NUMERICAL OPTIMISATION

ROOT FINDING METHODS

- Generalities
- Convergence rates, contraction, invariance, conditions for convergence

NONLINEAR OPTIMISATION

- Classes of problems
- First order optimality conditions
- second order optimality conditions

2

NEWTON-TYPE ALGORITHMS

- Equality constrained problems, convergence
- Inequality constrained problems
- Globalisation techniques

DERIVATIVES

- Algorithm differentiation
- Forward mode
- Backward mode

PARAMETER ESTIMATION

- Least-squares
- Convex penalty terms

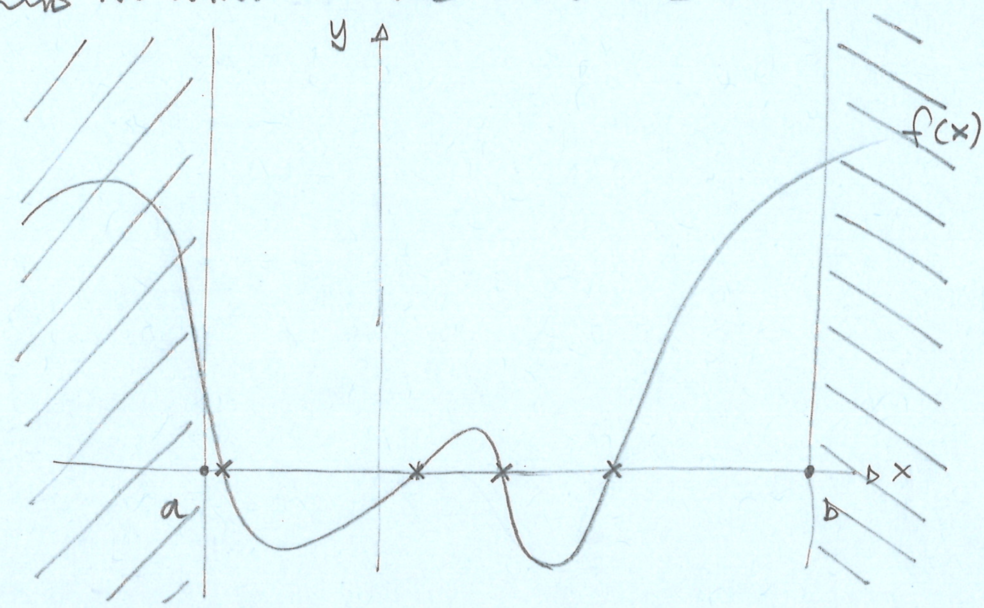
ROOT FINDING AND NEWTON-TYPE METHODS

2a

WE CONSIDER THE PROBLEM OF FINDING THE ZEROS OF SOME FUNCTION

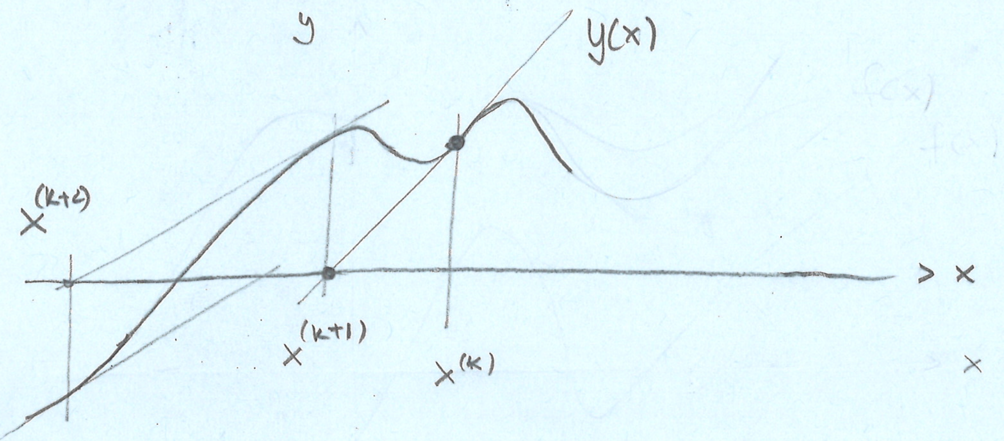
$$f : [a,b] \subset \mathbb{R} \longrightarrow \mathbb{R}$$

