Newton Type Optimization (Unconstrained)

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(some slide material was provided by W. Bangerth and K. Mombaur)

Aim of Newton type optimization algorithms

$$\min f(x) \quad (x \in R^n)$$

- Find a local minimizer x^* of f(x), i.e. a point satisfying

$$\nabla f(x^*) = 0$$

Derivative based algorithms

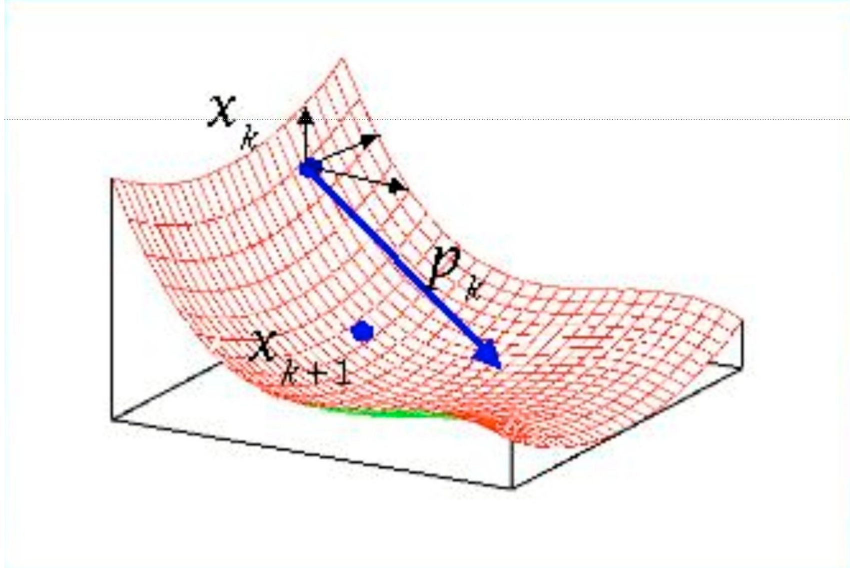
- **Fundamental underlying structure of most algorithms:**

  - choose start value x_0
  - for i=1, ...:
    - determine direction of search (descent) p
    - determine step length α
    - new iterate $x_{i+1} = x_i + \alpha p$
    - check convergence

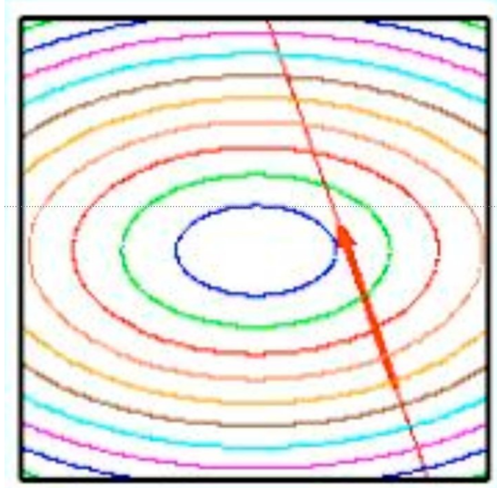
- Optimization algorithms differ in the choice of p und α

Basic algorithm:

Search direction:
choose descent direction
(f should be decreased)



