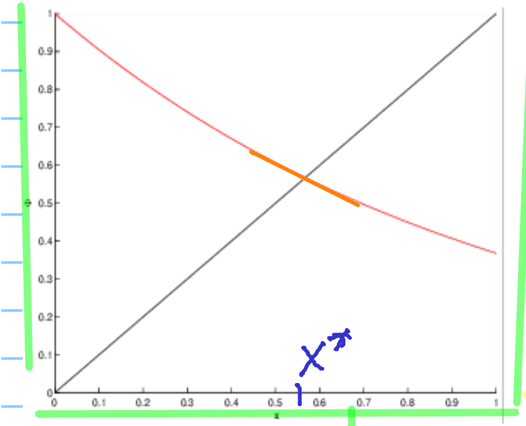
$x^{(0)} = 0.5$:

Φ_2 : order 2-cvg

Φ_1 : lin cvg.

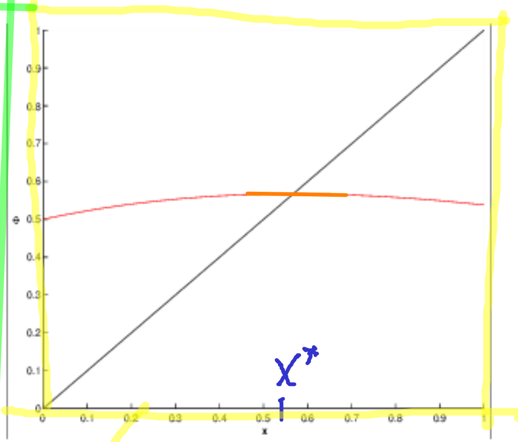
Φ_3 : no cvg.

k	Φ_1: $\lvert x_1^{(k+1)} - x^*\rvert$	Φ_2: $\lvert x_2^{(k+1)} - x^*\rvert$	Φ_3: $\lvert x_3^{(k+1)} - x^*\rvert$
0	0.067143290409784	0.067143290409784	0.067143290409784
1	0.039387369302849	0.000832287212566	0.108496074240152
2	0.021904078517179	0.000000125374922	0.219330611898582
3	0.012559804468284	0.000000000000003	0.288178118764323
4	0.007078662470882	0.000000000000000	0.723649245792953
5	0.004028858567431	0.000000000000000	0.410183132337935
6	0.002280343429460	0.000000000000000	1.186907542305364
7	0.001294757160282	0.000000000000000	0.146569797006362
8	0.000733837662863	0.000000000000000	0.310516641279937
9	0.000416343852458	0.000000000000000	0.357777386500765
10	0.000236077474313	0.000000000000000	0.974565695952037



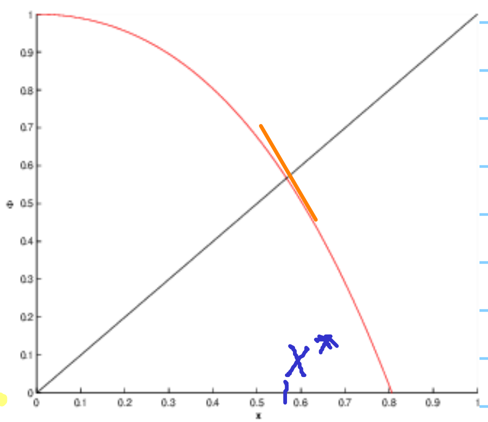
function Φ_1

$|\Phi_1'(x^*)| < 1$



function Φ_2

$\Phi_2'(x^*) = 0$



function Φ_3

$|\Phi_3'(x^*)| > 1$

▷ Slope of Φ at x^* matters! Taylor argument

$$x^{(k+1)} - x^* = \Phi(x^{(k)}) - \Phi(x^*)$$

$$= \Phi'(x^*)(x^{(k)}-x^*) + \tfrac{1}{2}\Phi''(x^*)(x^{(k)}-x^*)^2 + \underbrace{\tfrac{1}{6}\Phi'''(\xi)(x^{(k)}-x^*)^3}$$

If $|x^{(k)}-x^*| \ll 1$ ⟶ neglect

• and $\Phi'(x^*)=0$ (Φ "flat") $\Rightarrow$ $|x^{(k+1)}-x^*| \approx |\tfrac{1}{2}\Phi''(x^*)|\,|x^{(k)}-x^*|^2$

$\hat{=}$ order-2 cvg.

• and $|\Phi'(x^*)| < 1$ $\Rightarrow$ $|x^{(k+1)}-x^*| \leq |\Phi'(x^*)|\,|x^{(k)}-x^*|$ + small terms

$\hat{=}$ Linear convergence with rate $\approx |\Phi'(x^*)|$

Generalization to n-dim.:

Lemma 8.2.10. Sufficient condition for local linear convergence of fixed point iteration → **[?, Thm. 17.2], [?, Cor. 5.12]**

If $\Phi : U \subset \mathbb{R}^n \mapsto \mathbb{R}^n$, $\Phi(\mathbf{x}^*) = \mathbf{x}^*$, Φ differentiable in $\mathbf{x}^*$, and $\|D\,\Phi(\mathbf{x}^*)\| < 1$, then the fixed point iteration

$$\mathbf{x}^{(k+1)} := \Phi(\mathbf{x}^{(k)}) , \tag{8.2.2}$$

converges locally and at least linearly.

matrix norm, Def. 1.5.76 !

predictor for rate of lin. cvg.

If $D\Phi(x^*) = 0$ $\Rightarrow$ local order-2 cvg.

2.3. Zero Finding

Find $x^* \in I \subset \mathbb{R}$: $F(x^*) = 0$ for $F: I \to \mathbb{R}$

[F continuous]

2.3.1. Bisection

Input: $a, b \in I$ such that $F(a)F(b) < 0$ (different signs !)

$\Rightarrow$ $\exists\, x^* \in]\min\{a,b\}, \max\{a,b\}[$: $F(x^*) = 0$,

as we conclude from the intermediate value theorem.

