

# Nonlinear Programming



**UNIVERSITÄT  
HEIDELBERG**  
ZUKUNFT  
SEIT 1386

Ekaterina A. Kostina

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# Outline

- 1 Basic definitions, optimality conditions
- 2 Algorithms for unconstrained problems
- 3 Algorithms for constrained problems

# Nonlinear Programming Problem

- ▶ General problem formulation:

$$\begin{array}{ll} \min f(x) & f : D \in \mathbb{R}^n \rightarrow \mathbb{R} \\ \text{s.t. } g(x) = 0 & g : D \in \mathbb{R}^n \rightarrow \mathbb{R}^m \\ h(x) \geq 0 & h : D \in \mathbb{R}^n \rightarrow \mathbb{R}^k \end{array}$$

- ▶  $x$  variables
- ▶  $f$  objective function/ cost function/  $\min -f(x) \equiv -\max f(x)$
- ▶  $g$  equality constraints
- ▶  $h$  inequality constraints
- ▶  $f, g, h$  shall be sufficiently smooth (e.g. twice differentiable) functions

# Derivatives

- ▶ First and second derivatives of the objective function or the constraints play an important role in optimization
- ▶ The first order derivatives are called the gradient (of the resp. fct)

$$\nabla f(x) = \left( \frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \dots, \frac{\partial f}{\partial x_n} \right)^T$$

- ▶ and the second order derivatives are called the Hessian matrix

$$\nabla^2 f(x) = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \cdots & \cdots & \cdots & \cdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{pmatrix}$$

# Local and Global Solutions

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- ▶ Feasible set:  $S = \{x \in \mathbb{R}^n : g(x) = 0, h(x) \geq 0\}$

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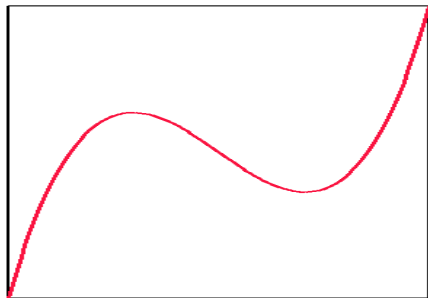
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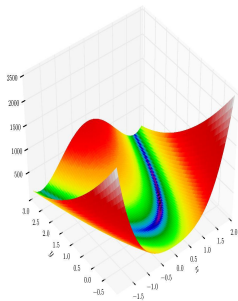
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- ▶  $x^*$  local minimizer of  $f$  over  $S \iff x^* \in S$  and there exists  $\mathcal{N}(x^*, \delta)$  such that  $f(x) \geq f(x^*)$ ,  $\forall x \in S \cap \mathcal{N}(x^*, \delta)$  where  $\mathcal{N}(x^*, \delta) := \{x \in \mathbb{R}^n : \|x - x^*\|_2 \leq \delta\}$



# Local and Global Solutions



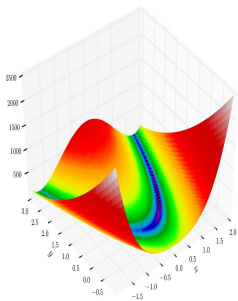
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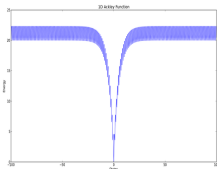
Rosenbrock's test function

see Wikipedia

# Local and Global Solutions



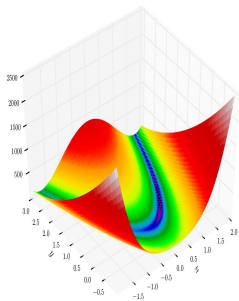
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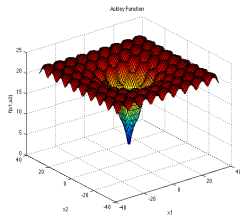
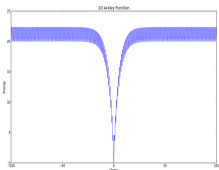
Ackley's test function

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# Local and Global Solutions



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# Main Classes of Continuous Optimization Problems

