$f(x) = 0$

$x = x + f(x) = \phi_1(x)$ $\qquad x = \phi_1(x)$ Fix point problem.

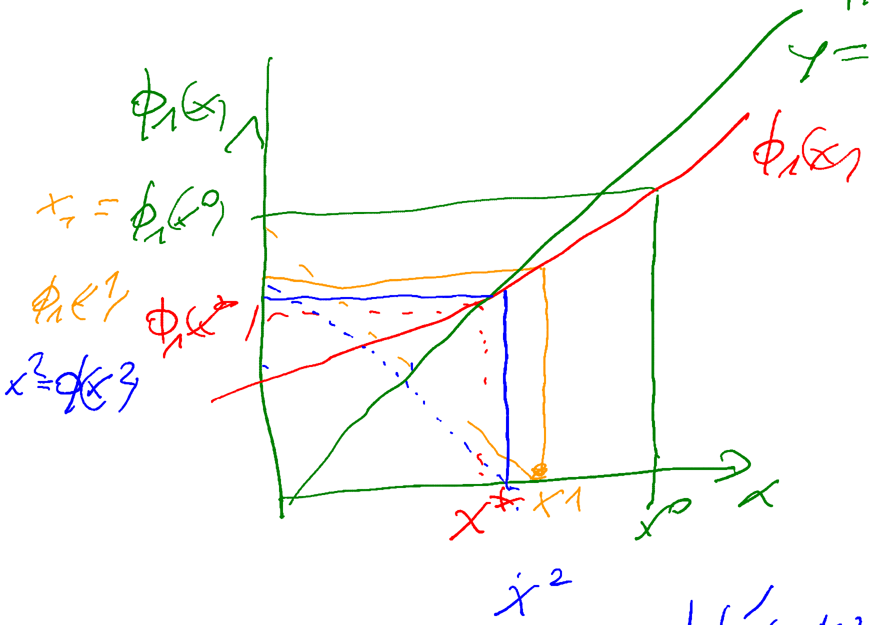
choose $x^0$

$x^1 = \phi_1(x^0)$

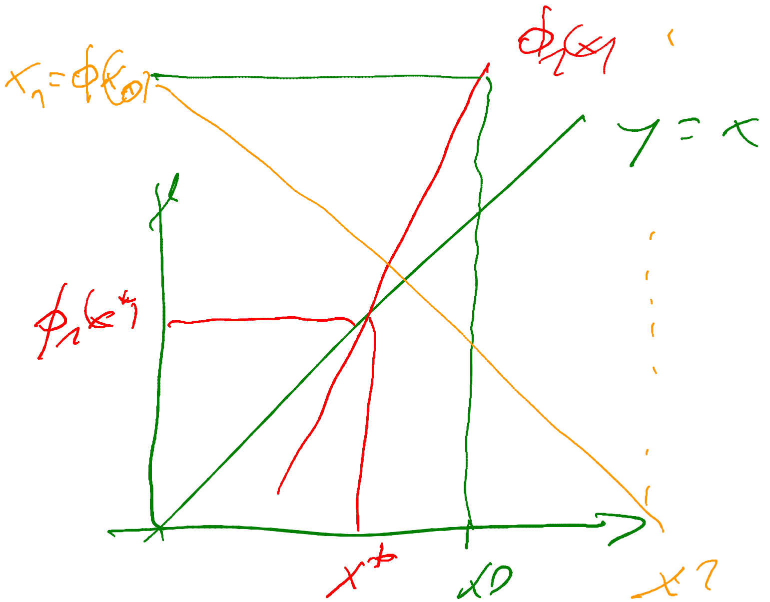
$x^2 = \phi_1(x^1)$

$\vdots$

hope: $x^n \xrightarrow{n\to\infty} x^*$ $\qquad x^* = \phi_1(x^*)$




$|\phi_1'(x^*)| < 1$




$|\phi_1'(x^*)| > 1$

Banach Fixed Point Theorem:

$$\|\phi(x) - \phi(y)\| < L \|x-y\| \quad \forall x,y \in D$$

Lipschitz continuity $\Longleftarrow$ $\phi$ differentiable

if $L < 1$ $\Longrightarrow$ $x^n \xrightarrow{n\to\infty} x^*$ $\quad x^* = \phi(x^*)$