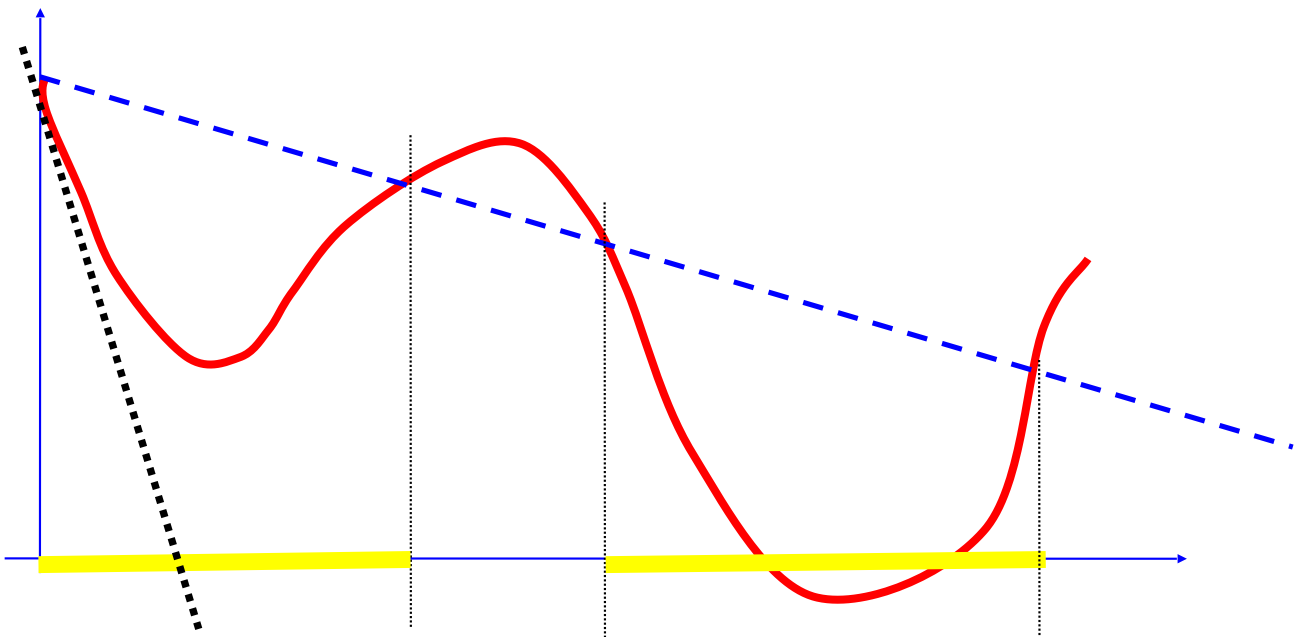
Step length:
solve1-d minimization approximately,
satisfy Armijo condition



Computation of step length

- Dream:
  - exact line search: $\alpha^k = \arg\min_{\alpha} f(x^k + \alpha p^k)$
- In practice:
  - **inexact line search:** $\alpha^k \approx \arg\min_{\alpha} f(x^k + \alpha p^k)$
  - ensure sufficient decrease, e.g. Armijo condition

$$f(x_k + \alpha_k p_k) \le f(x_k) + c_1 \alpha_k \nabla f_k^T p_k$$



How to compute search direction?

- We discuss three algorithms:
  - Steepest descent method
  - Newton‘s method
  - Newton type methods

Algorithm 1: Steepest descent method

- Based on first order Taylor series approximation of objective function

$$f(x_k + p_k) = f(x_k) + \underbrace{\nabla f(x_k)^T p_k}_{} + \ldots$$

  - maximum descent, if

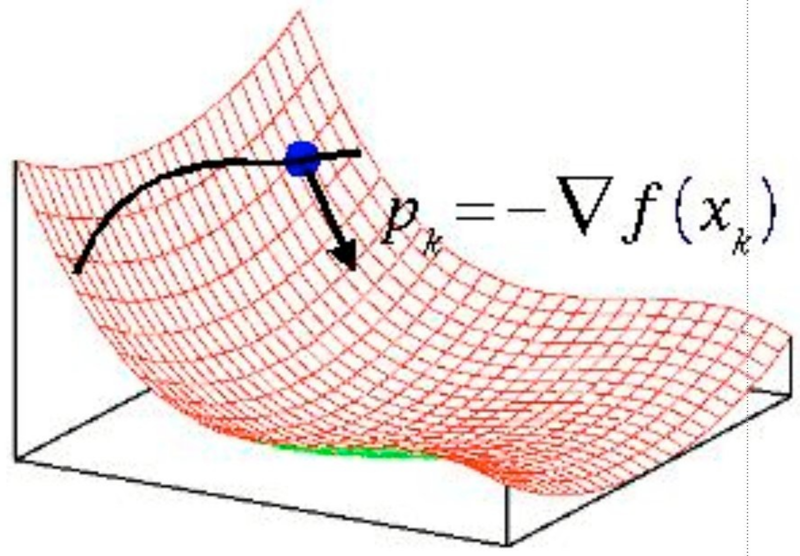
$$\begin{aligned} \frac{\nabla f(x_k)^T p_k}{||p_k||} &\rightarrow \quad \text{min!} \\ \Rightarrow p_k &= \quad -\nabla f(x_k) \end{aligned}$$