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- ▶ Linear programming: linear objective, linear constraints in the variables

$$\min_{x \in \mathbb{R}^n} c^T x \quad \text{subject to } a_i^T x = b_i, i \in E, a_i^T x \geq b_i, i \in I,$$

where  $c, a_i \in \mathbb{R}^n$ , for all  $i$ ,  $E$  and  $I$  are finite index sets,

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Quadratic programming: quadratic objective,  
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- ▶ Constrained nonlinear programming

$$\min_{x \in \mathbb{R}^n} \quad f(x) \quad \text{subject to } g(x) = 0, h(x) \geq 0.$$

# Optimality Conditions for Unconstrained Optimization

$$\min f(x), \quad x \in \mathbb{R}^n$$

- ▶ Optimality conditions:
  - ▶ give algebraic characterizations of solutions, suitable for computations
  - ▶ provide a way to guarantee that a candidate point is optimal (sufficient conditions)
  - ▶ indicate when a point is not optimal (necessary conditions)

# Optimality Conditions for Unconstrained Optimization

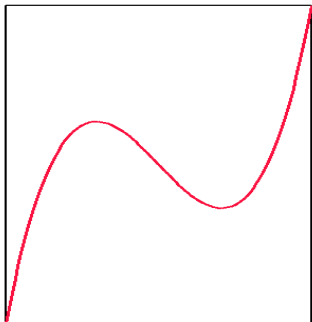
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# Optimality Conditions for Unconstrained Optimization

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- ▶ Necessary conditions:  
 $x^*$  is a local minimizer of  $f \Rightarrow \nabla f(x^*) = 0$  (stationarity)

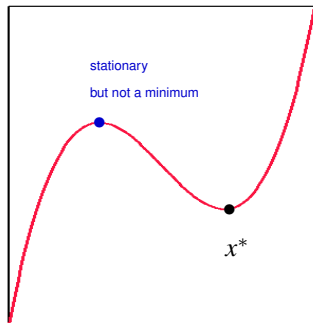
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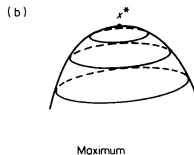
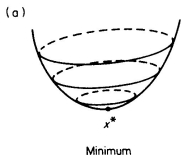
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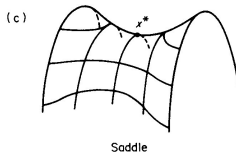
# Stationary Points

(a)-(c)  $x^*$  is stationary:  $\nabla f(x^*) = 0$

(a)  $\nabla^2 f(x^*)$  positive definite: local minimum



(b)  $\nabla^2 f(x^*)$  negative definite: local maximum



(c)  $\nabla^2 f(x^*)$  indefinite: saddle point



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  - ▶  $x^*$  is stationary  $\Rightarrow x^*$  is a global minimizer of  $f$
- ▶  $f$  nonconvex  $\rightarrow$  look at higher order derivatives

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 $x^*$  is a local minimizer of  $f \Rightarrow \nabla^2 f(x^*)$  positive semidefinite  
( $f$  locally convex)
- ▶ Sufficient conditions:  
 $x^*$  stationary and  $\nabla^2 f(x^*)$  positive definite  $\Rightarrow x^*$  is a (strict) local minimizer of  $f$

# Stability

# Stability

Let  $\varepsilon$  be a perturbation of the problem, then the solution  $x(\varepsilon)$  should be a small perturbation of the exact solution  $x^*$ :

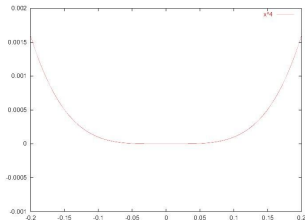
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$f(x) = x^4$ : Minimum at  $x^* = 0$

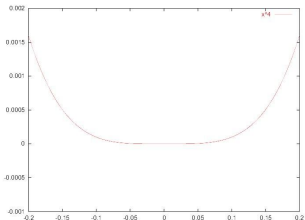


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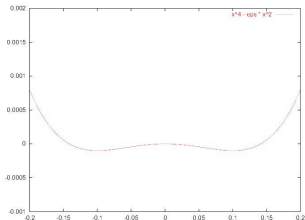
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$f(x) = x^4 - \varepsilon x^2$ : Maximum at  $x = 0$ ,  
Minima at  $x = \pm\sqrt{\varepsilon}$