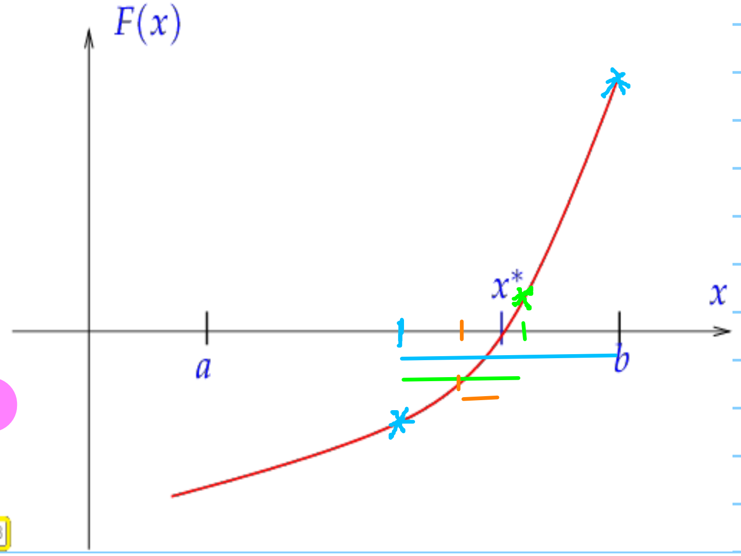


Fig. 288

C++11 code 8.3.2: Bisection method for solving $F(x) = 0$ on $[a, b]$

```
// Searching zero of F in [a,b] by bisection
template <typename Func>
double bisect(Func&& F, double a, double b, double tol)
{
  if (a > b) std::swap(a,b); // sort interval bounds
  double fa = F(a), fb = F(b);
  if (fa*fb > 0) throw "f(a) and f(b) have same sign";
  int v=1; if (fa > 0) v=-1;
  double x = 0.5*(b+a); // determine midpoint
  // termination, relies on machine arithmetic if tol = 0
  while (b-a > tol && ((a<x) && (x<b))) //
  {
    // sgn(f(x)) = sgn(f(b)), then use x as next right boundary
    if (v*F(x) > 0) b=x;
    // sgn(f(x)) = sgn(f(a)), then use x as next left boundary
    else a=x;
    x = 0.5*(a+b); // determine next midpoint
  }
  return x;
}
```

tol = 0 : Loop will stop, when

$a \mp \frac{1}{2}(b-a) = a$

$\hookrightarrow$ happens, if $|\frac{1}{2}(b-a)| \leq EPS \cdot |a|$

Convergence: "linear type"

Intervals shrink by factor 2 in each step

$|a^{(k)} - b^{(k)}| \leq 2^{-k} |a^{(0)} - b^{(0)}|$

$\Rightarrow$ $|x^{(k)} - x^*| \leq 2^{-k} |a^{(0)} - b^{(0)}|$

$\Rightarrow$ robust method

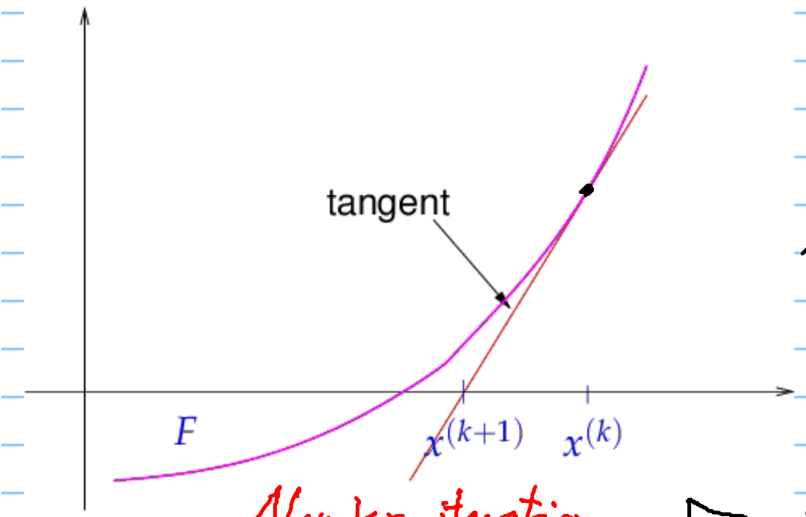
2.3.2 Model Function Methods

Idea: Replace F with $\tilde{F}: I \to \mathbb{R}$ (model function)

- depending on point values of F / F'
- whose zeros are easy to compute

↳ do this in every step of an iteration

2.3.2.1. Newtons method



Model function $\hat{F}$

≙ tangent at graph of F in $x^{(k)}$

$$\hat{F}(x) = F(x^{(k)}) + F'(x^{(k)})(x - x^{(k)})$$

$$x^{(k+1)}: \quad \hat{F}(x^{(k+1)}) = 0$$

Newton iteration ▷ $x^{(k+1)} = x^{(k)} - F(x^{(k)}) / F'(x^{(k)})$

[if $F'(x^{(k)}) \neq 0$]

↳ ≙ fixed point iteration with $\phi(x) = x - \frac{F(x)}{F'(x)}$

(Local) cvg. of Newton's method:

$$\phi'(x) = 1 - \frac{[F'(x)]^2 - F''(x)F(x)}{[F'(x)]^2} = \frac{F''(x)}{[F'(x)]^2} F(x)$$

▷ $F(x^*) = 0 \Rightarrow \phi'(x^*) = 0$, if $F'(x^*) \neq 0$

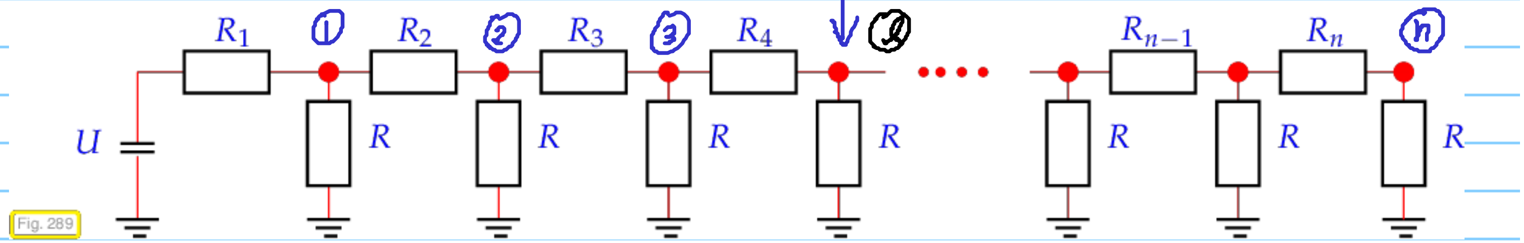
$\Rightarrow$ local 2nd-order cvg.

