Model Predictive Control and Reinforcement Learning - Lecture 3: Numerical Optimization -

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Slides contain some figures provided by W. Bangerth and K. Mombaur.





1 Optimization: basic definitions and concepts

- 2 Introduction to some classes of optimization problems
- **3** Newton-type optimization





1 Optimization: basic definitions and concepts

- 2 Introduction to some classes of optimization problems
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What is optimization?

- Optimization = search for the best solution
- in mathematical terms:

minimization or maximization of an objective function f (x) depending on variables x subject to constraints

Equivalence of maximization and minimization problems: (from now on only minimization)



Constrained optimization

• Often variable x shall satisfy certain constraints, e.g.:

- x ≥)
- $x_1^2 + x_2^2 = C$
- General formulation:

 $\min f(x)$ subject to (s.t.) g(x) = 0 $h(x) \ge 0$

f objective function / cost function g equality constraints h inequality constraints



Simple example: Ball hanging on a spring



Feasible set



Feasible set = collection of all points that satisfy all constraints:



The "feasible set" Ω is $\{x \in \mathbb{R}^n | g(x) = 0, h(x) \ge 0\}$.

Local and global minima



The point $x^* \in \mathbb{R}^n$ is a "local minimizer" iff $x^* \in \Omega$ and there exists a neighborhood \mathcal{N} of x^* (e.g an open ball around x^*) so that $\forall x \in \Omega \cap \mathcal{N} : f(x) \ge f(x^*)$.

MPC and RL - Lecture 3: Optimization

J. Boedecker and M. Diehl, University Freiburg

MPC and RL - Lecture 3: Optimization



• The first order derivatives are called the gradient (of the resp. fct)

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

• and the second order derivatives are called the Hessian matrix

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



Optimality conditions (unconstrained)



Types of stationary points



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



Ball on a spring without constraints





Sometimes there are many local minima





Global optimization is a very hard issue - most algorithms find only the next local minimum. But there is a favourable special case...

of macromolecule

Convex functions







Convex: all connecting lines are above graph

Non-convex: some connecting lines are not above graph

$$f:\Omega \to \mathbb{R} \text{ convex} \quad \Leftrightarrow \quad \forall x,y \in \Omega, t \in [0,1]: f(x+t(y-x)) \leq f(x)+t(f(y)-f(x))$$

Convex feasible sets







Convex: all connecting lines between feasible points are in the feasible set

Non-convex: some connecting line between two feasible points is not in the feasible set

$$\Omega$$
 convex $\Leftrightarrow \forall x, y \in \Omega, t \in [0, 1] : x + t(y - x) \in \Omega$

Convex optimization problems







Convex problem if

f(x) is convex **and** the feasible set is convex

One can show: For convex problems, every local minimum is also a global minimum. It is sufficient to find local minima!

Characteristics of optimization problems 1

- size / dimension of problem n , i.e. number of free variables
- continuous or discrete search space

• number of minima





Characteristics of optimization problems 2

- Properties of the objective function:
 - type: linear, nonlinear, quadratic ...
 - · smoothness: continuity, differentiability
- Existence of constraints
- Properties of constraints:
 - equalities / inequalities
 - type: "simple bounds", linear, nonlinear, dynamic equations (optimal control)
 - smoothness



Summary Basic Definitions and Concepts



Optimization problems can be:

- unconstrained or constrained
- convex or non-convex
- linear or non-linear
- differentiable or non-smooth
- continuous or (mixed-)integer
- finite or infinite dimensional

▶





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Problem Class 1: Linear Programming (LP)

 Linear objective, linear constraints: Linear Optimization Problem (convex)

$$\begin{array}{ll} \min_{x} & c^{T}x \\ \text{s. t.} & Ax = b \\ & x \ge 0 \end{array}$$

- Example: Logistics Problem
 - shipment of quantities a₁, a₂, ... a_m of a product from m locations
 - to be received at n detinations in quantities $b_1, b_2, ... b_n$
 - shipping costs c_{ij}
 - determine amounts x_{ij}



Problem Class 2: Quadratic Programming (QP)

 Quadratic objective and linear constraints: Quadratic Optimization Problem (convex, if Q pos. def.)