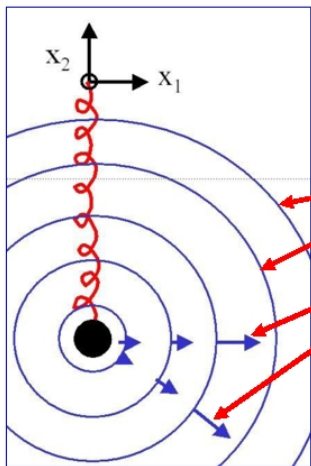


# Stability

- ▶ In the example problem the sufficient optimality conditions were not satisfied ( $\nabla^2 f(x^*)$  is not positive definite)
- ▶ One can show:

Optima that satisfy the sufficient optimality conditions are stable against perturbations

# Ball on a spring without constraints



$$\min_{x \in \mathbb{R}^2} x_1^2 + x_2^2 + mx_2$$

contour lines of  $f(x)$

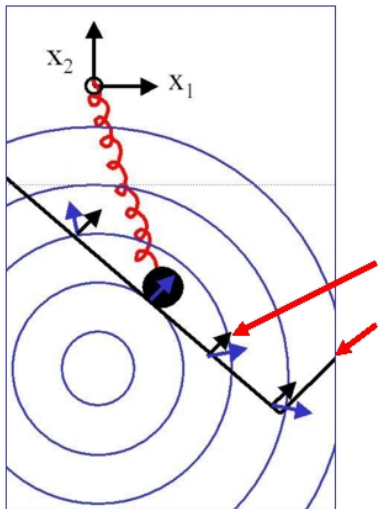
gradient vector

$$\nabla f(x) = (2x_1, 2x_2 + m)$$

unconstrained minimum:

$$0 = \nabla f(x^*) \Leftrightarrow (x_1^*, x_2^*) = \left(0, -\frac{m}{2}\right)$$

# Ball on a spring with constraints



$$\min_{x \in \mathbb{R}^2}$$

$$x_1^2 + x_2^2 + mx_2$$

$$h_1(x) = 1 + x_1 + x_2 \geq 0$$

$$h_2(x) = 3 - x_1 + x_2 \geq 0$$

gradient  $\nabla h_1$  of active constraint

inactive constraint  $h_2$

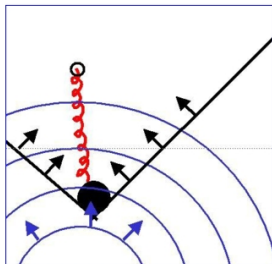
constrained minimum:

$$\nabla f(x^*) = \mu_1 \nabla h_1(x^*)$$

$\mu_1$  is Lagrange multiplier



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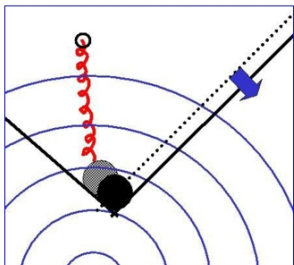
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“equilibrium of forces”

$$\nabla f(x^*) = \mu_1 \nabla h_1(x^*) + \mu_2 \nabla h_2(x^*), \quad \mu_1 \geq 0, \mu_2 \geq 0$$

$\mu_1, \mu_2$ , are Lagrange multipliers

# Multipliers as “shadow prices”



old constraint:  $h_2(x) \geq 0$

new constraint:  $h_2(x) + \varepsilon \geq 0$

- ▶ What happens if we relax a constraint?
- ▶ Feasible set becomes larger, so new minimum  $f(x_\varepsilon^*)$  becomes smaller.
- ▶ How much would we gain?

$$f(x_\varepsilon^*) \approx f(x^*) - \varepsilon \mu_2$$

- ▶ Multipliers show the hidden cost of constraints.

