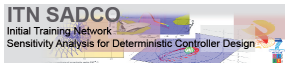


Numerical algorithms for nonlinear optimization problems

Sonja Rauški

22. Januar 2013



Outline

- Nonlinear optimization
- Numerical methods for nonlinear optimization
 - Newton-type optimization
 - Active set method
 - Sequential Quadratic Programming
 - Primal-dual interior point method
- Examples

Nonlinear optimization

$$\begin{array}{ll} \min_x & f(x) \\ \text{s.t.} & g(x) = 0, \\ & h(x) \leq 0. \end{array}$$

where: $x \in \mathbb{R}^n$, $f \in \mathbb{R}$, $g \in \mathbb{R}^{m_e}$, $h \in \mathbb{R}^{m_i}$

- Function f is the cost/ objective function
- Functions g and h equality and inequality constraints, resp.
- The set of indices i for which $h_i(x) = 0$ is named the active set
- f, g, h may be nonlinear
- Nonlinear optimization \Leftrightarrow Nonlinear programming (NLP)

KKT conditions

- A most of solvers try to find an approximate KKT point.
- Find the "primal-dual" variables x^*, ν^*, λ^* such that:

$$g(x^*) = 0, h(x^*) \leq 0$$

Primal feasibility

$$\nu^* \geq 0$$

Dual feasibility

$$\nu_i^* h_i(x^*) = 0, i = 1, \dots, m_i$$

Complementary slackness

$$\nabla \mathcal{L}(x^*, \nu^*, \lambda^*) = 0$$

Stationarity

where:

Lagrangian function:

$$\mathcal{L}(x, \nu, \lambda) = f(x) + \sum_{i=1}^{m_e} \lambda_i g_i(x) + \sum_{i=1}^{m_i} \nu_i h_i(x)$$

Lagrangian multipliers: λ_j, ν_j

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Numerical methods for nonlinear optimization

- Unconstrained optimization

$$\min_x f(x)$$

- Equality constrained optimization

$$\begin{aligned} \min_x \quad & f(x) \\ \text{s.t.} \quad & g(x) = 0, \end{aligned}$$

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Newton-type optimization

- Find x^* such that $\nabla f(x^*) = 0$
- $x_{k+1} = x_k + d_k$
- Linearizing the non-linear equations at x_k
 $\nabla f(x_k) + \nabla^2 f(x_k)d_k = 0$
- Newton step: $d_k = -\nabla^2 f(x_k)^{-1} \nabla f(x_k)$

- Hessian matrix $\nabla^2 f(x_k)$ expensive $\rightarrow B_k \approx \nabla^2 f(x_k)$

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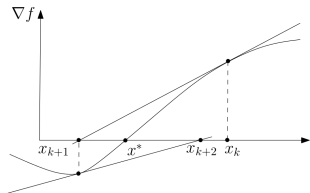
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Steepest descent

- $B_k = \alpha_k^{-1} I$
- $d_k = -B_k^{-1} \nabla f(x_k) = -\alpha_k \nabla f(x_k)$
- How to choose α_k ? → Line search
- Linear convergence when x_k is close to x^*

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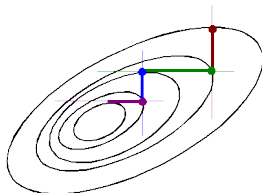
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Quasi-Newton methods

- Computing $\nabla^2 f(x)$ numerically
- BFGS

$$s_k = x_{k+1} - x_k, \quad y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$$

Secant condition: Find B_{k+1} such that $B_{k+1}s_k = y_k$

BFGS formula:
$$B_{k+1} = B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \frac{y_k y_k^T}{s_k^T y_k}, \quad B_0 = I$$

- Quadratic convergence when x_k is close to x^*

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Line search strategy

Problem: situation $f(x_k + d_k) > f(x_k)$ can occur

Idea: making the steps in the iteration shorter to ensure descent

$$f(x_k + d_k) < f(x_k)$$

Find the step size such that: $t = \arg \min_{s \in (0,1]} f(x_k + sd_k)$

But, steps shouldn't get too short either!

Armijo's backtracking line search:

Given d_k , $0 < \alpha \leq \frac{1}{2}$ and $0 < \beta \leq 1$

$t = 1$

while $f(x_k + td_k) \geq f(x_k) + \alpha t \nabla f(x_k)^T d_k$ do

$t = \beta t$

end while

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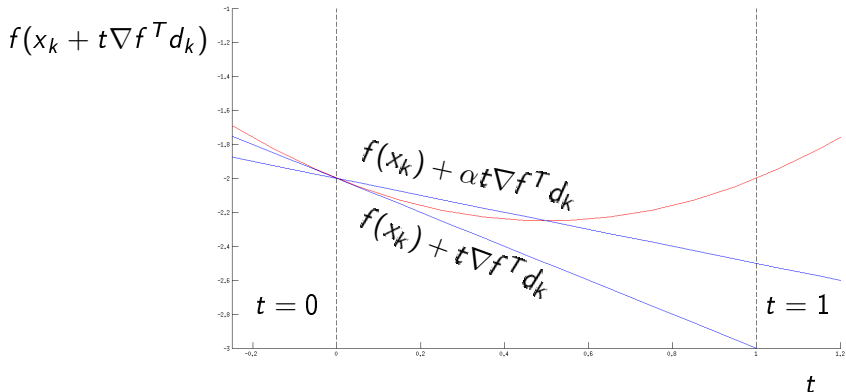
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Newton method for equality constrained problems