-) converges slowly

+) no derivatives

$\pm$) no unique $\quad f(x) = 0$

$$x = x + f(x) = \phi_1(x)$$

$$x = x - f(x) = \phi_2(x)$$

$$1 = 1 + f(x) \qquad x = \frac{x}{1+f(x)} = \phi_3(x)$$

## 2.4 the Newton–method

**Aim:** We look for the zero's of a function $\mathbf{f} : D \to \mathbb{R}^n$, $D \subset \mathbb{R}^n$:

$$\mathbf{f}(\mathbf{x}) = \mathbf{0}$$

- We already know the fixed-point iteration

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

  with starting point $\mathbf{x}^0$ and iteration map $\Phi : \mathbb{R}^n \to \mathbb{R}^n$.
- Convergence results are given by the Banach Fixed Point Theorem.

**Advantage:** this method is **derivative-free**.

**Disadvantages:**

- the numerical scheme converges to slow (only linear),
- there is no unique iteratin map.

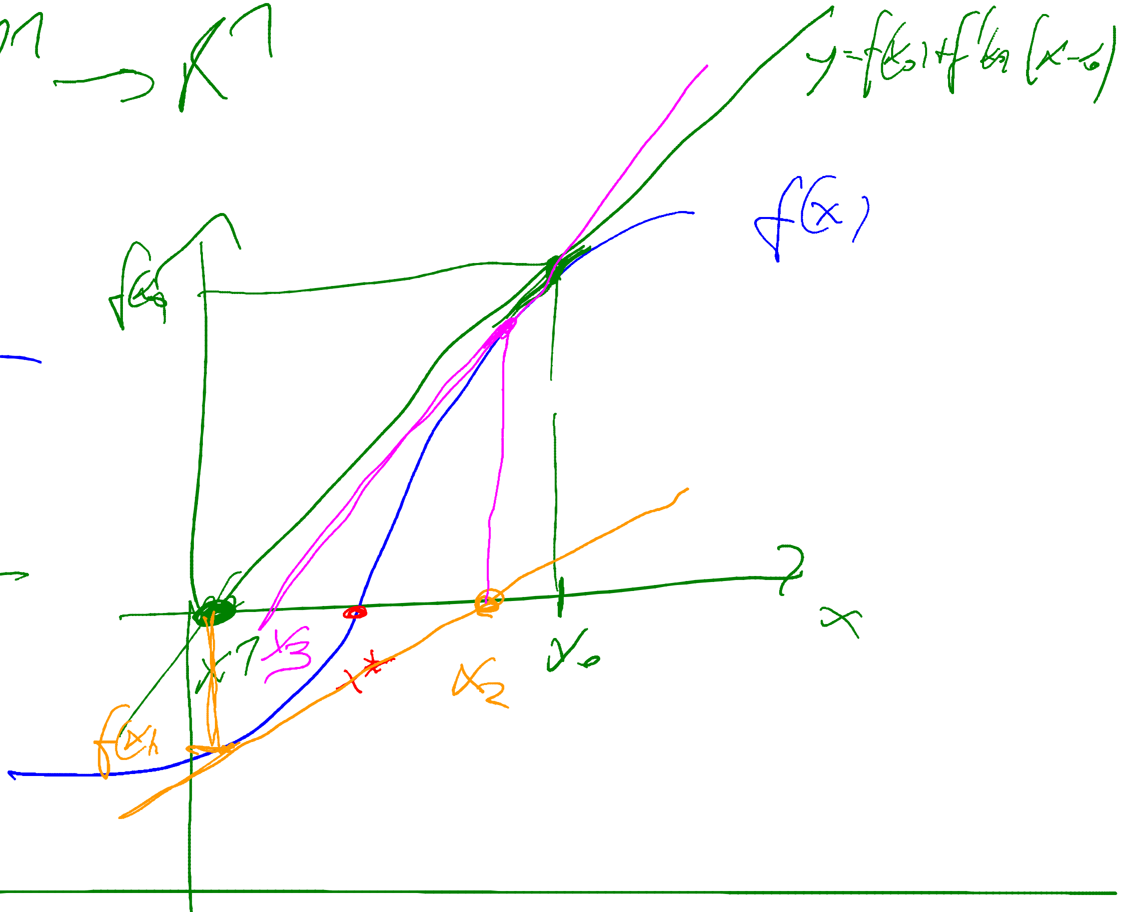
Newton $n=1$ $f: D \subset \mathbb{R}^1 \to \mathbb{R}^1$