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- ▶ Lagrangian function  $\mathcal{L} : \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^k \rightarrow \mathbb{R}$

$$\mathcal{L}(x, \lambda, \mu) := f(x) - \sum_i \lambda_i g_i(x) - \sum_i \mu_i h_i(x)$$

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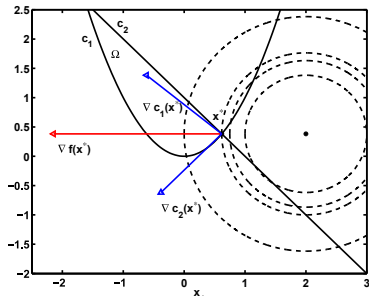
- ▶ Karush-Kuhn-Tucker (KKT) point:  
 $x$  is a KKT point if there exist  $\lambda \in \mathbb{R}^m$  and  $\mu \in \mathbb{R}^k$  such that  $(x, \lambda, \mu)$  satisfies

$$g(x) = 0, h(x) \geq 0$$

$$\nabla_x \mathcal{L}(x, \lambda, \mu) = 0 \Leftrightarrow \nabla f(x) = \sum_i \lambda_i \nabla g_i(x) + \sum_i \mu_i \nabla h_i(x)$$

$$\mu \geq 0, \mu_i h_i(x) = 0, i = 1, \dots, k \Leftrightarrow \mu_i = 0 \text{ or } h_i(x) = 0$$

# KKT Conditions: Illustration



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  - ▶ **All active constraints (equalities and active inequalities) are linear**
  - ▶ **Mangansarian-Fromovitz CQ** at  $x \Rightarrow \nabla g_i(x), i = 1, \dots, m$  linearly independent / or linear and  $\exists p \in \mathbb{R}^n$  such that  $\nabla g(x)^T p = 0, \nabla h_i(x)^T p > 0, i \in I(x)$

# No CQ: Example from Fiacco, McCormick

$$h_1(x) := (1 - x_1)^3 - x_2 \geq 0 \quad x_2 \leq (1 - x_1)^3$$

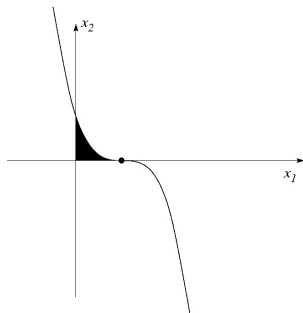
$$h_2(x) := x_1 \geq 0$$

$$h_3(x) := x_2 \geq 0$$

$$\nabla h_1 = \begin{pmatrix} -3(1 - x_1)^2 \\ -1 \end{pmatrix}$$

$$\nabla h_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\nabla h_3 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$



Active inequalities in  $(1, 0)^T$ :

$$h_3(x) = 0 \text{ and } h_1(x) = 0$$

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$$p^T \nabla^2 \mathcal{L}(x^*, \lambda^*, \mu^*) p \geq 0, \forall p \in T(x^*)$$
$$T(x^*) := \{s : s^T \nabla g_i(x^*) = 0, i = 1, \dots, m, \\ s^T \nabla h_i(x^*) \geq 0, i \in I(x^*)\}$$

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- ▶ Sufficient optimality conditions: if KKT conditions hold and  $\nabla^2 \mathcal{L}(x^*, \lambda^*, \mu^*)$  is positive definite at  $\tilde{T}(x^*, \lambda^*)$ , then  $x^*$  is optimal,  $\tilde{T}(x^*, \lambda^*) := \{s \in T(x^*) : s^T \nabla h_i(x^*) = 0, i \in I(x^*) \text{ with } \mu_i > 0\}$

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

- ▶ Find a local minimizer  $x^*$  of  $f(x)$ , i.e. a point satisfying
  - ▶  $\nabla f(x^*) = 0$  (stationarity)
  - ▶ and  $\nabla^2 f(x^*)$  positive definite

# Algorithms for Unconstrained Optimization

- ▶ Basic structure of most algorithms:
  - ▶ choose start value  $x^0$
  - ▶ for  $k = 1, \dots$ ,
    - determine search (descent) direction  $p^k$
    - determine steplength  $\alpha^k$
    - new iterate  $x^{k+1} = x^k + \alpha^k p^k$
    - check for convergence
- ▶ Optimization algorithms differ in the choice of  $p^k$  and  $\alpha^k$

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- ▶ Two types of convergence:
  - ▶ **Local convergence:** convergence of the full-step ( $\alpha_k \equiv 1$ ) algorithm near the solution
  - ▶ **Global convergence:** convergence of an algorithm starting from an any arbitrary point  $x^0$