$$\min_{x} \qquad c^{T}x + \frac{1}{2}x^{T}Qx \\ \text{s. t.} \qquad Ax = b \\ Cx \ge d$$

- Example: Markovitz mean variance portfolio optimization
 - quadratic objective: portfolio variance (sum of the variances and covariances of individual securities)
 - · linear constraints specify a lower bound for portfolio return
- QPs play an important role as **subproblems in nonlinear optimization**

Important: Linear MPC is based on online solution of QP for changing data



Problem Class 3: Nonlinear Programming (NLP)

• Nonlinear Optimization Problem (in general nonconvex)

$$\min_{x} \quad f(x) \\ \text{s. t.} \quad h(x) = 0 \\ g(x) \ge 0$$

• E.g. the famous nonlinear Rosenbrock function

$$f(x) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

Nonlinear MPC is based on online solution of NLP via Newton-type methods



Problem Class 4: Non-smooth optimization

• objective function or constraints are non-differentiable or not continuous e.g.

$$f(x) = |x|$$

$$f(x) = \max_{i} f_{i}(x), \quad i = 1, ..n$$

$$f(x) = \begin{cases} \cos x & \text{für } x \le \frac{\pi}{2} \\ 0 & \text{für } x > \frac{\pi}{2} \end{cases}$$

$$f(x) = i \quad \text{for} \quad i \le x < i + 1, \ i = 0, 1, 2, ...$$

derivative-based methods can still be useful e.g. stochastic gradient descent (SGD) or penalty methods for mathematical programs with complementarity constraints (MPCC)

Problem Class 5: (Mixed) Integer Programming (MIP)

• Some or all variables are integer (e.g. linear integer problems)

$$\min_{x} c^{T}x \\ \text{s. t.} Ax = b \\ x \in Z_{+}^{n}$$

- Special case: combinatorial optimization problems -- feasible set is finite
- Example: traveling salesman problem
 - determine fastest/shortest round trip through n locations



Problem Class 6: Continuous Optimal Control



 Optimization problems including dynamics in form of differential equations (infinite dimensional)



Variables
$$x(t), u(t), p$$
 (partly ∞-dim.)

$$\min_{x,u,p} \int_0^T \phi(t, x(t), u(t), p) dt$$
s. t. $\dot{x} = f(t, x(t), u(t), p)$
....

THIS COURSE'S MAIN TOPIC!

Continuous Time NMPC Problem

$$\min_{s(\cdot),a(\cdot)} \int_0^T c_c(s,a) dt + E(s(T))$$

s.t. $s(0) = \bar{s}_0$
 $\dot{x}(t) = f_c(s(t),a(t))$
 $0 \ge h(s(t),a(t)), t \in [0,T]$
 $0 \ge r(s(T))$

Direct methods like multiple shooting first discretize, then optimize.

Continuous Time NMPC Problem

$$\min_{s(\cdot),a(\cdot)} \int_0^T c_c(s,a) \, \mathrm{d}t + E(s(T))$$

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Direct methods like multiple shooting first discretize, then optimize.

Discrete time NMPC Problem (an NLP)

$$\min_{s,a} \sum_{k=0}^{N-1} c(s_k, a_k) + E(s_N)$$

s.t.
$$s_0 = \bar{s}_0$$

 $s_{k+1} = f(s_k, a_k)$
 $0 \ge h(s_k, a_k), \ k = 0, \dots, N-1$
 $0 \ge r(s_N)$

Variables $s = (s_0, ...)$ and $a = (a_0, ..., a_{N-1})$ can be summarized in vector $x = (s, a) \in \mathbb{R}^n$.

Nonlinear MPC solves Nonlinear Programs (NLP)



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Variables $s = (s_0, ...)$ and $a = (a_0, ..., a_{N-1})$ can be summarized in vector $x = (s, a) \in \mathbb{R}^{n_x}$.

Nonlinear Program (NLP)

$$\min_{x \in \mathbb{R}^{n_x}} F(x)$$

s.t. $G(x) = 0$
 $H(x) \ge 0$



"The great watershed in optimization isn't between linearity and nonlinearity, but convexity and nonconvexity"

R. Tyrrell Rockafellar

- · For convex optimization problems we can efficiently find global minima.
- For non-convex, but smooth problems we can efficiently find local minima.