Convergence of Newton's method in 1D

Newton's method locally quadratically converges (→ Def. 8.1.17) to a zero x^* of F, if $F'(x^*) \neq 0$

Example: F' by implicit differentiation

achieve prescribed voltage = 1 here



[Nodal analysis] ⇒ LSE for nodal voltages u_i

$$(A + xI)\,u(x) = b \in \mathbb{R}^n$$

s.p.d. tridiagonal matrix $\in \mathbb{R}^{n,n}$

$= 1/R$ [→ unknown]

n.v.

Task: $x \in \mathbb{R}$: $\mathbf{w}^T \mathbf{u}(x) = 1$, $\mathbf{w} = \mathbf{e}_\ell$

$\Updownarrow$

Find zero of $F(x) = \mathbf{w}^T\mathbf{u}(x) - 1 = \mathbf{w}^T(A+xI)^{-1}\mathbf{b} - 1$

$F'(x) = \mathbf{w}^T \mathbf{u}'(x)$

$\mathbf{u}(x)$: $(A+xI)\mathbf{u}(x) = \mathbf{b} \quad \Big| \frac{d}{dx}$

$I\cdot\mathbf{u}(x) + (A+xI)\cdot\mathbf{u}'(x) = 0$

with product rule: $(fg)' = f'\cdot g + f\cdot g'$

$\Rightarrow \quad \mathbf{u}'(x) = -(A+xI)^{-1}\mathbf{u}(x)$

▷ Newton iteration:

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

$$= x^{(k)} - \frac{\mathbf{w}^T\mathbf{u}(x^{(k)}) - 1}{\mathbf{w}^T\mathbf{z}}$$

where: $(A + x^{(k)}I)\,\mathbf{u}(x^{(k)}) = \mathbf{b}$

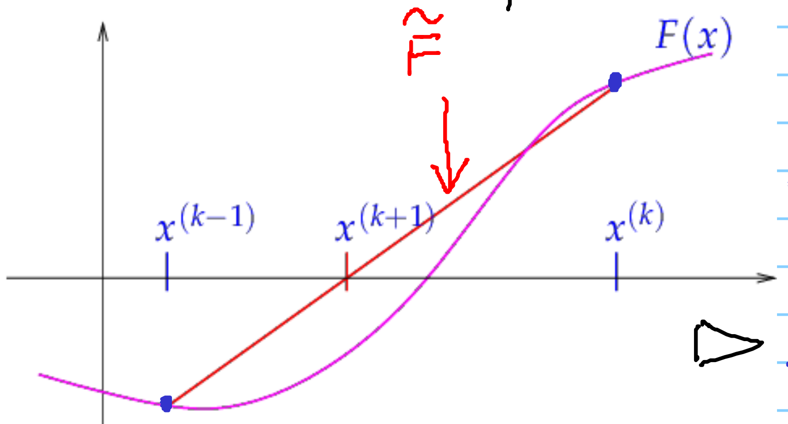
$$(A + x^{(k)}I)\,\underbrace{\mathbf{z}}_{:=\,\mathbf{u}'(x^{(k)})} = -\mathbf{u}(x^{(k)})$$

2.3.2.2. Multi-point methods

m-point method: $x^{(k+1)} = \phi(x^{(k)}, \dots, x^{(k-m+1)})$

↳ m initial $x^{(j)}$ required

Secant method: 2-point method



$\tilde{F}(x) = F(x^{(k)}) + \Delta s \cdot (x - x^{(k)})$

$$\Delta s = \frac{F(x^{(k)}) - F(x^{(k-1)})}{x^{(k)} - x^{(k-1)}}$$

▷ $$x^{(k+1)} = x^{(k)} - \underbrace{\frac{F(x^{(k)})}{\Delta s}}_{=:\,s}$$

1 F-evaluation per step

C++11 code 8.3.25: Secant method for 1D non-linear equaton

```
// Secant method for solving F(x) = 0 for F : D ⊂ ℝ → ℝ,
// initial guesses x0, x1,
// tolerances atol (absolute), rtol (relative)
template<typename Func>
double secant(double x0, double x1, Func&& F,
              double rtol, double atol, unsigned int maxIt)
{
  double fo = F(x0);
  for (unsigned int i=0; i<maxIt; ++i) {
      double fn = F(x1);
      double s = fn*(x1-x0)/(fn-fo); // secant correction
      x0 = x1; x1 = x1-s;
      // correction based termination (relative and absolute)
      if (abs(s) < max(atol,rtol*min(abs(x0),abs(x1))))
     return x1;
      fo = fn;
  }
  return x1;
}
```

(Empiric) convergence of secant method :

$F(x) = xe^x - 1$, $x^{(0)} = 0$, $x^{(1)} = 5$

estimate for order of cvg.

k	$x^{(k)}$	$F(x^{(k)})$	$e^{(k)} := x^{(k)} - x^*$	$\dfrac{\log\lvert e^{(k+1)}\rvert - \log\lvert e^{(k)}\rvert}{\log\lvert e^{(k)}\rvert - \log\lvert e^{(k-1)}\rvert}$
2	0.00673794699909	-0.99321649977589	-0.56040534341070	
3	0.01342122983571	-0.98639742654892	-0.55372206057408	24.43308649757745
4	0.98017620833821	1.61209684919288	0.41303291792843	2.70802321457994
5	0.38040476787948	-0.44351476841567	-0.18673852253030	1.48753625853887
6	0.50981028847430	-0.15117846201565	-0.05733300193548	1.51452723840131
7	0.57673091089295	0.02670169957932	0.00958762048317	1.70075240166256
8	0.56668541543431	-0.00126473620459	-0.00045787497547	1.59458505614449
9	0.56713970649585	-0.00000990312376	-0.00000358391394	1.62641838319117
10	0.56714329175406	0.00000000371452	0.00000000134427	
11	0.56714329040978	-0.00000000000001	-0.00000000000000	