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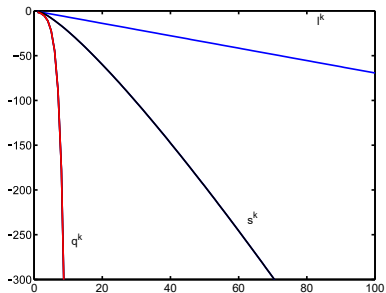
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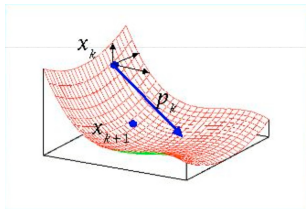
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- ▶  $r = 2$  : quadratic convergence
- ▶ superlinear convergence:  $\frac{\|x^{k+1} - x^*\|}{\|x^k - x^*\|} \rightarrow 0$  as  $k \rightarrow \infty$

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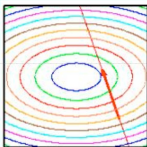
# Generic Linesearch Algorithm

Search direction  $p^k$ :  
 $f$  must decrease  
along the direction  $p^k$   
 $\nabla f(x^k)p^k < 0$



Steplength  $\alpha^k$   
to guarantee global convergence:  
solve 1D minimization problem  
(exact or inexact):

$$\alpha^k = \arg \min_{\alpha} f(x^k + \alpha p^k)$$



# Computation of Steplength

- ▶ Ideal: Move to (global) minimum on the selected line (univariate optimization, exact line search)

$$\alpha^k = \arg \min_{\alpha} f(x^k + \alpha p^k)$$

- ▶ In practice: approximate solution may guarantee global convergence, perform only inexact line search

$$\alpha^k \approx \arg \min_{\alpha} f(x^k + \alpha p^k)$$

- ▶ Problem: how to guarantee sufficient decrease?
  - ▶ Answer: Check e.g. if  $\alpha^k$  satisfies Armijo-Wolfe conditions

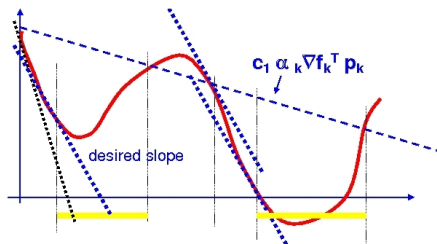
# Armijo-Wolfe Conditions for Inexact Line Search

- ▶ Armijo condition (sufficient decrease condition):

$$f(x^k + \alpha p^k) \leq f(x^k) + c_1 \alpha^k \nabla^T f(x^k) p^k, \quad c_1 \in (0, 1)$$

- ▶ Curvature condition:

$$\nabla^T f(x^k + \alpha p^k) p^k \geq c_2 \nabla^T f(x^k) p^k, \quad c_2 \in (c_1, 1)$$



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  - ▶ either there exist  $l \geq 0$  such that  $\nabla f(x^l) = 0$
  - ▶ or  $\min\left\{\frac{|\nabla f(x^k)^T p^k|}{\|s^k\|}, |\nabla f(x^k)^T p^k|\right\} \rightarrow 0$  as  $k \rightarrow \infty$

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- ▶ not only  $p^k$  to be descent direction
  - ▶ but also  $\cos \theta^k \geq \delta > 0$  for all  $k$   
(i.e.  $p^k$  and  $\nabla f(x^k)$  should not become nearly orthogonal!



# Computation of the Search Direction

- ▶ For the determination of  $p^k$  frequently first and second order derivatives of  $f(x^k)$  are used
- ▶ We discuss:
  - ▶ Steepest descent method
  - ▶ Newton's method
  - ▶ Quasi-Newton methods
- ▶ Left out: conjugate gradients

# Algorithm 1: Steepest Descent Method

- ▶ Based on first order Taylor series approximation of objective function

$$f(x^k + p^k) = f(x^k) + \underbrace{\nabla^T f(x^k) p^k}_{\text{first order approximation}} + \dots$$