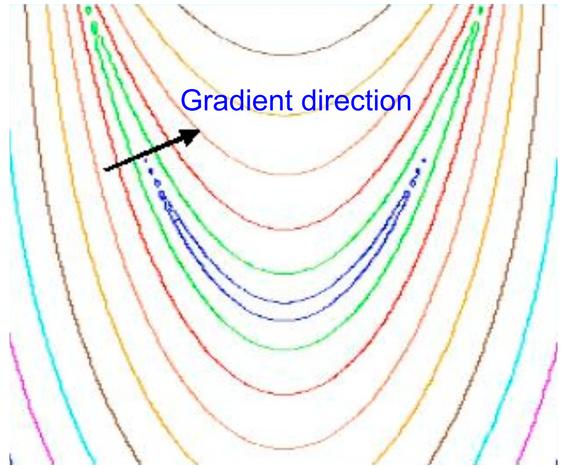
Steepest descent method

Choose steepest descent search direction, perform (exact) line search:

$$p^k = -\nabla f(x^k) \qquad\qquad x^{k+1} = x^k - \alpha^k \nabla f(x^k)$$

search direction is perpendicular to level sets of *f(x)*





Convergence of steepest descent method

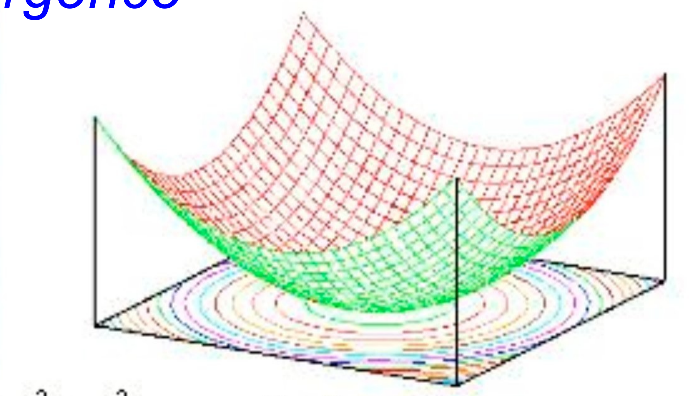
steepest descent method has *linear convergence*

i.e. $\left\| x^k - x^* \right\| \leq C \left\| x^{k-1} - x^* \right\|$

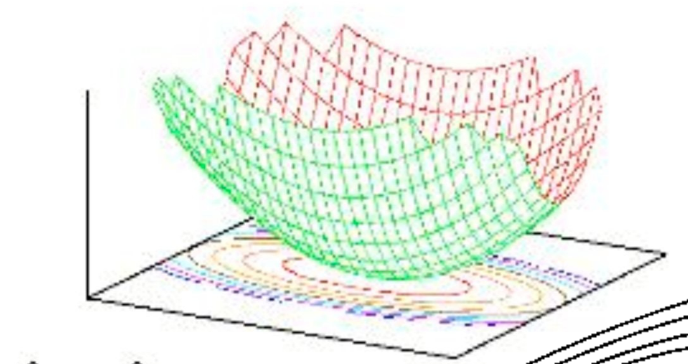
- gain is a fixed factor *C*<1
- convergence can be very slow
  if *C* close to 1

If f(x) = $x^T Ax$, *A* positive definite,
λ eigenvalues of *A, one can show that*

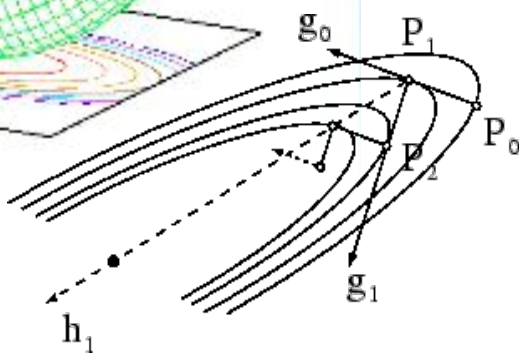
$$\Rightarrow \quad C \approx \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}}$$