$\rightsquigarrow$ WE WANT TO FIND $\alpha \in [a,b]$ such that $f(a) = 0$



WE KNOW THE EQUATION OF THE TANGENT LINE TO THE FUNCTION AT POINT $x^{(k)}$

$$y(x) = f[x^{(k)}] + f'[x^{(k)}][x - x^{(k)}]$$



- WE CAN FIND THE POINT WHERE THE TANGENT LINE EQUALS ZERO
- AND ITERATE

$$0 = f[x^{(k)}] + f'[x^{(k)}][x - x^{(k)}]$$

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

$$\rightsquigarrow \quad x = \frac{-f[x^{(k)}] + f'[x^{(k)}]\,x^{(k)}}{f'[x^{(k)}]}$$

$$= x^{(k)} - f(x^{(k)})/f'(x^{(k)})$$

- THE SEQUENCE $\{x^{(k)}\}$ IS THE NEWTON'S METHOD FOR FINDING THE ZEROS OF FUNCTION f

RFO

NOW CONSIDER A SET OF FUNCTIONS, NOW ALSO MULTIVARIATE

$$
\begin{cases}
f_1(x_1, x_2, \_\_\_, x_N) = 0 \\
f_2(x_1, x_2, \_\_\_, x_N) = 0 \\
\vdots \\
f_M(x_1, x_2, \_\_\_, x_N) = 0
\end{cases}
$$

WE WANT TO FIND THE VALUE $x \in \mathbb{R}^N$ SUCH THAT $f(x) = 0$

⤳ WE CAN EXTEND NEWTON'S METHOD

⤳ WE REPLACE THE FIRST DERIVATIVE OF f WITH THE JACOBIAN OF f

$$
\text{let } J_f = \begin{bmatrix}
\partial f_1/\partial x_1 & \partial f_1/\partial x_2 & \_\_\_ & \partial f_1/\partial x_N \\
\partial f_2/\partial x_1 & \partial f_2/\partial x_2 & \_\_\_ & \partial f_2/\partial x_N \\
\vdots & \vdots & \ddots & \vdots \\
\partial f_N/\partial x_1 & \partial f_N/\partial x_2 & \_\_\_ & \partial f_N/\partial x_N
\end{bmatrix}
$$

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

IT BECOMES $x^{(k+1)} = x^{(k)} - J^{-1}[x^{(k)}]\, f[x^{(k)}]$ (**)

<u>Example</u>

$$
\begin{cases}
f_1(x_1, x_2) = x_1^2 + x_2^2 = 1 \\
f_2(x_1, x_2) = \sin(\pi/2\, x_1) + x_2^3 = 0
\end{cases}
\qquad J = ?
$$

The system has two solutions $\begin{cases} (0.47, -0.88) \\ (-0.47, 0.88) \end{cases}$

RF 0a

WHY IS A METHOD FOR ROOT FINDING IMPORTANT IN OPTIMISATION?

⤳ WE CAN HAVE $f(x) = 0$ WITH $f(x)$ THE GRADIENT OF SOME OBJECTIVE FUNCTION $f(x)$

⤳ THE JACOBIAN OF THE SYSTEM IS THUS GIVEN BY THE HESSIAN $H(x)$ OF $f(x)$

WE GET THE ITERATES $$x^{(k+1)} = x^{(k)} - H^{-1}[x^{(k)}]\nabla f[x^{(k)}]$$

Example

$R(z) = z^{16} - 1$ such that $\dfrac{\partial R(z)}{\partial z} = 16 z^{15}$

→ THE ITERATES OF THE NEWTON'S METHOD ARE

$$z_{k+1} = z_k - \underbrace{\left(16 z_k^{15}\right)}_{\text{Jacobian } \left.\frac{\partial R}{\partial z}\right|_{z_k}}^{-1} \underbrace{\left(z_k^{16} - 1\right)}_{R(z)}$$