- ▶ maximum descent, if

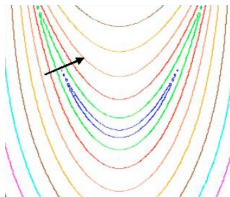
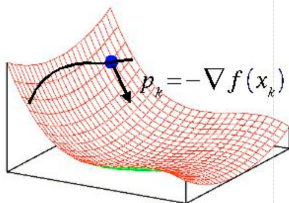
$$\frac{\nabla^T f(x^k) p^k}{\|p^k\|} \rightarrow \min!$$
$$\Rightarrow p^k = -\nabla f(x^k)$$

# Algorithm 1: Steepest Descent Method

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

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

- ▶ search direction is perpendicular to level sets of  $f(x)$



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- ▶ If  $f(x) = x^T A x$ ,  $A$  positive definite (quadratic convex)  $\lambda_i$  are eigenvalues of  $A$ , one can show that

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



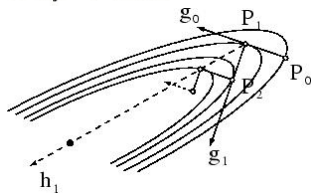
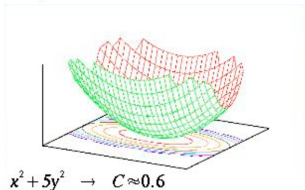
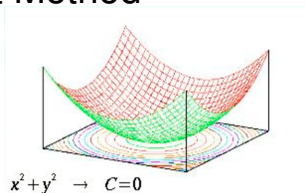
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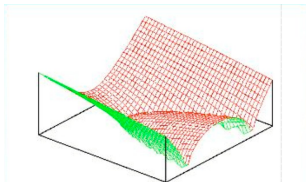
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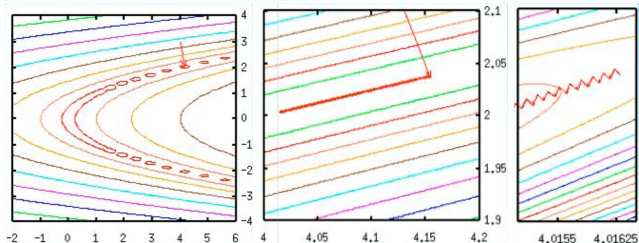
# Example - Steepest Descent Method



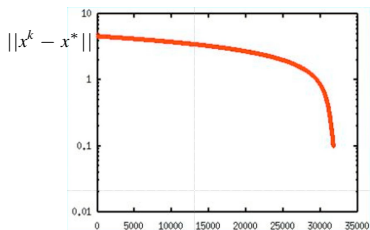
$$f(x, y) = \left( (x - y^2)^2 + \frac{1}{100} \right)^{\frac{1}{4}} + \frac{1}{100} y^2$$

banana valley function

global minimum at  $x = y = 0$



# Example - Steepest Descent Method



Convergence of steepest descent method:

- ▶ needs almost 35.000 iterations to come closer than 0.1 to the solution
- ▶ mean value of convergence rate  $C \approx 0.99995$
- ▶ it holds at  $(x = 4, y = 2)$

$$\lambda_{min} = 0.1, \lambda_{max} = 268, C \approx \frac{268 - 0.1}{268 + 0.1} \approx 0.9993$$

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- ▶ useful for some special applications (e.g. in data analysis)



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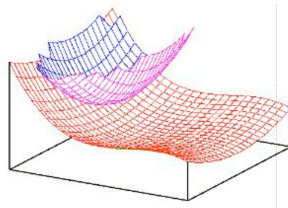
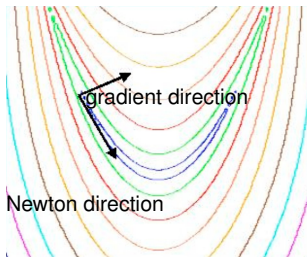
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- ▶  $p^k$  is decrease direction if the hessian  $\nabla^2 f(x^k)$  is positive definite!