$$f(x) = f(x_0) + f'(x_0)(x-x_0) \, \boxed{+ \dots}$$

$$y = f(x_0) + f'(x_0)(x-x_0)$$

look for $y=0 \iff x^1 = x_0 - \frac{f(x_0)}{f'(x_0)}$

$$y'(x_0) = f'(x_0)$$

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$n>1$ $f(x^*)=0$ $f(x) = f(x_0) + \underbrace{Jf(x_0)}_{n\times n}(x-x_0) \, \boxed{+}$ $f: \mathbb{R}^n \to \mathbb{R}^n$

$$y = f(x_0) + Jf(x_0)(x-x_0)$$

$y=0 \iff \begin{cases} \underline{Jf(x_0)}(x_1-x_0) = -f(x_0) & \Rightarrow \text{linear system for } (x_1-x_0) \Rightarrow x_1 \; \checkmark \\ x = x_0 - (Jf(x_0))^{-1} f(x_0) & \text{calculate inverse of } Jf(x_0) \; ↯ \end{cases}$

# The construction of the Newton method.

Starting point: Let $\mathcal{C}^1$–function $\mathbf{f} : D \to \mathbb{R}^n$, $D \subset \mathbb{R}^n$ open.

We look for a zero of $\mathbf{f}$, i.e. a $\mathbf{x}^* \in D$ with

$$\mathbf{f}(\mathbf{x}^*) = \mathbf{0}$$

Construction of the Newton–method:

The Taylor–expansion of $\mathbf{f}(\mathbf{x})$ at $\mathbf{x}^0$ is given by

$$\mathbf{f}(\mathbf{x}) = \mathbf{f}(\mathbf{x}^0) + \mathbf{Jf}(\mathbf{x}^0)(\mathbf{x} - \mathbf{x}^0) + \mathbf{o}(\|\mathbf{x} - \mathbf{x}^0\|)$$

Setting $\mathbf{x} = \mathbf{x}^*$ we obtain

$$\mathbf{Jf}(\mathbf{x}^0)(\mathbf{x}^* - \mathbf{x}^0) \approx -\mathbf{f}(\mathbf{x}^0)$$

An approximative solution for $\mathbf{x}^*$ is given by $\mathbf{x}^1$, $\mathbf{x}^1 \approx \mathbf{x}^*$, the solution of the linear system of equations

$$\mathbf{Jf}(\mathbf{x}^0)(\mathbf{x}^1 - \mathbf{x}^0) = -\mathbf{f}(\mathbf{x}^0)$$

# The Newton–method as algorithm.

The Newton–method can be formulated as algorithm.

**Algorithm** (Newton–method)**:**

**(1) FOR** $k = 0, 1, 2, \dots$

**(2a) Solve** $\mathbf{Jf}(\mathbf{x}^k) \cdot \Delta\mathbf{x}^k = -f(\mathbf{x}^k)$**;**

**(2b) Set** $\mathbf{x}^{k+1} = \mathbf{x}^k + \Delta\mathbf{x}^k$**;**

- In *every* Newton–step we solve a set of linear equations.
- The solution $\Delta\mathbf{x}^k$ is called Newton–correction.
- The Newton–method is scaling-invariant.

# Scaling-invariance of the Newton–method.

**Theorem:** the Newton–method is invariant under linear transformations of the form

$$\mathbf{f}(\mathbf{x}) \to \mathbf{g}(\mathbf{x}) = \mathbf{A}\mathbf{f}(\mathbf{x}) \qquad \text{for } \mathbf{A} \in \mathbb{R}^{n\times n} \text{ regular,}$$

i.e. the iterates for **f** and **g** are identical.