$\Rightarrow$ order 1.6 convergence

Generalization: Inverse interpolation

Assume: $F : I \subset \mathbb{R} \mapsto \mathbb{R}$ one-to-one (monotone)

$$F(x^*) = 0 \quad \Rightarrow \quad F^{-1}(0) = x^* .$$

- Interpolate F^{-1} by polynomial p of degree $m-1$ determined by

$$p(F(x^{(k-j)})) = x^{(k-j)} , \quad j = 0, \dots, m-1 .$$

- New approximate zero $x^{(k+1)} := p(0)$

The graph of F^{-1} can be obtained by reflecting the graph of F at the angular bisector. ▷

$$F(x^*) = 0 \quad \Leftrightarrow \quad F^{-1}(0) = x^*$$

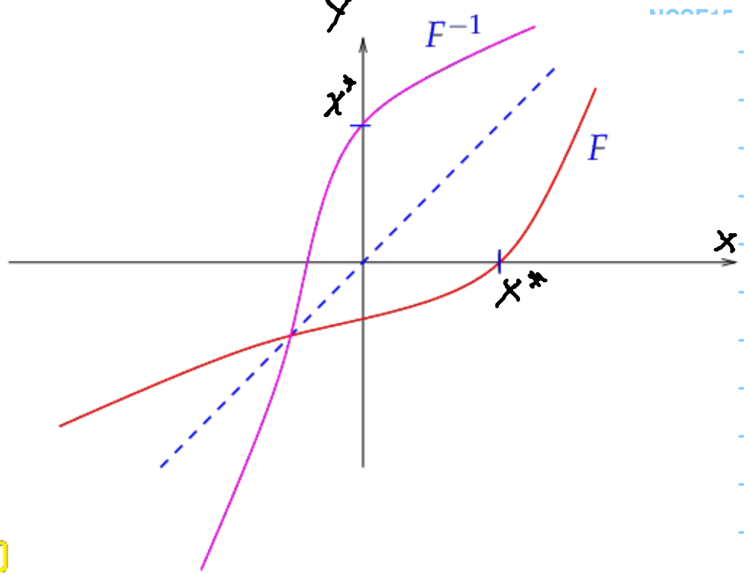


Fig. 292

Case $m = 2$ (2-point method)
➢ secant method

The interpolation polynomial is a line. In this case we do not get a new method, because the inverse function of a linear function (polynomial of degree 1) is again a polynomial of degree 1.

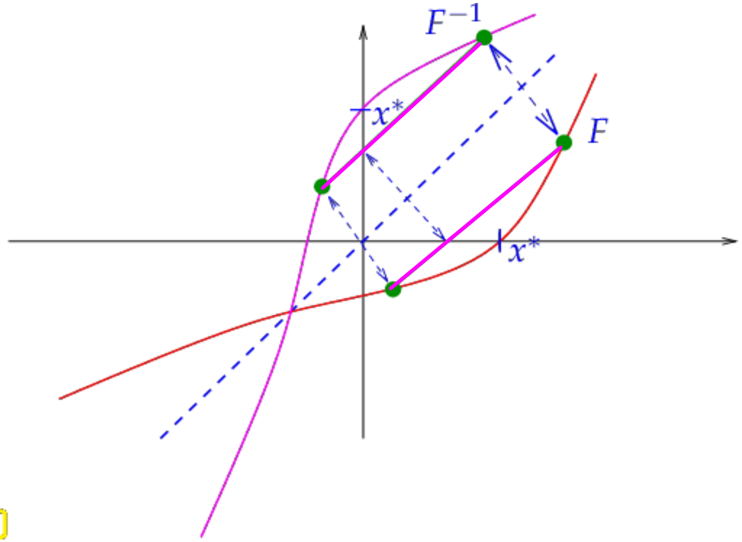


Fig. 293

m = 3 :

$$x^{(k+1)} = \frac{F_0^2(F_1x_2 - F_2x_1) + F_1^2(F_2x_0 - F_0x_2) + F_2^2(F_0x_1 - F_1x_0)}{F_0^2(F_1 - F_2) + F_1^2(F_2 - F_0) + F_2^2(F_0 - F_1)} .$$

$$\left(F_0 := F(x^{(k-2)}), F_1 := F(x^{(k-1)}), F_2 := F(x^{(k)}), x_0 := x^{(k-2)}, x_1 := x^{(k-1)}, x_2 := x^{(k)} \right)$$

$F(x) = xe^x - 1$, $x^{(0)} = 0$, $x^{(1)} = 2.5$, $x^{(2)} = 5$.

k	$x^{(k)}$	$F(x^{(k)})$	$e^{(k)} := x^{(k)} - x^*$	$\frac{\log\lvert e^{(k+1)}\rvert - \log\lvert e^{(k)}\rvert}{\log\lvert e^{(k)}\rvert - \log\lvert e^{(k-1)}\rvert}$
3	0.08520390058175	-0.90721814294134	-0.48193938982803	
4	0.16009252622586	-0.81211229637354	-0.40705076418392	3.33791154378839
5	0.79879381816390	0.77560534067946	0.23165052775411	2.28740488912208
6	0.63094636752843	0.18579323999999	0.06380307711864	1.82494667289715
7	0.56107750991028	-0.01667806436181	-0.00606578049951	1.87323264214217
8	0.56706941033107	-0.00020413476766	-0.00007388007872	1.79832936980454
9	0.56714331707092	0.00000007367067	0.00000002666114	1.84841261527097
10	0.56714329040980	0.00000000000003	0.00000000000001	

fractional order

2.3.3. Asymptotic efficiency

$\hookrightarrow \frac{\text{gain}}{\text{work}}$ ← [no. of digits] prescribed error reduction ← #F-eval + #F'-eval

gain: $\boxed{\|e^{(k)}\| \le \rho \|e^{(0)}\|}$ with $\rho \ll 1$ (*)