→ ALTERNATIVELY, WE COULD USE AN APPROXIMATION OF THE JACOBIAN FOR EXAMPLE A CONSTANT VALUE, $M_K = 16$

ROOT FINDING AND NEWTON'S TYPE METHODS

WE ARE INTERESTED IN SOLVING A SYSTEM OF EQUATIONS $R(z) = 0$ (POTENTIALLY NONLINEAR)

⤳ FUNCTION $R : \mathbb{R}^n \to \mathbb{R}^n$ (so $z \in \mathbb{R}^n$)

WE KNOW THAT THIS FUNCTION IS DIFFERENTIABLE

Example

SOME CONSTANT VALUE (say, 2)

i) $R(z) = z^{16} - \text{Const}$ (1 variable, 1 equation) $z \in \mathbb{R}$

ii) $R(z) = \begin{pmatrix} z_1^4 - z_2 \\ z_2^4 - \text{Const} \end{pmatrix} \begin{matrix} R_1(z) \\ R_2(z) \end{matrix}$ (2 variables, 2 equations) $z \in \mathbb{R}^2$

The derivative(s) of $R(z)$

i) $\dfrac{\partial R}{\partial z} = 16 z^{15}$

ii) $\dfrac{\partial R}{\partial z} = \begin{bmatrix} 4z_1^3 & -1 \\ 0 & 4z_2^3 \end{bmatrix}$ ← The Jacobian matrix

$\dfrac{\partial R_1}{\partial z_1}$ $\quad \partial R_1 / \partial z_2 \quad$ $\dfrac{\partial R_2}{\partial z_1}$ $\quad \dfrac{\partial R}{\partial z_2}$

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IDEA BEHIND NEWTON'S METHODS ⤳ USE A TAYLOR SERIES (1st) EXPANSION OF R AND SOLVE A LINEAR SYSTEM (easier)

1. GUESS $z_k \in \mathbb{R}^n$
2. GET NEW z_{k+1} AS SOLUTION OF $\underbrace{R(z_k) + \dfrac{\partial R}{\partial z}(z_k)(z - z_k) \approx R(z)}_{\text{1st ORDER TAYLOR SERIES APPROX OF } R(z)} = 0$

↓ THIS CAN BE EXPLICITLY COMPUTED

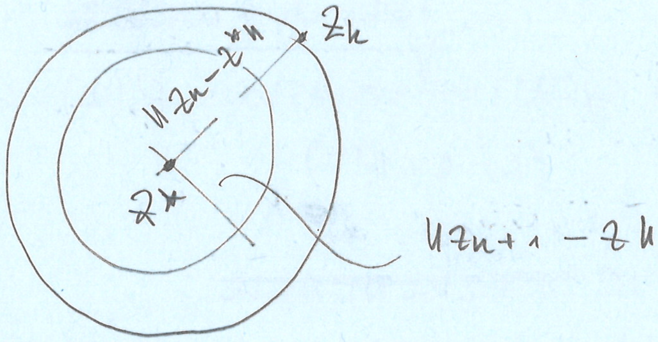
$$z_{k+1} = z_k - \underbrace{\left[\left. \frac{\partial R}{\partial z} \right|_{z_k} \right]^{-1}}_{\substack{\text{THE JACOBIAN MUST BE INVERTIBLE} \\ J_k}} R(z_k)$$

← NEWTON'S ITERATION

3. REPEAT 2.

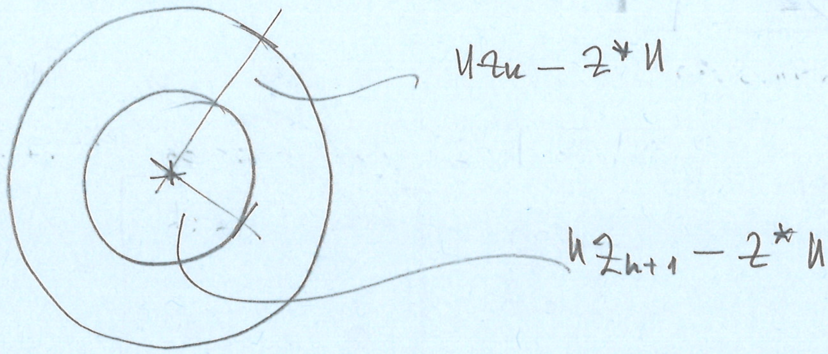
↳ STOPS IF $J_k = 0$ OR $R(z_k) = 0$

Q-LINEAR CONVERGENCE (After local convergence rate, when in class)