**Proof:** Constructing the Newton–method for $\mathbf{g}(\mathbf{x})$, then the Newton–correction is given by

$$(*) = J[Af(x^k)](x^{k+1}-x^k) = \boxed{Jg(x^k)(x^{k+1}-x^k) = -g(x^k)} = \boxed{-Af(x^k)}$$

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

$A^{-1}$

$$\boxed{Jf(x^k)(x^{k+1}-x^k) = -f(x^k)}$$

$$\begin{aligned}
\Delta\mathbf{x}^k &= -(\mathbf{Jg}(\mathbf{x}^k))^{-1} \cdot \mathbf{g}(\mathbf{x}^k) \\
&= -(\mathbf{AJf}(\mathbf{x}^k))^{-1} \cdot \mathbf{Af}(\mathbf{x}^k) \\
&= -(\mathbf{Jf}(\mathbf{x}^k))^{-1} \cdot \mathbf{A}^{-1}\mathbf{A} \cdot \mathbf{f}(\mathbf{x}^k) \\
&= -(\mathbf{Jf}(\mathbf{x}^k))^{-1} \cdot \mathbf{f}(\mathbf{x}^k)
\end{aligned}$$

and thus the Newton–correction of **f** and **g** conincide.

Using the same starting point $\mathbf{x}^0$ we obtain the same iterates $\mathbf{x}^k$.

# Local convergence of the Newton–method.

**Theorem:** Let $\mathbf{f} : D \to \mathbb{R}^n$ be a $\mathcal{C}^1$–function, $D \subset \mathbb{R}^n$ open and convex. Let $\mathbf{x}^* \in D$ a zero of $\mathbf{f}$, i.e. $\mathbf{f}(\mathbf{x}^*) = 0$.

Let the Jacobi–matrix $\mathbf{Jf}(\mathbf{x})$ be regular for $\mathbf{x} \in D$, and suppose the Lipschitz–condition for $\phi(z) = (\mathbf{J}f(x))^{-1} \mathbf{J}f(z)$

$$\|(\mathbf{Jf}(\mathbf{x})^{-1}(\mathbf{Jf}(\mathbf{y}) - \mathbf{Jf}(\mathbf{x}))\| \leq L\|\mathbf{y} - \mathbf{x}\| \qquad \text{for all } \mathbf{x}, \mathbf{y} \in D,$$

holds true with $L > 0$. Then the Newton–method is well defined for all starting points $\mathbf{x}^0 \in D$ with

$$\boxed{\|\mathbf{x}^0 - \mathbf{x}^*\| < \frac{2}{L} =: r} \text{ and } \quad K_r(\mathbf{x}^*) \subset D$$

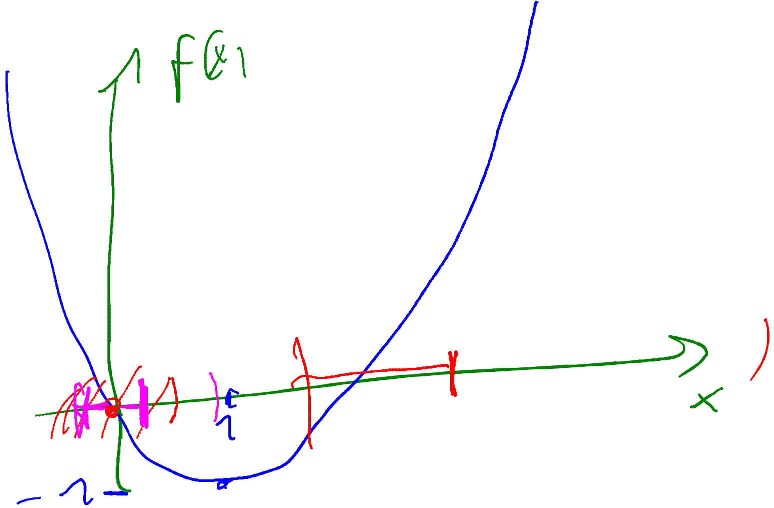
with $\mathbf{x}^k \in K_r(\mathbf{x}^*)$, $k = 0, 1, 2, \ldots$, and the Newton–iterates $\mathbf{x}^k$ converge quadratically to $\mathbf{x}^*$, i.e.

$$\boxed{\|\mathbf{x}^{k+1} - \mathbf{x}^*\| \leq \frac{L}{2} \|\mathbf{x}^k - \mathbf{x}^*\|^2}$$

$\mathbf{x}^*$ is the unique zero of $\mathbf{f}(\mathbf{x})$ within the ball $K_r(\mathbf{x}^*)$.