$K(\rho)$: minimal no. of iterations required for (*)

▷ Efficience : $\frac{|\log \rho|}{K(\rho) \cdot W}$, $W \hat{=}$ work/iteration

• Linearly cvgt. iteration: $\|e^{(k)}\| \le L^k \|e^{(0)}\|$, $L<1$

$\Rightarrow K(\rho) \ge \frac{\log \rho}{\log L} \Rightarrow \text{Eff.} = \frac{|\log L|}{W}$

• order $p>1$: $\|e^{(k)}\| \le C\|e^{(k-1)}\|^p$

$\|e^{(k)}\| \le \underbrace{C^{1+p+p^2+\dots+p^{k-1}}}_{= C^{\frac{p^k-1}{p-1}}} \|e^{(0)}\|^{p^k-1} \cdot \|e^{(0)}\|$

▷ $K(\rho)$: $\Big(\underbrace{C^{\frac{1}{p-1}} \|e^{(0)}\|}_{=: L_0}\Big)^{p^k-1} \le \rho$

$p^k \ge \frac{\log \rho}{\log L_0} + 1 \qquad | \cdot \log$

$k \ge \log\left(\frac{\log \rho}{\log L_0} \cancel{+1}\right) / \log p$

$\rho \ll 1$: $k \cdot \log p \ge \log\log\rho - \cancel{\log\log L_0}$

$K(\rho) = \frac{\log\log\rho}{\log p}$

$\text{Efficiency} = \frac{\log p}{W} \frac{\log \rho}{\log\log\rho}$

$\hookrightarrow$ different for different methods

$W_{\text{Newton}} = 2W_{\text{secant}}$, $p_{\text{Newton}} = 2$, $p_{\text{secant}} = 1.62$ $\Rightarrow \frac{\log p_{\text{Newton}}}{W_{\text{Newton}}} : \frac{\log p_{\text{secant}}}{W_{\text{secant}}} = 0.71$.

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NCSE15

▷ "Secant method is 30% more efficient than Newton"

2.4. Newton's Method (for $n > 1$)

$\underline{x}^* \in \mathbb{R}^n$: $\quad F(\underline{x}^*) = 0$, $F : D \subset \mathbb{R}^n \to \mathbb{R}^n$

differentiable

"Tangent plane" at $x^{(k)}$ $\hat{=}$ model function by linearization

$\underline{x}^{(k+1)}$: $\quad \hat{F}(x) = F(\underline{x}^{(k)}) + DF(x^{(k)})(\underline{x} - \underline{x}^{(k)}) \overset{!}{=} 0$

Jacobian $\in \mathbb{R}^{n,n}$

Newton iteration $\quad \boxed{\underline{x}^{(k+1)} = \underline{x}^{(k)} - \underbrace{DF(\underline{x}^{(k)})^{-1} F(\underline{x}^{(k)})}}$

Newton correction $\Delta x^{(k)}$: by solving a LSE

Affine invariance :

Newton iterations for $\to F(x) = \underline{0}$; $\to A F(x) = \underline{0}$, $A \in \mathbb{R}^{n,n}$ regular

produce the same iterates, if started with the same value

$[\ G(x) := AF(x) \Rightarrow DG(x) = A\,DF(x)\ ]$

N.I. for $G(x) = 0$:

$$x^{(k+1)} = x^{(k)} - [\cancel{A} DF(x^{(k)})]^{-1} [\cancel{A} F(x^{(k)})]$$

2.4.2. Convergence of Newton's method

→ = Fixed point iteration with iteration function

$$\Phi(\underline{x}) := \underline{x} - DF(\underline{x})^{-1} \cdot F(\underline{x}) \ , \ x \in D$$

[product rule]

$$D\Phi(x^*) = \cancel{I} - ? \cdot \overbrace{F(x^*)}^{=0} - \cancel{DF(x)^{-1} DF(x)} = 0$$

$\Rightarrow$ $\boxed{\text{local quadratic cvg.}}$

Example : Quasi-linear system of equation

$$A(\underline{x})\underline{x} = \underline{b} \ , \quad A : \mathbb{R}^n \to \mathbb{R}^{n,n}$$

$$\boxed{\mathbf{A}(\mathbf{x})\mathbf{x} = \mathbf{b}}\ , \quad \mathbf{A}(\mathbf{x}) = \begin{pmatrix} \gamma(\mathbf{x}) & 1 & & & \\ 1 & \gamma(\mathbf{x}) & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & 1 & \gamma(\mathbf{x}) & 1 \\ & & & 1 & \gamma(\mathbf{x}) \end{pmatrix} \in \mathbb{R}^{n\times n}\ , \tag{8.4.20}$$

$\gamma(x) = 3 + \|x\|$

$$\Longleftrightarrow \quad F(\underline{x}) = \underline{b} - A(\underline{x})\underline{x} = \underline{0}$$

$$\mathbf{A}(\mathbf{x})\mathbf{x} = \mathbf{T}\mathbf{x} + \mathbf{x}\|\mathbf{x}\|_2\ , \quad \mathbf{T} := \begin{pmatrix} 3 & 1 & & & \\ 1 & 3 & 1 & & \\ & \ddots & 3 & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & 3 & 1 \\ & & & & 1 & 3 \end{pmatrix}.$$

$$\Rightarrow \quad F(\underline{x}) = \underline{b} - T\underline{x} - \|x\|\cdot\underline{x}$$

$$\Rightarrow \quad DF(\underline{x}) = -T - D\{\underbrace{x \to \|x\|\cdot x}_{=:\, g(\underline{x})}\}$$