# Visualization of Newton's method

- ▶  $p^k$  minimizes **quadratic approximation** of the objective

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



# Why is it called Newton's method?

- ▶ Newton's method finds zeros of nonlinear equations. Here: find solution of the equation

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

- ▶ Newton's idea: use Taylor series of  $\nabla f$  at  $x^k$ :

$$\nabla f(x^k + p^k) \approx \nabla f(x^k) + \nabla^2 f(x^k)p^k = 0!$$

- ▶ and to make this zero, set:

$$p^k = \underbrace{-\left(\nabla^2 f(x^k)\right)^{-1} \nabla f(x^k)}_{\text{Newton direction}}$$

- ▶ (Full step) Newton's method: iterate

$$x^{k+1} = x^k + p^k$$

# Convergence of Newton's method



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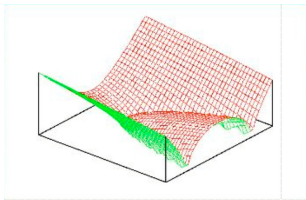
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  - ▶ Line search helps, but is only possible if  $p$  is descent direction, i.e. if  $\nabla^2 f$  positive definite.
  - ▶ Ensure this by: Levenberg-Marquardt, or trust-region methods

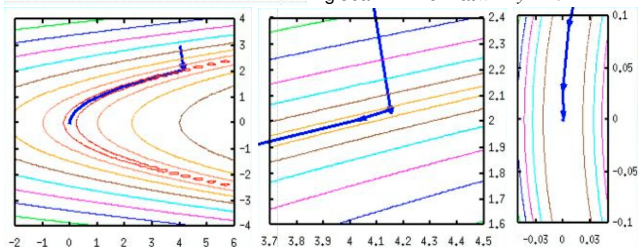
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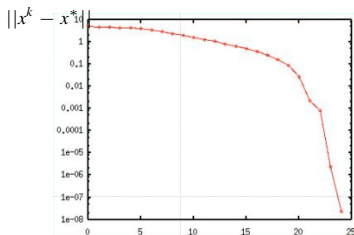
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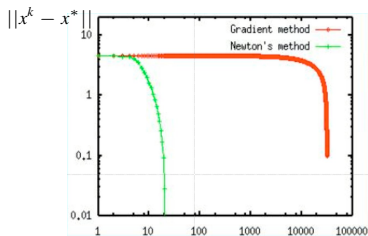
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► Convergence of Newton's method:

- 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  $\alpha^k = 1$

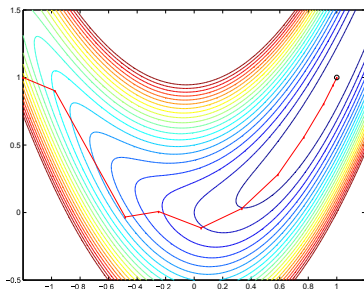
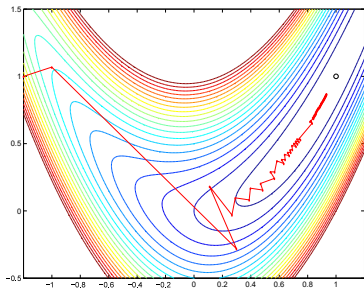
# Comparison of the Steepest Descent and Newton's Methods



- ▶ 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



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# Summary: Newton's Methods

- ▶ Fast (i.e. quadratic) local rate of convergence
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- ▶ Line search, trust region



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- ▶ special case: steepest descent method:  $B = I$

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- ▶ or, even cheaper: use update-formulas for Hessian...

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- ▶ **Examples:**

- ▶ Symmetric Broyden-update
- ▶ DFP-update (Davidon, Fletcher, Powell)
- ▶ BFGS-update (Broyden, Fletcher, Goldfarb, Shanno) (most widely used)

# Convergence Properties

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- ▶ Quasi-Newton methods most popular method for medium scale problems

# Constrained Optimization: SQP-method

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- ▶ Constrained problem:

$$\begin{array}{ll} \min f(x) & f : D \in \mathbb{R}^n \rightarrow \mathbb{R} \\ \text{s.t. } g(x) = 0 & g : D \in \mathbb{R}^n \rightarrow \mathbb{R}^l \\ h(x) \geq 0 & h : D \in \mathbb{R}^n \rightarrow \mathbb{R}^k \end{array}$$

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- ▶ Idea: Consider successively quadratic approximations of the problem:

$$\begin{array}{ll} \min_p & f(x^k) + \nabla^T f(x^k)p + \frac{1}{2}p^T H^k p \\ \text{s.t.} & g(x^k) + \nabla g(x^k)p = 0 \\ & h(x^k) + \nabla h(x^k)p \geq 0 \end{array}$$