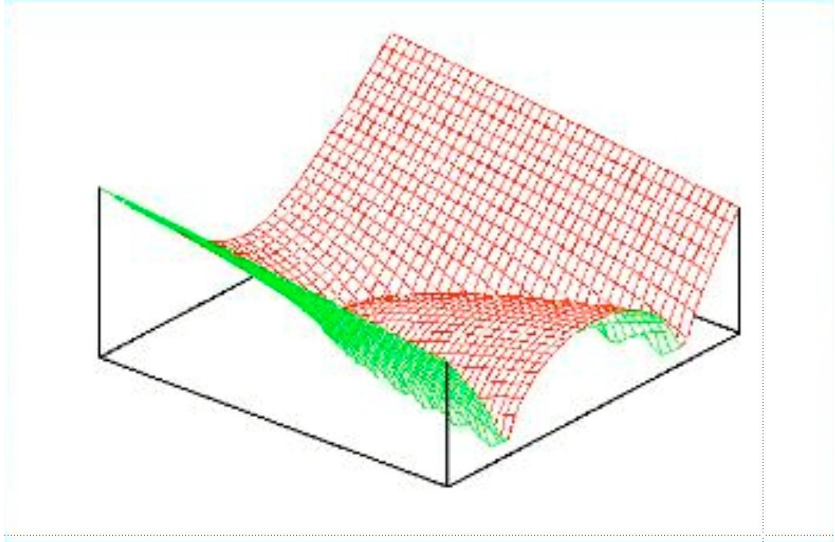
$x^2 + y^2 \rightarrow C=0$



$x^2 + 5y^2 \rightarrow C \approx 0.6$

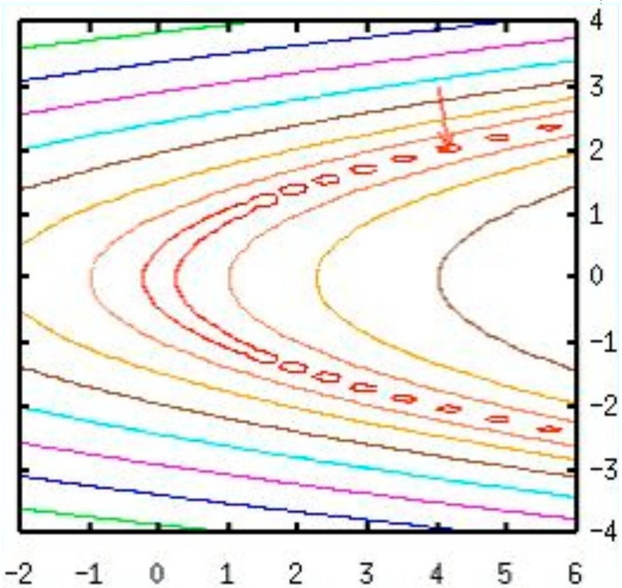


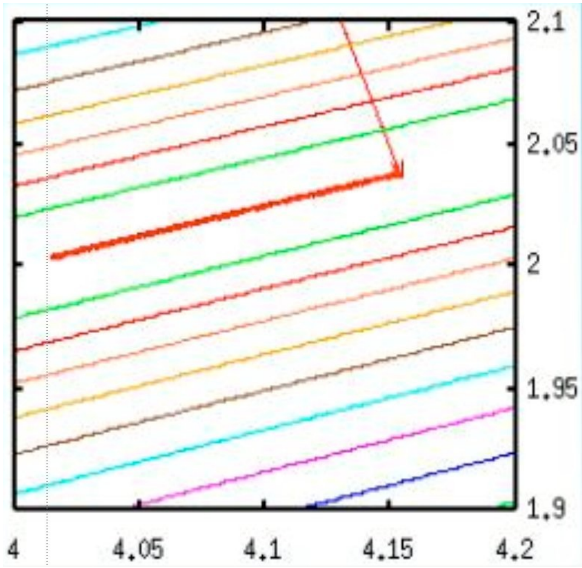
Example - steepest descent method

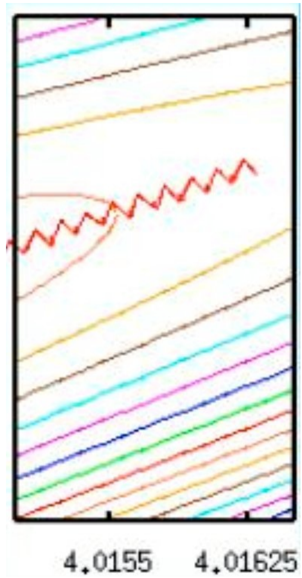


$$f(x,y) = \sqrt[4]{(x-y^2)^2 + \frac{1}{100}} + \frac{1}{100} y^2$$

banana valley function,
global minimum at $x=y=0$

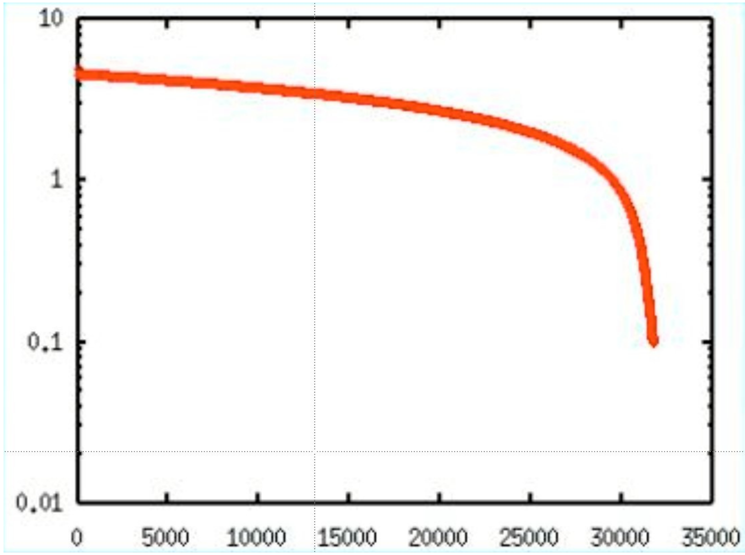






Example - steepest descent method

$\|x^k - x^*\|$



Convergence of steepest descent method:

- needs almost 35.000 iterations to come closer than 0.1 to the solution