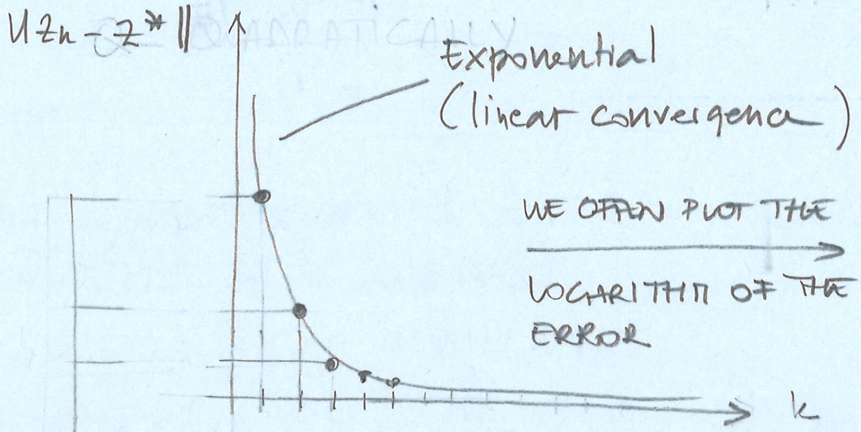


THE NEXT ITERATE MUST BE WITHIN THE k-TH BALL (SHRINKS)

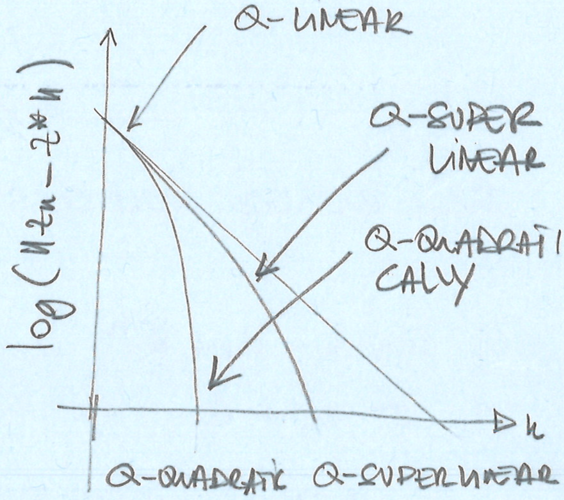
Q-SUPERLINEAR CONVERGENCE



THE SHRINKING FACTOR ITSELF CONVERGES TO ZERO



WE OFTEN PLOT THE → LOGARITHM OF THE ERROR



→ Q-LINEARLY WITH c=2 (at each iteration we contract by a factor equal c=2)

(it is exponential, so linear in log scale)