Find the "primal-dual" variables x^*, λ^* such that:

$$\begin{aligned}\nabla \mathcal{L}(x^*, \lambda^*) &= 0 \\ g(x^*) &= 0\end{aligned}$$

Applying a Newton search, we get Newton recursion for solving the KKT conditions:

$$\begin{pmatrix} \nabla^2 \mathcal{L}(x_k, \lambda_k) & \nabla g(x_k) \\ \nabla g(x_k)^T & 0 \end{pmatrix} \begin{pmatrix} x_{k+1} - x_k \\ -(\lambda_{k+1} - \lambda_k) \end{pmatrix} + \begin{pmatrix} \nabla \mathcal{L}(x_k, \lambda_k) \\ g(x_k) \end{pmatrix} = 0$$

replacing $x_{k+1} = x_k + d_k$ and $\nabla \mathcal{L}(x_k, \lambda_k) = \nabla f(x_k) + \nabla g(x_k) \lambda_k$

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KKT system is equivalent to the KKT of Quadratic Program (QP)

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Equality and inequality constrained problems

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- Active set method
- Sequential Quadratic Programming
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Active set method

Guess the active set \mathbb{A}

Solve:

$$\begin{aligned} h_i(x^*) &= 0, \quad i \in \mathbb{A} \\ g_i(x^*) &= 0, \quad \nabla \mathcal{L}(x^*, \nu^*, \lambda^*) = 0 \end{aligned}$$

If $\nu^* \geq 0$ and $h_i(x^*) \leq 0, i \in \mathbb{A}^c$ then

Solution found

else

Add or remove constraints indices of \mathbb{A}

end if

Efficient only for Quadratic programs!

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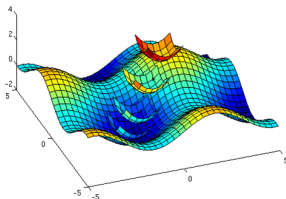
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Sequential Quadratic Programming

L_1 merit function:

$$T_1(x_k) = f(x_k) + \mu \|g(x_k)\|_1 + \mu \sum_{i=1}^{m_i} |\min(0, h(x_k))|$$