- mean value of convergence constant *C*: 0.99995
- at *(x*=4,*y*=2*)*, there holds

$$\lambda_1 = 0.1, \lambda_2 = 268 \quad \Rightarrow \quad C \approx \frac{268 - 0.1}{268 + 0.1} \approx 0.9993$$

Algorithm 2: Newton's Method

- Based on **second order** Taylor series approximation of f(x)

$$f(x_k + p_k) = f(x_k) + \underbrace{\nabla f(x_k)^T p_k + \frac{1}{2} p_k^T \nabla^2 f(x_k)\, p_k}_{} + \ldots$$

$$\nabla f(x_k)^T p_k + \frac{1}{2} p_k^T \nabla^2 f(x_k)\, p_k \to \min!$$

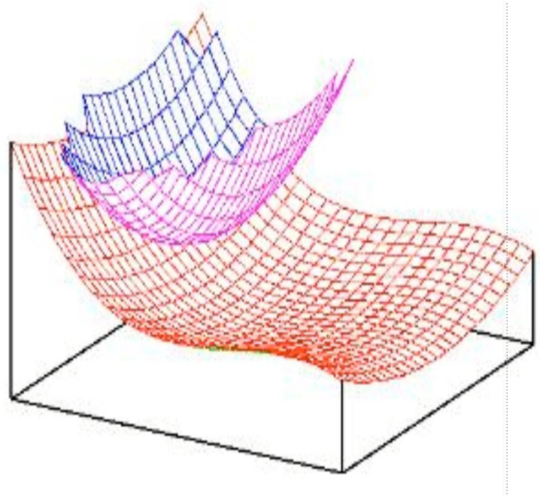
$$\Leftrightarrow \qquad \nabla^2 f(x_k)\, p_k = -\nabla f(x_k)$$