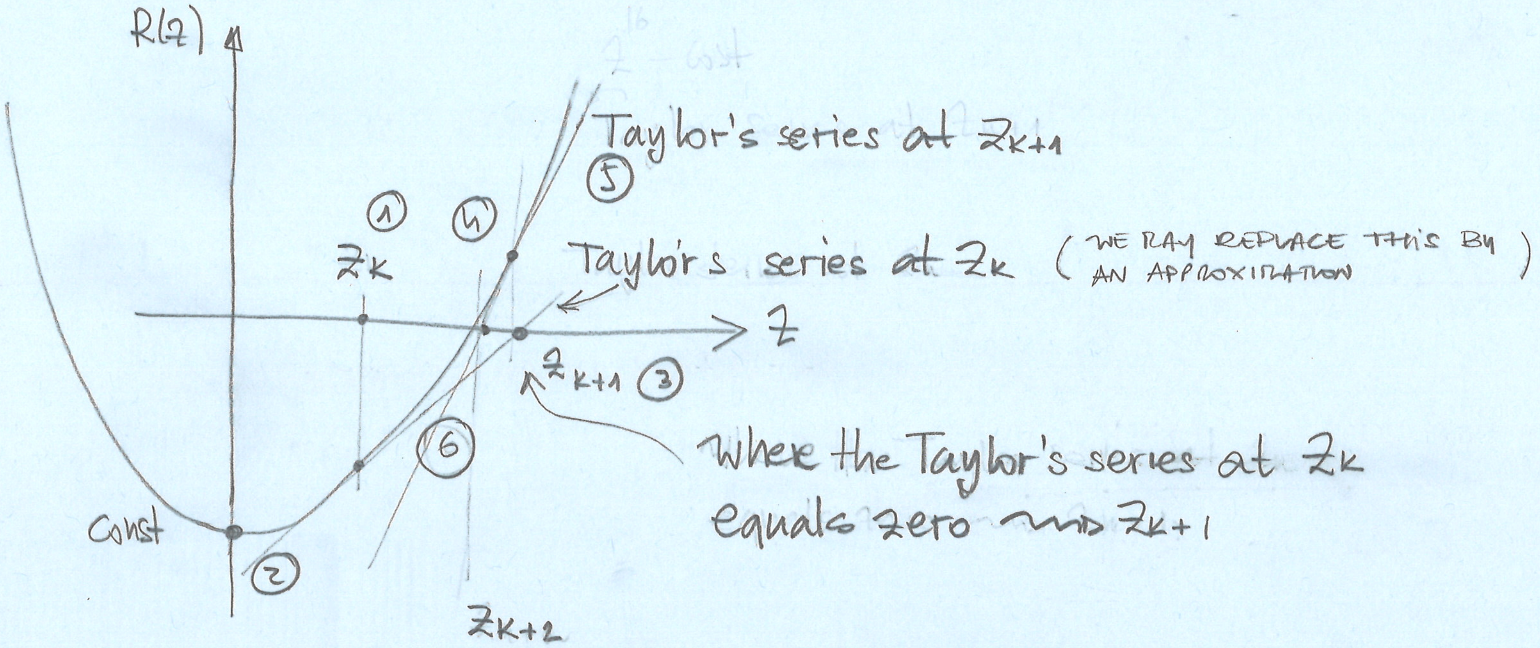
On a general level, we can use some <u>invertible approximation</u> M_k of the Jacobian J_k

$$\rightsquigarrow z_{k+1} = z_k - \left[M_k \right]^{-1} R(z_k)$$

NEWTON-TYPE ITERATION

APPROXIMATES THE JACOBIAN

GENERAL FORM OF A NEWTON'S TYPE METHOD $\left(M_k \approx \frac{\partial R}{\partial z}\Big|_{z_k}\right)$



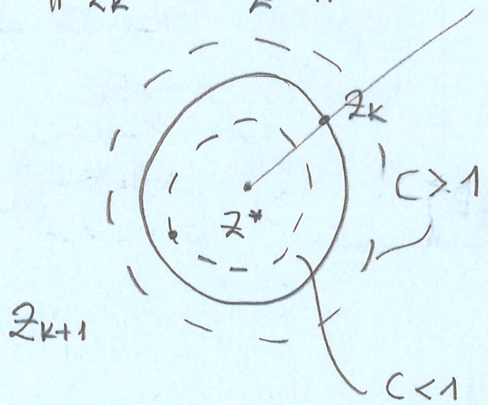
THE SEQUENCE OF ITERATES $\{z_k\}_{k=0}^{\infty}$ WILL CONVERGE TO THE SOLUTION

⇝ WE NEED TO DEFINE THE CONVERGENCE RATE!