$DF(x)$: (i) product rule

(ii) direct computation

$$(g(\underline{x}))_i = \sqrt{x_1^2 + \dots + x_n^2}\cdot x_i$$

$$(Dg(\underline{x}))_{i,j} = \frac{\partial g_i(x)}{\partial x_j} = \begin{cases} * & j = i \\ \dfrac{x_j}{\sqrt{x_1^2 + \dots + x_n^2}}\, x_i\ , & j \neq i \end{cases}$$

$$\frac{\partial}{\partial x_i}(\mathbf{x}\|\mathbf{x}\|)_i = \underbrace{\sqrt{x_1^2 + \cdots + x_n^2}}_{=\|x\|} + x_i \frac{x_i}{\sqrt{x_1^2 + \cdots + x_n^2}}\ ,$$

$$\frac{\partial}{\partial x_j}(\mathbf{x}\|\mathbf{x}\|)_i = x_i \frac{x_j}{\sqrt{x_1^2 + \cdots + x_n^2}}\ , \quad j \neq i\ .$$

$$\boxed{DF(\mathbf{x})} = \mathbf{T} + \|\mathbf{x}\|_2 + \mathbf{x}\frac{\mathbf{x}^\top}{\|\mathbf{x}\|_2} = \boxed{\left(\mathbf{A}(\mathbf{x}) + \frac{\mathbf{x}\mathbf{x}^\top}{\|\mathbf{x}\|_2}\right)}\ .$$

rank-1-modification of tridiagonal matrix A

$\Rightarrow$ Use Sherman-Morrison-Woodbury formula for computing Newton correction : cost $O(n)$

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Example: Matrix inversion via Newton

$A \in \mathbb{R}^{n,n}$ regular: $F(X) = A - X^{-1} \overset{!}{=} 0$

$F : \mathbb{R}^{n,n} \to \mathbb{R}^{n,n}$

Newton iteration for $F(X) = 0$?

Trick: implicit differentiation $\quad F(X)\cdot X = AX - I$

[product rule]

[" General derivative of $\phi : V \to W$

$$D\phi(v)h = \lim_{\tau \to 0} \frac{\phi(v+\tau h) - \phi(v)}{\tau}$$]

h ↑ direction of differentiation

Product rule: $F : D \subset V \mapsto W$, $G : D \subset V \mapsto U$ sufficiently smooth, $b : W \times U \mapsto Z$ bilinear, *ie.*, linear in each argument:

$$T(\mathbf{x}) = b(F(\mathbf{x}), G(\mathbf{x})) \quad \Rightarrow \quad \mathrm{D}\,T(\mathbf{x})\mathbf{h} = b(\mathrm{D}\,F(\mathbf{x})\mathbf{h}, G(\mathbf{x})) + b(F(\mathbf{x}), \mathrm{D}\,G(\mathbf{x})\mathbf{h}) , \qquad (8.4.9)$$

$\mathbf{h} \in V, \mathbf{x} \in D$.

$$(f\cdot g)' = f'\cdot g + f\cdot g'$$

"$\frac{d}{dX}$" $F(X)\cdot X = AX - I$

$\Rightarrow \quad D(F(X)\cdot X)H = D(AX - I)H$

- General product rule with $b \Leftrightarrow$ matrix multiplication.
- $D\{X \to X\}H = H$ $\qquad H \in \mathbb{R}^{n,n}$

$$DF(X)(H)\cdot X + F(X)\cdot H = A\cdot H$$

$$\triangleright \quad \underbrace{DF(X)(H)}_{\in \mathbb{R}^{n,n}} = (A\cdot H - F(X)\cdot H)X^{-1} = X^{-1}HX^{-1}$$

Newton iteration: $DF(X)$ is not a matrix!

$$X^{(k+1)} = X^{(k)} - S, \quad DF(X^{(k)})(S) = F(X^{(k)})$$

$$\Updownarrow$$

$$(X^{(k)})^{-1}S(X^{(k)})^{-1} = A - (X^{(k)})^{-1}$$

$$\Leftrightarrow \quad S = X^{(k)}AX^{(k)} - X^{(k)}$$

$$\triangleright \quad X^{(k+1)} = 2X^{(k)} - X^{(k)}AX^{(k)}$$

General notion of derivative and Newton's method

For $f : \mathbb{R} \to \mathbb{R}$ smooth: local linear approximation

$$f(x+h) \approx f(x) + f'(x)h \quad , h \in \mathbb{R}$$

General: $F : V \to W$, $V, W \hat{=}$ vector space

$$F(\underline{x}+\underline{h}) \approx F(\underline{x}) + DF(\underline{x})(\underline{h}) \quad , \forall \underline{h} \in V$$

$\uparrow$ = linear mapping $V \longrightarrow W$

Note:
- $c \in \mathbb{R} \iff$ linear mapping $\mathbb{R} \to \mathbb{R}$, $t \to c \cdot t$
- $V = W = \mathbb{R}^n$: Jacobi matrix describes linear mapping $DF(x) : \mathbb{R}^n \to \mathbb{R}^n$

Abstract Newton iteration for solving $F(x) = 0$ for $F : D \subset V \to W$

$$\underline{x}^{(k+1)} = \underline{x}^{(k)} + \underline{s} \quad , \quad DF(x^{(k)})\underline{s} = -F(x^{(k)})$$

$\to$ To state Newton iteration we have to find expressions for $DF(x^{(k)})\underline{h}$, $\underline{h} \in V$

Application: Derivative of matrix inversion

Tool: Product rule for general derivatives

- Vector spaces: V, W, U, Z
- $F : V \to W$, $G : V \to U$ differentiable mappings
- $b : W \times U \to Z$ bilinear (linear in each argument)
- $T(\underline{x}) := b(F(x), G(x))$, $T : V \to Z$

Simplest setting: $V = W = U = Z = \mathbb{R}$, $b(\xi, \eta) = \xi \cdot \eta$

$$T(x) = F(x) \cdot G(x) \quad , x \in \mathbb{R}$$

std. prod. rule $\Rightarrow$ $T'(x) = F'(x) \cdot G(x) + F(x) \cdot G'(x) \in \mathbb{R}$

Regarded as linear mappings: $T'(x)h = F'(x)h \cdot G(x) + F(x) \cdot (G'(x)h) \quad \forall h \in \mathbb{R}$

$\uparrow$ linear mapping $\mathbb{R} \to \mathbb{R}$

Product rule: $F : D \subset V \mapsto W$, $G : D \subset V \mapsto U$ sufficiently smooth, $b : W \times U \mapsto Z$ bilinear, *ie.*, linear in each arguent:

linear map $V \to W$ linear map $V \to U$

$$T(\mathbf{x}) = b(F(\mathbf{x}), G(\mathbf{x})) \quad \Rightarrow \quad DT(\mathbf{x})\mathbf{h} = b(\underbrace{DF(\mathbf{x})\mathbf{h}}_{\in W}, G(\mathbf{x})) + b(F(\mathbf{x}), \underbrace{DG(\mathbf{x})\mathbf{h}}_{\in U}) \,, \tag{8.4.9}$$

$\forall \mathbf{h} \in V, \mathbf{x} \in D$.