Example $f(x)=0$

$$f(x) = (x-1)^2 - 1$$




$$Jf(x) = 2(x-1)$$

$$(Jf(x))^{-1} = \frac{1}{2(x-1)}$$

$L>0$?

$$\|(Jf(x))^{-1}(Jf(y) - Jf(x))\|_2 = \left\| \frac{1}{2(x-1)}\big(2(y-1) - 2(x-1)\big)\right\| = \left\| \frac{1}{x-1}(y-x)\right\| \le$$

$$\le \left\|\frac{1}{x-1}\right\| \|y-x\| \le L\,\|y-x\|$$

$x^* = 0$

$$\begin{cases} \left|\frac{1}{x-1}\right| < 2 = L & \text{if } x \in \left(-\infty, \frac{1}{2}\right) \\ \left|\frac{1}{x-1}\right| < 10 & \text{if } x \in \left(-\infty, \frac{9}{10}\right) \end{cases}$$

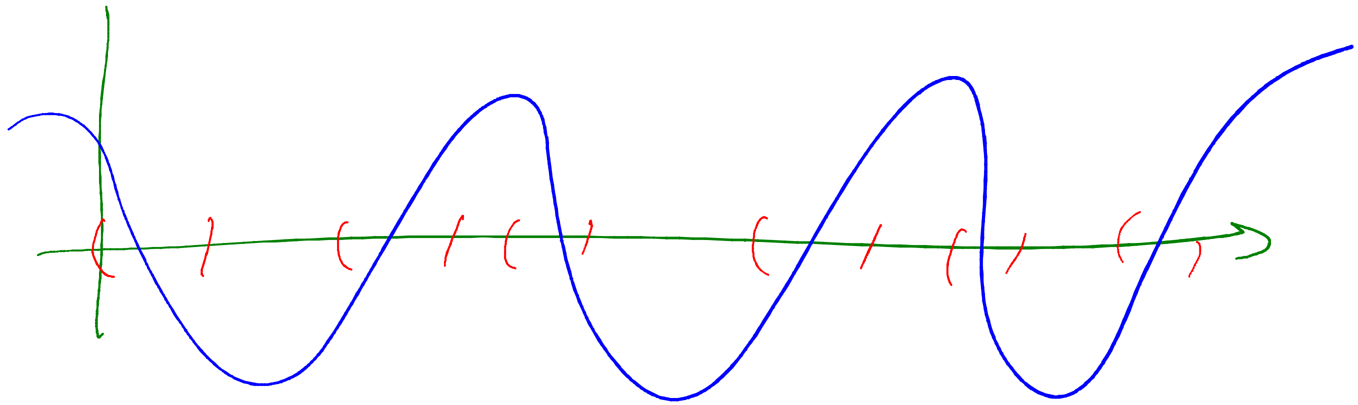
$|x^0 - x^*| = |x^0 - 0| < \frac{2}{L} = 1$

$|x^0 - x^*| = |x^0 - 0| < \frac{2}{10} = \frac{1}{5}$

$x^* = 1$

$$\left\{ \left|\frac{1}{x-1}\right| < 2 \quad \text{if } x \in \left(\frac{3}{2}, \infty\right) \right.$$