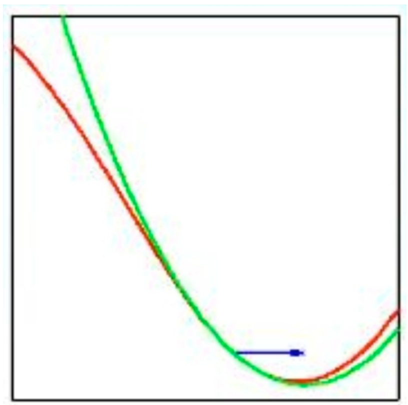
„Newton-Direction" $p_k = -(\nabla^2 f(x_k))^{-1}\, \nabla f(x_k)$

Visualization of Newton's method

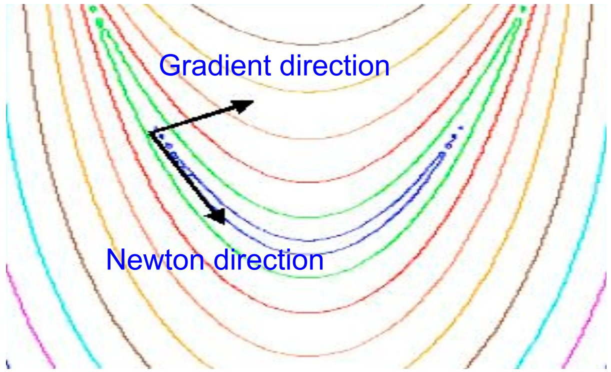
p_k minimizes **quadratic approximation** of the objective

$$Q(p^k) = f(x^k) + \nabla f(x^k) p^k + \frac{1}{2} p^{k^T} \nabla^2 f(x^k) p^k$$





if quadratic model is good, then take full step with $\alpha^k = 1$



Convergence of Newton‘s method

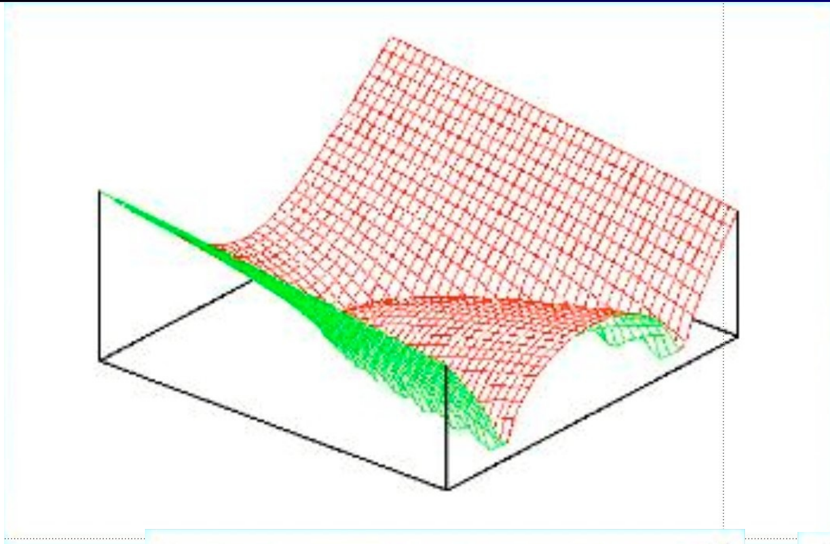
Newton‘s method has *quadratic convergence*

i.e. $$\left\| x^k - x^* \right\| \leq C \left\| x^{k-1} - x^* \right\|^2$$

This is ***very fast*** close to a solution:

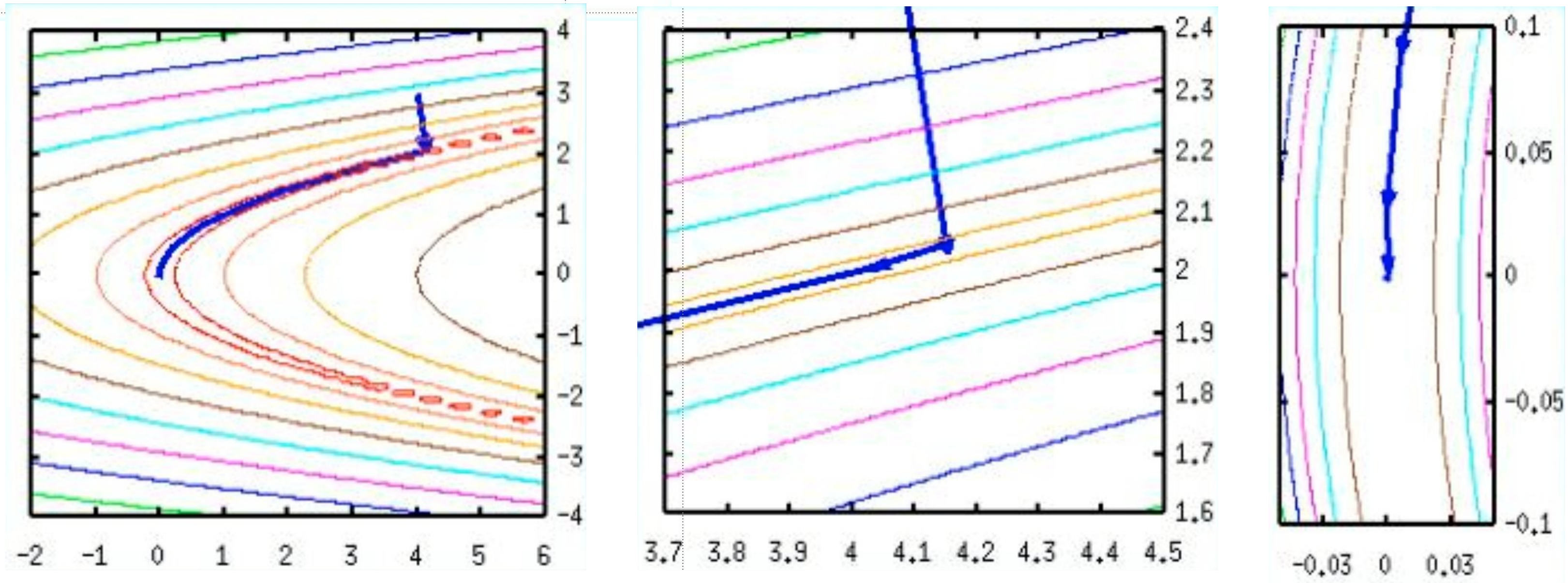
Correct digits double in each iteration!