Matrix inversion :

invertible $n\times n$ matrices

$$\mathrm{inv} := \begin{cases} \mathbb{R}^{n,n}_{reg} \longrightarrow \mathbb{R}^{n,n} \\ X \longrightarrow X^{-1} \end{cases}$$

$\Rightarrow$ $D\mathrm{inv}(X) \hat{=}$ linear mapping $\mathbb{R}^{n,n} \to \mathbb{R}^{n,n}$

Here : Basis free approach

Implicit differentiation & product rule

[Here, $I \hat{=}$ identity matrix is a const. mapping $\mathbb{R}^{n,n} \to I$]

diff.

$$T(X) := \mathrm{inv}(X)\cdot X = I$$

$$DT(X)H = D\mathrm{inv}(X)(H)\cdot X + \mathrm{inv}(X)\cdot H = O$$

$$\boxed{D\,\mathrm{inv}(X)H = -X^{-1}HX^{-1}}\ , H\in\mathbb{R}^{n,n}$$

Product rule: $F : D \subset V \mapsto W$, $G : D \subset V \mapsto U$ sufficiently smooth, $b : W \times U \mapsto Z$ bilinear, *ie.*, linear in each argument:

$$T(\mathbf{x}) = b(F(\mathbf{x}), G(\mathbf{x})) \quad\Rightarrow\quad \mathrm{D}\,T(\mathbf{x})\mathbf{h} = b(\mathrm{D}\,F(\mathbf{x})\mathbf{h}, G(\mathbf{x})) + b(F(\mathbf{x}), \mathrm{D}\,G(\mathbf{x})\mathbf{h})\ , \qquad (8.4.9)$$
$$\mathbf{h}\in V, \mathbf{x}\in D\,.$$

applied with : $F \hat{=} \mathrm{inv}$, $G \hat{=} \mathrm{Id}$ ($\Rightarrow DG(X)H = H$)

$b \Leftrightarrow$ matrix multiply

$V = U = W = Z = \mathbb{R}^{n,n}$

! We never use that matrices can represent linear maps

Note : $D\,\mathrm{id} = \mathrm{id}$:

$$\mathrm{id}(x+h) = x + h = \mathrm{id}(x) + \mathrm{id}(h)$$
$$\Updownarrow \qquad\qquad \Updownarrow \qquad \Updownarrow$$
$$F(x+h) \approx F(x) + DF(x)(h)$$

Newton iteration for matrix inversion

$$F : \mathbb{R}^{n,n}_{reg} \to \mathbb{R}^{n,n}\ , \quad F(X) = A - X^{-1}$$

$[\ A \in \mathbb{R}^{n,n}_{reg}\ ]$

$$F(X^*) = O \iff X^* = A^{-1}$$

Derivative of F : $F(X) = A - \mathrm{inv}(X)$

$$DF(X)\cdot H = O + X^{-1}\cdot H\cdot X^{-1}$$

Newton correction :

$$DF(X^{(k)})S = (X^{(k)})^{-1}S\,(X^{(k)})^{-1} = -F(X^{(k)}) = -A + (X^{(k)})^{-1}$$

$$\Rightarrow \quad S = -X^{(k)}AX^{(k)} + X^{(k)}$$

$\Rightarrow$ Newton it. :

$$X^{(k+1)} = X^{(k)} - X^{(k)}AX^{(k)} + X^{(k)}$$
$$= X^{(k)}(2I - A\cdot X^{(k)})$$

2.4.3. Termination of Newton Iteration

Asymptotic quadratic cvg:

$\Rightarrow \quad \|x^{(k+1)} - x^*\| \ll \|x^{(k)} - x^*\|$

$\Rightarrow \quad \|x^{(k)} - x^*\| \approx \|x^{(k)} - x^{(k+1)}\|$

$\Rightarrow$ correction based termination

↳ One redundant Newton step → significant additional cost.

→ often very few steps only

Cheaper: use simplified Newton correction
(for $n \gg 1$)

$$\Delta\bar{x}^{(k)} := DF(x^{(k-1)})^{-1} F(x^{(k)})$$

LU-dec. available

▶ Economical correction based termination criterion for Newton's method:

STOP, as soon as $\left\|\Delta\bar{\mathbf{x}}^{(k)}\right\| \le \tau_{\mathrm{rel}}\left\|\mathbf{x}^{(k)}\right\|$ **or** $\left\|\Delta\bar{\mathbf{x}}^{(k)}\right\| \le \tau_{\mathrm{abs}}$, (8.4.42)

with simplfied Newton correction $\Delta\bar{\mathbf{x}}^{(k)} := \mathrm{D}F(\mathbf{x}^{(k-1)})^{-1}F(\mathbf{x}^{(k)})$.

2.4.4. Damped Newton Method

Problem: Annoyingly local convergence

Causes:

1

$$F(x) = xe^x - 1 \quad \Rightarrow \quad F'(-1) = 0$$

$x^{(0)} < -1 \quad \Rightarrow \quad x^{(k)} \to -\infty$,
$x^{(0)} > -1 \quad \Rightarrow \quad x^{(k)} \to x^*$,

because all Newton corrections for $x^{(k)} < -1$ make the iterates decrease even further.