$|x^0 - x^*| = |x^0 - 1| < 1$



Proof:

$$\rho(t) = (Jf(x))^{-1} f(x+t(y-x)) \qquad t\in[0,1] \qquad \rho:\mathbb{R}^1\to\mathbb{R}^n$$

$$\rho(0) = (Jf(x))^{-1} f(x)$$

$$\rho(1) = (Jf(x))^{-1} f(y)$$

$$\rho'(t) = (Jf(x))^{-1} \overbrace{Jf(x+t(y-x))\cdot(y-x)}^{\text{chain rule}}$$

$$\boxed{\|\rho'(t)-\rho'(0)\|} = \|(Jf(x))^{-1} Jf(x+t(y-x))\cdot(y-x) - (Jf(x))^{-1} Jf(x)(y-x)\|$$

$$= \|(Jf(x))^{-1}\left[Jf(x+t(y-x)) - Jf(x)\right]\cdot(y-x)\|$$

$$\le \underbrace{\|(Jf(x))^{-1}\left[Jf(x+t(y-x)) - Jf(x)\right]\|}_{y\,=\,x+t(y-x)} \|y-x\| \qquad \leftarrow \text{condition of the theorem}$$

$$\le L\|\cancel{x}+t(y-x)-\cancel{x}\|$$

$$\le Lt\|y-x\|\,\|y-x\| \le \boxed{Lt\|y-x\|^2}$$

$$\boxed{\|Jf(x)^{-1}(f(y)-f(x)-Jf(x)(y-x))\|} = \|\rho(1)-\rho(0)-\rho'(0)\| = \left\|\int_0^1 \rho'(t)\,dt - \rho'(0)\right\| = \left\|\int_0^1 (\rho'(t)-\rho'(0))\,dt\right\|$$

$$\le \int_0^1 \|\rho'(t)-\rho'(0)\|\,dt \le \int_0^1 Lt\|y-x\|^2\,dt = L\|y-x\|^2\int_0^1 t\,dt$$

$$\boxed{= \frac{L}{2}\|y-x\|^2}$$

$$x^{k+1} - x^* = x^k - (Df(x^k))^{-1} f(x^k) - x^* =$$

$$= (Df(x^k))^{-1} \big( f(x^k) - \underbrace{f(x^*)}_{=0} \big) + (Df(x^k))^{-1} Df(x^k)(x^k - x^*)$$

$$= (Df(x^k))^{-1} \big[ f(x^*) - f(x^k) - Df(x^k)(x^* - x^k) \big]$$

$y = x^*$ $\quad x = x^k$

$$\boxed{\| x^{k+1} - x^* \| \leq \frac{L}{2} \| x^k - x^* \|^2}$$

# The damped Newton–method.

**Additional obserrvations:**

- The Newton–method converges quadratically, but only locally.
- Global convergence can be obtained - if applicable - by a damping term:

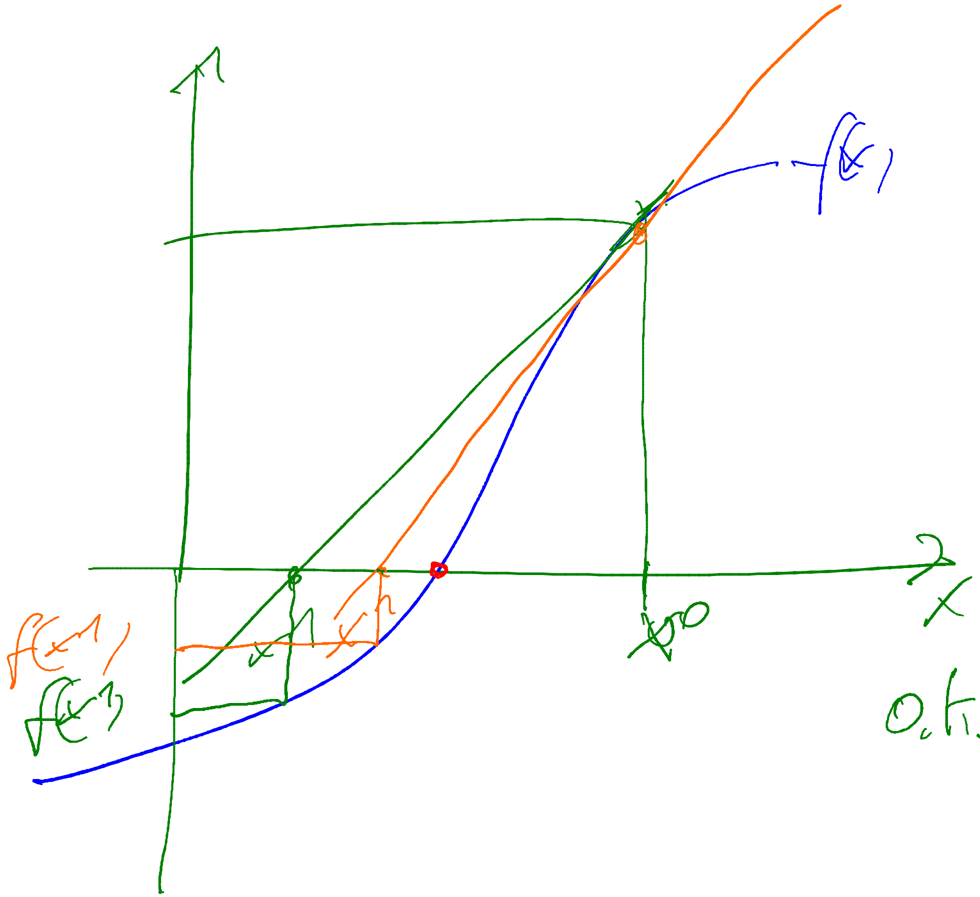
**Algorithm** (Damped Newton–method)**:**