Line-search SQP algorithm:

```
while  $T_1(x_k) > TOL$  do
  get  $\nabla f(x_k), \nabla g(x_k), \nabla h(x_k), B_k \approx \nabla^2 \mathcal{L}(x_k, \nu_k, \lambda_k)$ 
  solve the QP, get  $d_k, \lambda_{QP}, \nu_{QP}$ 
  perform line search on  $T_1(x_k + d_k)$ , get step length  $t_k$ 
  update:  $x_{k+1} = x_k + t_k d_k$ 
  update:  $\lambda_{k+1} = \lambda_k + t_k \lambda_{QP}, \nu_{k+1} = \nu_k + t_k \nu_{QP}$ 
end while
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Primal-dual interior point method

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Primal-dual interior point method

$$\begin{array}{ll} \min_x & f(x) \\ \text{s.t.} & g(x) = 0, \\ & h(x) + s = 0 \\ & s \geq 0 \end{array}$$

Primal-dual interior point method

$$\begin{array}{ll} \min_{x,s} & f(x) - \tau \sum_{i=1}^{m_i} \log s_i \\ \text{s.t.} & g(x) = 0, \\ & h(x) + s = 0 \end{array}$$

Barrier function $f(x) - \tau \sum_{i=1}^{m_i} \log s_i$ prevents the iterates from leaving the feasible region defined by the inequalities.

Hanging Chain



- mass points

$$(x_i, y_i), i = 1, \dots, N_p$$

- potential energy of each spring

$$V_{ij}^s = \frac{1}{2} D_{ij} ((x_i - x_{i+1})^2 + (y_i - y_{i+1})^2)$$

- gravitational potential energy of each mass

$$V_i^g = m_i g y_i$$

- total potential energy

$$V_{tot}(x, y) = \sum_{i=1}^{N_p} m_i g y_i + \sum_{i=1}^{N_s} \frac{1}{2} D_{ij} ((x_i - x_{i+1})^2 + (y_i - y_{i+1})^2)$$

- equilibrium position (x^*, y^*)

Hanging Chain



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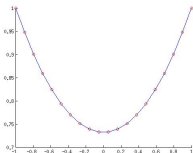
$$V_g^i = m_i g y_i$$

- total potential energy

$$V_{chain}(x, y) =$$

$$\frac{1}{2} \sum_{i=1}^{N_p-1} D_i ((x_i - x_{i+1})^2 + (y_i - y_{i+1})^2) + g \sum_{i=1}^{N_p} m_i y_i$$

- Equilibrium point? $\rightarrow \min_{x,y} V_{chain}(x, y)$



Hanging Chain



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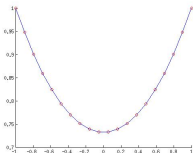
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- Equilibrium point? $\rightarrow \min_{x,y} V_{chain}(x, y)$



Hanging Chain



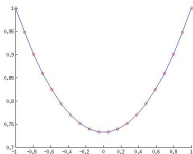
- mass points
 $(x_i, y_i), i = 1, \dots, N_p$
- potential energy of each spring
 $V_{el}^i = \frac{1}{2} D_i ((x_i - x_{i+1})^2 + (y_i - y_{i+1})^2)$
- gravitational potential energy of each mass
 $V_g^i = m_i g y_i$

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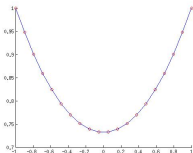


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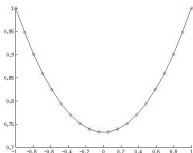


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$$V_{chain}(x, y) = \sum_{i=1}^{N_p-1} D_i (\sqrt{((x_i - x_{i+1})^2 + (y_i - y_{i+1})^2 - \frac{L}{N_p})^2} + g \sum_{i=1}^{N_p} m_i y_i$$

$$N_p = 20, m_i = 20/N_p \text{ kg}, D_i = 75 N_p N/m, g = 9.81 \text{ m/s}^2$$

$$q = (x, y)$$

$$\min_q \sum_{i=1}^{N_p-1} D_i (\|q_{i+1} - q_i\| - \frac{L}{N_p})^2 + mg \sum_{i=1}^{N_p} \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T q_i$$

Unconstrained case

$$V_{chain}(x, y) = \sum_{i=1}^{N_p-1} D_i \left(\sqrt{((x_i - x_{i+1})^2 + (y_i - y_{i+1})^2 - \frac{L}{N_p})^2} + g \sum_{i=1}^{N_p} m_i y_i \right)$$

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$$q_{k+1} = q_k - t_k B_k^{-1} \nabla f(q_k)$$

t_k → backtracking line search using the Armijo condition

$\nabla f(q_k)$ → finite differences

- Steepest descent method
 - B_k → identity matrix
 - 1323 iterations
- Quasi-Newton method
 - B_k → BFGS formula
 - 42 iterations

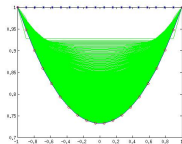
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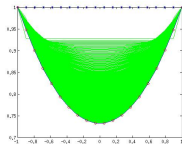
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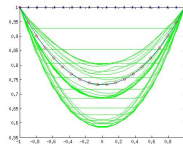
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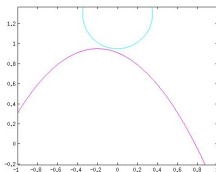


Constrained Optimization

$$\min_q \sum_{i=1}^{N_p-1} D_i \left(\|q_{i+1} - q_i\| - \frac{L}{N_p} \right)^2 + mg \sum_{i=1}^{N_p} \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T q_i$$

$$\text{s.t. } \|q_{(N_p+1)/2} - (0, 1.3)^T\|^2 - 0.35^2 = 0,$$

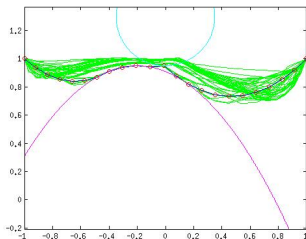
$$0.95 - \begin{pmatrix} 0 \\ 1 \end{pmatrix}^T q_i - \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}^T q_i + 0.2 \right)^2 \leq 0, \quad i = 1, \dots, N_p.$$



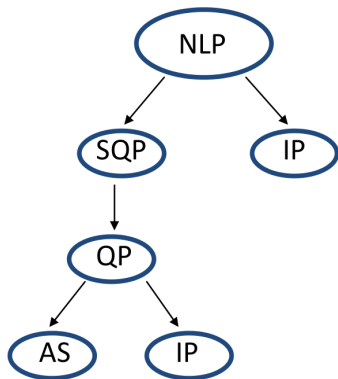
Constrained Optimization

SQP method

- $q_{k+1} = q_k - t_k d_k$
- $t_k \rightarrow$ line search with Armijo's condition using L_1 merit function
- $d_k \rightarrow$ solution of QP problem
- $B_k \rightarrow$ BFGS formula
- 54 iterations

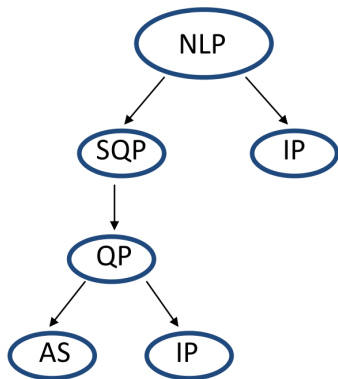


Summary



- Sequential Quadratic Programming(SQP): very powerful for parametric optimization problems, warm start, optimal control
- Interior Point methods(IP): broadly used for convex and non-convex problems, well suited for large-scale problems

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Thank you for your attention!