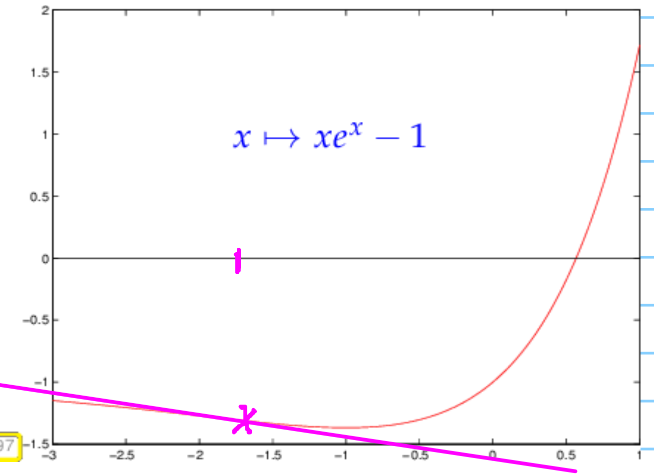

Fig. 297

→ Newton correction in the wrong direction

→ Beyond repair

2

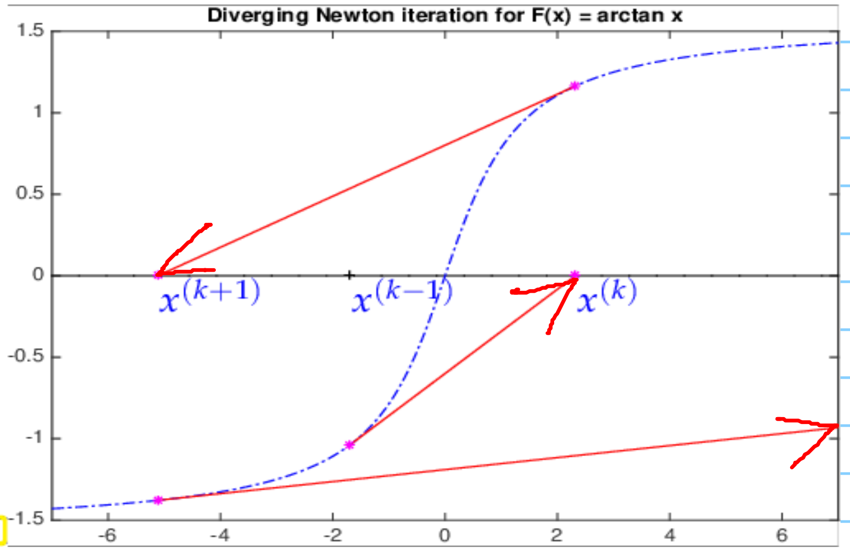

Fig. 299

Overshooting of Newton correction

Remedy: damping

▶ we observe "overshooting" of Newton correction

Idea: **damping** of Newton correction:

With $\lambda^{(k)} > 0$: $\mathbf{x}^{(k+1)} := \mathbf{x}^{(k)} - \lambda^{(k)} \, D F(\mathbf{x}^{(k)})^{-1} F(\mathbf{x}^{(k)})$. (8.4.47)

Terminology: $\lambda^{(k)}$ = damping factor , $\lambda^{(k)} \in]0,1]$

Affine invariant* damping strategy

Choice of damping factor: affine invariant **natural monotonicity test** [?, Ch. 3]: (NMT)

choose "maximal" $0 < \lambda^{(k)} \leq 1$: $\left\| \Delta\overline{\mathbf{x}}(\lambda^{(k)}) \right\| \leq \left(1 - \frac{\lambda^{(k)}}{2}\right) \left\| \Delta\mathbf{x}^{(k)} \right\|_2$ (8.4.49)

where
$\Delta\mathbf{x}^{(k)} := D F(\mathbf{x}^{(k)})^{-1} F(\mathbf{x}^{(k)})$ → current Newton correction ,
$\Delta\overline{\mathbf{x}}(\lambda^{(k)}) := D F(\mathbf{x}^{(k)})^{-1} F(\underbrace{\mathbf{x}^{(k)} + \lambda^{(k)} \Delta\mathbf{x}^{(k)}}_{})$ → tentative simplified Newton correction .

↳ tentative next iterate

* The same damping factor for $AF(x) = 0$ $\forall A \in \mathbb{R}^{n,n}_{reg}$

"Theory": If quad. cvg $\Rightarrow \|\Delta\overline{x}(1)\| \leq \frac{1}{2} \|\Delta x^{(k)}\|$

If NMT passed $\Rightarrow$ reduce damping : $\lambda \leftarrow 2 \cdot \lambda$
failed $\Rightarrow$ increase damping : $\lambda \leftarrow \lambda/2$

C++11 code 8.4.50: Generic damped Newton method based on natural monotonicity test

```cpp
template <typename FuncType, typename JacType, typename VecType>
void dampnewton(const FuncType &F, const JacType &DF,
                VecType &x, double rtol, double atol)
{
  using index_t = typename VecType::Index;
  using scalar_t = typename VecType::Scalar;
  const index_t n = x.size();
  const scalar_t lmin = 1E-3; // Minimal damping factor
  scalar_t lambda = 1.0; // Initial and actual damping factor
  VecType s(n), st(n); // Newton corrections
  VecType xn(n);       // Tentative new iterate
  scalar_t sn, stn;    // Norms of Newton corrections

  do {
    auto jacfac = DF(x).lu(); // LU-factorize Jacobian
    s = jacfac.solve(F(x));   // Newton correction
    sn = s.norm();            // Norm of Newton correction
    lambda *= 2.0;
    do {
      lambda /= 2;
      if (lambda < lmin) throw "No convergence: lambda -> 0";
      xn = x-lambda*s;          // Tentative next iterate
      st = jacfac.solve(F(xn)); // Simplified Newton correction
      stn = st.norm();
    }
    while (stn > (1-lambda/2)*sn); // Natural monotonicity test
    x = xn; // Now: xn accepted as new iterate
    lambda = std::min(2.0*lambda,1.0); // Try to mitigate damping
  }
  // Termination based on simplified Newton correction
  while ((stn > rtol*x.norm()) && (stn > atol));
}
```

tentatively reduce damping