⇝ (CONDITIONS FOR CONVERGENCE / DIVERGENCE)

$$\frac{\| z_{k+1} - z^* \|}{\| z_k - z^* \|} \leq C$$

Q-LINEAR CONVERGENCE



C IS A SHRINKING FACTOR
AND IT IS OF FIXED SIZE

Q-SUPERLINEAR CONVERGENCE

$$\frac{\| z_{k+1} - z^* \|}{\| z_k - z^* \|} \leq C_k$$

C_k IS A SHRINKING FACTOR
AND ITSELF SHRINKS (VARIABLE SIZE)
TO ZERO (IT GETS INFINITELY SMALLER)

Q-QUADRATIC CONVERGENCE

$$\| z_{k+1} - z^* \| \leq C \underbrace{\| z_k - z^* \| \| z_k - z^* \|}_{\| z_k - z^* \|^2}$$

LOCAL CONVERGENCE RATES

Def. (Types of convergence rates) Assume $z_k \in \mathbb{R}^n$ and $\underbrace{z_k \xrightarrow{\text{CONVERGES TO}} z^*}$ for $k \to \infty$

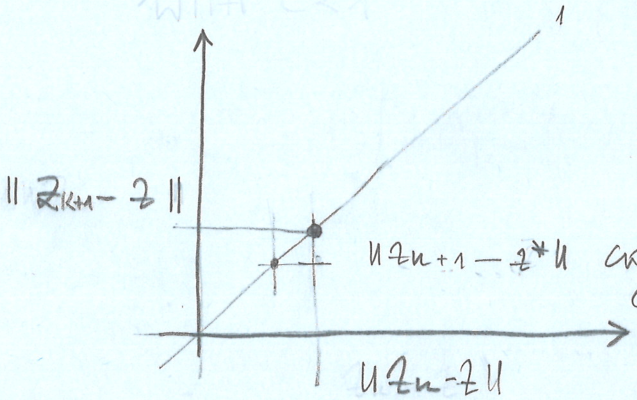
CONVERGENT TO SOMETHING FOR $k \to \infty$

We SAY:

1. (z_k) is CONVERGENT TO z^* Q-LINEARLY

IFF $\exists C < 1$ SUCH THAT $\|z_{k+1} - z^*\| \leq C\|z_k - z^*\|$

(for all $k \geq k_0$)



$$\rightsquigarrow \limsup_{k \to \infty} \underbrace{\frac{\|z_{k+1} - z^*\|}{\|z_k - z^*\|}}_{\text{"QUOTIENT"}} < 1$$

2. (z_k) is CONVERGENT TO z^* Q-SUPERLINEARLY (STRONGER)

IFF $\exists C_k$ SUCH THAT $\|z_{k+1} - z^*\| \leq C_k \|z_k - z^*\|$ WITH $C_k \to 0$

THE SEQUENCE $\{C_k\}$ CONVERGE TO ZERO

(for all $k \geq k_0$)

$$\rightsquigarrow \limsup_{k \to \infty} \frac{\|z_{k+1} - z^*\|}{\|z_k - z^*\|} = 0$$

3. (z_k) is CONVERGENT TO z^* Q-QUADRATICALLY

IFF $\exists C < \infty$ SUCH THAT $\|z_{k+1} - z^*\| \leq C \|z_k - z^*\|^2$

(for all $k \geq k_0$)

$$\leq \underbrace{C\,\|z_k - z^*\|}\,\|z_k - z^*\|$$

THE SIZE OF THE SHRINKING DEPENDS ON THE CLOSENESS (LINEARLY)

$$\rightsquigarrow \limsup_{k \to \infty} \frac{\|z_{k+1} - z^*\|}{\|z_k - z^*\|} < \infty$$

Proof.

$$
\begin{aligned}
z_{k+1} - z^* &= z_k - z^* - M_k^{-1} R(z_k) \\
&= z_k - z^* - M_k^{-1}\left[R(z_k) - R(z^*)\right] \\
&= M_k^{-1}\left[M_k(z_k - z^*)\right] - M_k^{-1}\int_0^1 J(z^* + t(z_k - z^*))(z_k - z^*)\,dt \\
&= M_k^{-1}\left[M_k - J(z_k)\right](z_k - z^*) + \\
&\quad - M_k^{-1}\int_0^1 \left[J(z^* + t(z_k - z^*)) - J(z_k)\right](z_k - z^*)\,dt
\end{aligned}
$$