Example - Newton's method

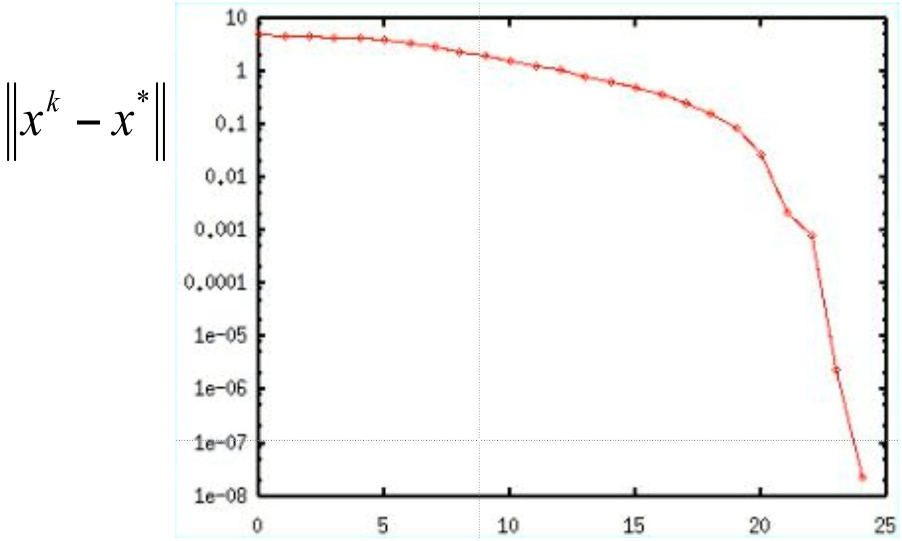


$$f(x,y) = \sqrt[4]{(x-y^2)^2 + \frac{1}{100}} + \frac{1}{100} y^2$$

banana valley function,
global minimum at *x*=*y*=*0*



Example - Newton‘s method



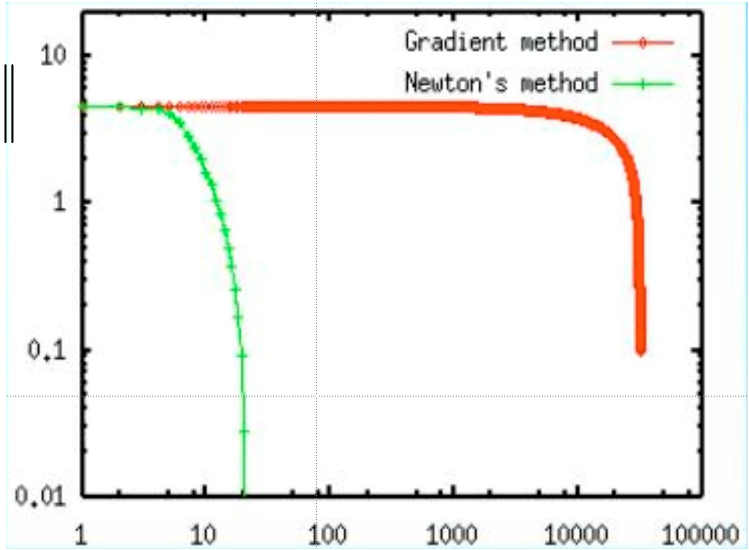
Convergence of Newton‘s method:

- less than 25 iterations for an accuracy of better than 10^{-7}!
- convergence roughly *linear* for first 15-20 iterations since step length $\alpha_k \neq 1$
- convergence roughly *quadratic* for last iterations with step length

$$\alpha_k = 1$$

Comparison of steepest descent and Newton

$\left\| x^k - x^* \right\|$



For banana valley example:

- Newton's method **much faster** than steepest descent method (factor 1000)
- Newton's method superior due to higher order of convergence
- steepest descent method converges too slowly for practical applications

Algorithm 3: Newton type methods

In practice, evaluation of second derivatives
for the hessian can be difficult!

➔ approximate hessian matrix $\nabla^2 f(x^k)$

➔ often methods ensure that the approximation B_k is positive definite

$$x^{k+1} = x^k - B_k^{-1} \nabla f(x^k)$$

$$B_k \approx \nabla^2 f(x^k)$$

methods are collectively known as *Newton type methods*

Newton type variants

Notation:

$$p_k \;:=\; x_{k+1} - x_k \;=\; -B_k^{-1} \nabla f(x^k)$$

- **Steepest Descent:**

$$B_k \;=\; I$$

Convergence rate: linear

- **Newton Method:**

$$B_k \;=\; \nabla^2 f(x^k)$$

Convergence rate: quadratic

Newton type variants (continued)

- **BFGS** update (Broyden, Fletcher, Goldfarb, Shanno)

$$\begin{aligned} B_{k+1} &= \underset{B_{k+1}}{\operatorname{argmin}} \, \|B_{k+1}^{-1} - B_k^{-1}\|_{W,F}^2 \\ & \text{s.t.} \quad B_{k+1}\, p_k = \nabla f(x^{k+1}) - \nabla f(x^k) \\ & \qquad\;\; B_{k+1} = B_{k+1}^T \end{aligned}$$

Convergence rate: super-linear

- For Least-Squares Problems: **Gauss-Newton Method**

$$f(x) = \frac{1}{2}\|F(x)\|^2 \quad J(x) = \frac{\partial F(x)^T}{\partial x}$$

$$B_k = J(x^k)^T J(x^k)$$

Convergence rate: linear

Summary: Unconstrained Newton Type Optimization

- Aim: find **local minima** of smooth nonlinear problems: $\nabla f(x^*)=0$

- Derivative based methods iterate $x_{i+1} = x_i + \alpha_i p_i$ with
  - **search direction** p_i and **step length** α_i .
  - start at **initial guess** x_0 ,

- Four Newton type methods:
  - steepest descent: intuitive, but slow linear convergence
  - exact Newton‘s method: very fast quadratic convergence
  - BFGS: fast superlinear convergence
  - Gauss-Newton (only for least-squares): fast linear convergence

Literature

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- P. E. Gill, W. Murray, M. H. Wright: Practical Optimization, Academic Press, 1981
- R. Fletcher, Practical Methods of Optimization, Wiley, 1987
- D. E. Luenberger: Linear and Nonlinear Programming, Addison Wesley, 1984