**(1) FOR** $k = 0, 1, 2, \dots$

**(2a) Solve** $\mathbf{Jf}(\mathbf{x}^k) \cdot \Delta\mathbf{x}^k = -f(\mathbf{x}^k)$**;**

**(2b) Set** $\mathbf{x}^{k+1} = \mathbf{x}^k + \lambda_k \Delta\mathbf{x}^k$**;**

**Frage:** How should we choose the damping parameters $\lambda_k$?




$x^1 = x^0 + \Delta x^0$ Newton classical

$x^1 = x^0 + \lambda \Delta x^0$

$\lambda \in [0,1]$

o.k. if $|f(x^1)| > |f(x^1)|$

## Choice of the damping paramter.

**Strategy:** Use a testfunction $T(\mathbf{x}) = \|\mathbf{f}(\mathbf{x})\|$ such that

$$\begin{aligned} T(\mathbf{x}) &\geq 0, \quad \forall \mathbf{x} \in D \\ T(\mathbf{x}) &= 0 \quad \Leftrightarrow \quad f(\mathbf{x}) = \mathbf{0} \end{aligned}$$

Choose $\lambda_k \in (0,1)$ such that the sequence $T(\mathbf{x}^k)$ decreases strictly monotonically, i.e.

$$\|\mathbf{f}(\mathbf{x}^{k+1})\| < \|\mathbf{f}(\mathbf{x}^k)\| \qquad \text{für } k \geq 0.$$

Close to the solution $\mathbf{x}^*$ we should choose $\lambda_k = 1$ to guarantee (local) quadratic convergence.

The following Theorem guarantees the existence of damping parameters.

**Theorem:** Let $\mathbf{f}$ a $\mathcal{C}^1$–function on the open and convex set $D \subset \mathbb{R}^n$. For $\mathbf{x}^k \in D$ with $\mathbf{f}(\mathbf{x}^k) \neq \mathbf{0}$ there exists a $\mu_k > 0$ such that

$$\|\mathbf{f}(\mathbf{x}^k + \lambda \Delta x^k)\|_2^2 < \|\mathbf{f}(\mathbf{x}^k)\|_2^2 \qquad \text{for all } \lambda \in (0, \mu_k).$$

# Damping strategy.

For the **initial iteration** $k = 0$: Choose $\lambda_0 \in \{1, \frac{1}{2}, \frac{1}{4}, \ldots, \lambda_{min}\}$ as big as possible such that

$$\|\mathbf{f}(\mathbf{x}^0)\|_2 > \|\mathbf{f}(\mathbf{x}^0 + \lambda_0 \Delta \mathbf{x}^0)\|_2$$

holds. For **subsequent iterations** $k > 0$: Set $\lambda_k = \lambda_{k-1}$.

**IF** $\|\mathbf{f}(\mathbf{x}^k)\|_2 > \|\mathbf{f}(\mathbf{x}^k + \lambda_k \Delta \mathbf{x}^k)\|_2$ **THEN**

- $\mathbf{x}^{k+1} := \mathbf{x}^k + \lambda_k \Delta \mathbf{x}^k$
- $\lambda_k := 2\lambda_k$, falls $\lambda_k < 1$.