Take the norm of both side, to get

$$
\begin{aligned}
\|z_{k+1} - z^*\| &\leq K_k \|z_k - z^*\| + \int_0^1 w \|z^* + t(z_k - z^*) - z_k\|\,dt\, \|z_k - z^*\| \\
&= \left[K_k + w \underbrace{\int_0^1 (1-t)\,dt}_{1/2} \|z_k - z^*\|\right] \|z_k - z^*\| \\
&= \left[K_k + \frac{w}{2}\|z_k - z^*\|\right] \|z_k - z^*\| \qquad \square
\end{aligned}
$$

THE LOCAL CONTRACTION THEOREM

Th. (Local contraction) CONSIDER A NONLINEAR DIFFERENTIABLE FUNCTION $R : \mathbb{R}^n \to \mathbb{R}^n$ AND A SOLUTION $z^* \in \mathbb{R}^n$ (THAT IS SUCH THAT $R(z^*) = 0$)

CONSIDER A NEWTON'S TYPE OF ITERATION $z_{k+1} = z_k - \underbrace{M_k^{-1}}_{\text{APPROXIMATE JACOBIAN / OR ACTUAL JACOBIAN}} R(z_k)$
WITH INITIAL ITERATE z_0

THE SEQUENCE $(z_k)_{k=0}^{\infty}$ CONVERGES TO z^* WITH CONTRACTION RATE

$$\| z_{k+1} - z^* \| \leq \underbrace{\left(K_k + \frac{w}{2} \| z_k - z^* \| \right)} \cdot \| z_k - z^* \|$$

IT GETS CLOSER WITH K :-)

IF THERE EXIST $w < \infty$ AND $K < 1$ SUCH THAT THE FOLLOWING HOLDS

$$\begin{cases} \| M_k^{-1} [\underbrace{J(z_k) - J(z)}_{(*)}] \| \leq w \| z_k - z \| & \text{(Lipschitz condition)} \\ \| M_k^{-1} [\underbrace{J(z_k) - M_k}_{(**)}] \| \leq K_k < K & \text{(Compatibility condition)} \end{cases}$$

$*$ DISTANCE BETWEEN JACOBIANS
$**$ DISTANCE WITH APPROXIMATION

FOR ALL z_k AND z IN $\mathbb{R}^n$

AND, IF $\| z_0 - z^* \|$ IS SMALL ENOUGH, THAT IS SUCH THAT

then $\to \| z_0 - z^* \| < \dfrac{2(1-K)}{w}$

ITERATIONS START CLOSE ENOUGH TO THE SOLUTION

FOR $K = 0$, THE METHOD IS THE EXACT NEWTON'S METHOD

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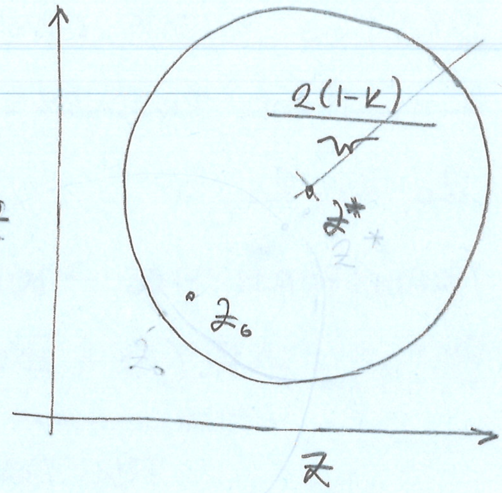
IT COMPARES DISTANCES TO THE OPTIMAL SOLUTION BETWEEN TWO SUCCESSIVE ITERATIONS z_{k+1} AND z_k

THE IDEA BEHIND THE CONTRACTION RATE



– Consider the two-dimensional case :

THE FIRST CONTRACTION FACTOR

$\left(K_0 + \frac{\nu}{2} \| z_k - z^* \|\right)$ IS SMALLER THAN

$\left(K + \frac{\nu}{2} \| z_k - z^* \|\right) < 1$

BECAUSE $\| z_0 - z^* \| < \frac{2(1-K)}{\nu}$

THIS IMPLIES THAT $\| z_1 - z^* \| \leq \delta \| z_0 - z^* \|$ WITH

$\delta = \left(K + \frac{\nu}{2} \| z_k - z^* \|\right)$

RECURSIVELY SO FOR ALL CONTRACTION FACTORS WE HAVE THE BOUND δ SUCH THAT

$$\underbrace{\| z_k - z^* \| \leq \delta_k \| z_0 - z^* \|}_{\text{This implies linear convergence with contraction rate } \delta}$$