- ▶  $H^k \approx \nabla^2 L(x, \lambda, \mu)$

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- ▶ global convergence can be achieved by using a stepsize strategy based on (inexact) 1D minimization of an appropriate merit function, e.g. **exact merit function**

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- ▶ alternatively, global convergence by trust region

# Constrained Optimization: SQP-method

1. Start with  $k = 0$ , start value  $x^0$  and  $H^0 = I$
2. Compute  $f(x^k), g(x^k), h(x^k), \nabla f(x^k), \nabla g(x^k), \nabla h(x^k)$
3. If  $x^k$  feasible and  $\|\nabla \mathcal{L}(x, \lambda, \mu)\| < \varepsilon$  then stop  $\rightarrow$  convergence achieved
4. Solve quadratic problem (QP) and get  $p^k$
5. Perform line search and get stepsize  $\alpha^k$
6. Iterate  $x^{k+1} = x^k + \alpha^k p^k$
7. Update Hessian of the Lagrange function
8.  $k = k + 1$ , goto step 2

# Solution of the Quadratic Program

- ▶ Unconstrained case:

$$\min_p g^T p + \frac{1}{2} p^T H p$$

- ▶ H must be positive definite, otherwise the optimization problem has no solution
- ▶ necessary optimality condition:

$$H p + g = 0$$

- ▶ => use cholesky-method or cg-method to solve

# Solution of the Quadratic Program

- ▶ equality constrained case:

$$\begin{aligned} \min_p \quad & g^T p + \frac{1}{2} p^T H p \\ & A p + a = 0 \end{aligned}$$

- ▶ necessary optimality condition (KKT-system):  $\exists \lambda$  such that

$$\begin{pmatrix} H & A^T \\ A & 0 \end{pmatrix} = - \begin{pmatrix} g \\ a \end{pmatrix}$$

- ▶ matrix is indefinite, use range- or nullspace-method to solve

# Solution of the Quadratic Program

- ▶ equality and inequality constrained case:

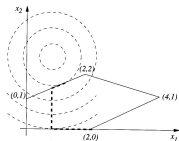
$$\begin{aligned} \min_p \quad & g^T p + \frac{1}{2} p^T H p \\ & A p + a = 0 \\ & B p + b \geq 0 \end{aligned}$$

- ▶ use active-set-strategy
- ▶ aim: find out which inequalities are active at the solution and which not
- ▶ idea: solve a sequence of equality constrained QPs

$$\begin{aligned} \min_p \quad & g^T p + \frac{1}{2} p^T H p \\ & A p + a = 0 \\ & B_i p + b_i = 0, \quad i \in W^k \end{aligned}$$

where  $W^k$  is a “guess” for an optimal active set

# Active-Set Strategy: Example



- ▶  $p^0 = (2, 0)^T$ ,  $W^0 = \{3, 5\}$ , negative multiplier with respect to constraint 3, remove constraint 3

$$\min(p_1 - 1)^2 + (p_2 - 2.5)^2$$

$$p_1 + 2p_2 + 2 \geq 0$$

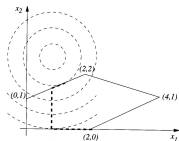
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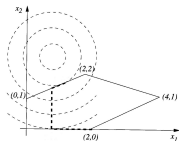
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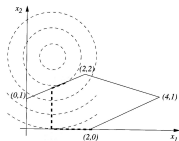
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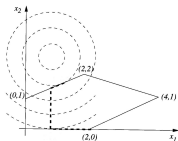
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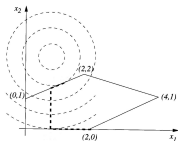
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- ▶  $p^5 = (1.4, 1.7)$ ,  $W^5 = \{3, 5\}$  all multipliers positive  $\rightarrow$  solution

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- ▶ Interior point methods for inequality constrained problems



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  - ▶ CG method (good for very large scale problems)
- ▶ Other methods: direct search, simulated annealing, genetic algorithms, ... useful for special optimization problems

# References

- ▶ J. Nocedal, S. Wright: Numerical Optimization, Springer, 1999
- ▶ 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

**Thank you for your attention!**