**ELSE**

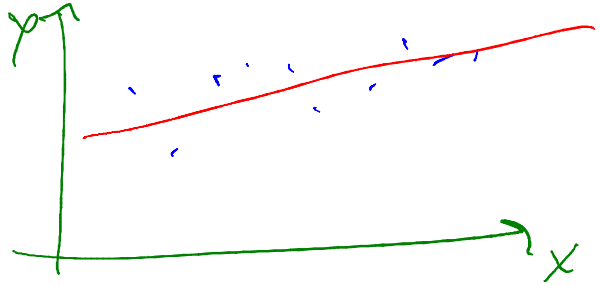
- Determine $\mu = \max\{\lambda_k/2, \lambda_k/4, \ldots, \lambda_{min}\}$ with

$$\|\mathbf{f}(\mathbf{x}^k)\|_2 > \|\mathbf{f}(\mathbf{x}^k + \lambda_k \Delta \mathbf{x}^k)\|_2$$

- $\lambda_k := \mu$

**END**

Date $(y_i, x_i)$ $\quad i = 1, \dots, m$




model $\quad \phi(x_1, \dots, x_m, \alpha_1, \dots, \alpha_n)$

e.g. $\quad \phi = \underbrace{A(x)}_{m \times n} \alpha$ $\qquad$ such as $\quad y_i = \alpha_1 + \alpha_2 x_i$

$$A = \underbrace{\begin{pmatrix} 1 & x_1 \\ \vdots & \\ 1 & x_m \end{pmatrix}}_{m \times 2} \qquad \alpha = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}$$

$$f(\alpha) = \| y - A(x)\alpha \|_2^2 \longrightarrow \min$$

$$\operatorname{grad}_\alpha f(\alpha) \overset{!}{=} 0$$

$$f(\alpha) = (y - A\alpha)^T (y - A\alpha) = y^T y - y^T A \alpha - \alpha^T A^T y + \alpha^T A^T A \alpha$$

$$\operatorname{grad}_\alpha f(\alpha) = \underbrace{-y^T A \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}}_{\left(y^T A \left(\begin{smallmatrix} 1 \\ \vdots \\ 1 \end{smallmatrix}\right)\right)^T = (1 \dots)A^T y} - (1 \dots 1) A^T y + \alpha^T \Big( \underbrace{\underbrace{A^T A}_{n \times m \ \ m \times n}}_{n \times n} + \underbrace{(A^T A)^T}_{A A^T} \Big)$$

$$= -2 \underbrace{y^T A \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}}_{y^T A} + 2 \alpha^T A^T A = 0$$

$$A^T A \alpha = A^T y \quad \Longrightarrow \quad \alpha = (A^T A)^{-1} A^T y$$

$$A = \begin{pmatrix} 1 & x_1 \\ \vdots & x_m \end{pmatrix}$$

$$A^T y = \begin{pmatrix} 1 & \cdot & 1 \\ x_1 & & x_m \end{pmatrix} \begin{pmatrix} y_1 \\ \\ y_m \end{pmatrix} = \begin{pmatrix} \sum y_i \\ \\ \sum y_i \cdot x_i \end{pmatrix}$$

$$A^T A = \begin{pmatrix} & \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ \\ 1 & x_m \end{pmatrix} = n \begin{pmatrix} 1 & \frac{1}{n} \sum x_i \\ \frac{1}{n} \sum x_i & \frac{1}{n} \sum x_i^2 \end{pmatrix}$$

$$\alpha = \frac{1}{\overline{x^2} - \bar{x}^2} \begin{pmatrix} \overline{x^2}\,\bar{y} + \bar{x}\,\overline{xy} \\ \\ -\bar{x}\,\bar{y} + \overline{xy} \end{pmatrix}$$

$$\bar{x} = \frac{1}{n} \sum x_i$$

$$\bar{y} = \frac{1}{n} \sum y_i$$

$$\overline{x^2} = \frac{1}{n} \sum x_i^2$$

$$\overline{xy} = \frac{1}{n} \sum x_i y_i$$