LOCAL CONTRACTION RATES WILL BE USUALLY FASTER THAN THIS

- $R(z)=0$ IS THE GIVEN PROBLEM
- A METHOD PRODUCES THE FOLLOWING SEQUENCE OF ITERATES

  $z_0, z_1, z_2, \dots$
- TRANSFORM THE PROBLEM (COORDINATE CHANGE)

$$\tilde{R}(y) = \underbrace{AR(b+By)}_{\text{THE TRANSFORMED RESIDUAL TAKES THIS FORM}} = 0$$

- APPLY THE METHOD TO $\tilde{R}(y)=0$ FROM $y_0 = B^{-1}(z_0 - b)$ (THE SAME INITIAL CONDITION IN THE NEW COORDINATE SYSTEM)

$\rightarrow$ $y_0, y_1, y_2, \dots$ SUCH THAT $y_k = B^{-1}(z_k - b)$ $\forall k$

From $z^* = b + By^*$

$\rightsquigarrow$ $By^* = z^* - b$

$\rightsquigarrow$ $B^{-1}By^* = B^{-1}(z^* - b)$

AFFINE INVARIANCE (CONDITIONS)

$$z_{k+1} = z_k - J(z_k)^{-1}R(z_k)$$

Does this update relate to $y_{k+1} = y_k - \tilde{J}(y_k)^{-1}\tilde{R}(y_k)$

$$\tilde{J}(y_k) = AJ(b+By)B$$

We obtain,

$$y_{k+1} = y_k - \underbrace{B^{-1}J(b+By)^{-1}\underbrace{A^{-1}A}_{I}R(b+By)}_{J(y_{k+1})^{-1}R(z_k)}$$

AFFINE INVARIANCE (of an algorithm)

Consider an iterative algorithm for rootfinding tasks $R(z)=0$

→ THE METHOD IS CALLED AFFINE INVARIANT, IF AFFINE BASIS TRANSFORMATIONS OF THE EQUATIONS OF THE VARIABLES WILL NOT CHANGE THE RESULTING ITERATIONS

Consider 2 invertible matrices A and $B \in \mathbb{R}^{n \times n}$ and a vector $b \in \mathbb{R}^n$

1/ → CONSIDER THE FOLLOWING ROOT FINDING PROBLEM

$$\tilde{R}(y) \equiv A R(\underbrace{b + By}) = 0 \qquad \boxed{z = By + b}$$

→ THE SOLUTION TO $R^*(z) = 0$ IS z^*

If we have the solution z^* we can construct it from y^* such that $\tilde{R}(y^*) = 0$, by inverting the relation $z^* = b + By^*$

→ THAT IS $y^* = B^{-1}(z^* - b)$

2/ → CONSIDER AN ITERATIVE ALGORITHM THAT STARTING FROM THE INITIAL SOLUTION, x_0, GENERATES THE ITERATES $z_0, z_1, \dots$ THAT CONVERGE TO THE SOLUTION OF $R(z)=0$

The method is called AFFINE INVARIANT IF, WHEN APPLIED TO $\tilde{R}(y) = 0$ from the initial solution $y_0 = B^{-1}(z_0 - b)$, the resulting iterates $y_0, y_1, \dots$ all satisfy $y_k = B^{-1}(z_k - b)$

EXACT NEWTON'S METHOD IS AFFINE INVARIANT, AS MANY OTHERS

RFS

AFFINE INVARIANCE IS AN IMPORTANT PROPERTY OF ITERATIVE METHODS FOR ROOT FINDING (~ NUMERICAL OPTIMISATION)

SUPPOSE THAT YOUR TASK IS TO FIND THE EQUILIBRIUM TEMPERATURE IN A CHEMICAL REACTION SYSTEM

→ The problem can be formulated by considering temperatures expressed in different units (K, C, and F)

→ K, C, F formulations will lead to different numerical results corresponding to the same physical temperature

→ The different solutions can be obtained by affine transformations from one another