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Linearization of F at linearization point \bar{x} equals First order Taylor series at \bar{x} equals

$$F_{\rm L}(x;\bar{x}) := F(\bar{x}) + \frac{\partial F}{\partial x}(\bar{x}) \quad (x-\bar{x})$$

(for continuously differentiable $F : \mathbb{R}^{n_x} \to \mathbb{R}^{n_F}$)





Linearization of F at linearization point \bar{x} equals First order Taylor series at \bar{x} equals

$$F_{\mathrm{L}}(x;\bar{x}) := F(\bar{x}) + \nabla_x F(\bar{x})^{\top} (x-\bar{x})$$

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- Equality Constrained Optimization
- Inequality Constrained Optimization
- How to solve QP subproblems?



We want to solve the discretized optimal control problem, which is a Nonlinear Program (NLP)

$$\min_{x} F(x) \text{ s.t. } \begin{cases} G(x) = 0, \\ H(x) \ge 0. \end{cases}$$

We first treat the case without inequalities

$$\min_{x} F(x) \quad \text{s.t.} \quad G(x) = 0,$$

Introduce Lagrangian function

$$\mathcal{L}(x,\lambda) = F(x) - \lambda^{\top} G(x)$$

Then for an optimal solution x^* exist multipliers λ^* such that

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



How to solve nonlinear equations

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

Linearize.

$$\begin{aligned} \nabla_x \mathcal{L}(x^k, \lambda^k) &+ \nabla_x^2 \mathcal{L}(x^k, \lambda^k) \Delta x &- \nabla_x G(x^k) \Delta \lambda &= 0, \\ G(x^k) &+ \nabla_x G(x^k)^\top \Delta x &= 0. \end{aligned}$$

This is equivalent, due to $\nabla \mathcal{L}(x^k, \lambda^k) = \nabla F(x^k) - \nabla G(x^k)\lambda^k$, with the shorthand $\lambda^+ = \lambda^k + \Delta \lambda$, to

$$\begin{aligned} \nabla_x F(x^k) &+ \nabla_x^2 \mathcal{L}(x^k, \lambda^k) \Delta x &- \nabla_x G(x^k) \lambda^+ &= 0, \\ G(x^k) &+ \nabla_x G(x^k)^\top \Delta x &= 0, \end{aligned}$$



Conditions

$$\begin{aligned} \nabla_x F(x^k) &+ \nabla_x^2 \mathcal{L}(x^k, \lambda^k) \Delta x &- \nabla_x G(x^k) \lambda^+ &= 0, \\ G(x^k) &+ \nabla_x G(x^k)^\top \Delta x &= 0, \end{aligned}$$

are optimality conditions of a quadratic program (QP), namely:

$$\min_{\Delta x} \quad \nabla F(x^k)^\top \Delta x + \frac{1}{2} \Delta x^\top B_k^{\text{ex}} \Delta x$$

s.t.
$$G(x^k) + \nabla G(x^k)^\top \Delta x = 0,$$

with

$$B_k^{\rm ex} = \nabla_x^2 \mathcal{L}(x^k, \lambda^k)$$



The full step Newton's Method iterates by solving in each iteration the Quadratic Program

$$\min_{\Delta x} \quad \nabla F(x^k)^\top \Delta x + \frac{1}{2} \Delta x^\top B_k^{\text{ex}} \Delta x$$

s.t.
$$G(x^k) + \nabla G(x^k)^\top \Delta x = 0,$$

with $B_k^{\text{ex}} = \nabla_x^2 \mathcal{L}(x^k, \lambda^k).$

Obtain as QP solution step Δx^k and new multiplier λ_{OP}^+ , and iterate:

$$\begin{array}{rcl} x^{k+1} & = & x^k + \Delta x^k \\ \lambda^{k+1} & = & \lambda^+_{\rm QP} \end{array}$$

The full step Newton's Method iterates by solving in each iteration the Quadratic Program

$$\min_{x} \qquad F_{\mathrm{L}}(x;x^{k}) + \frac{1}{2}(x-x^{k})^{\top}B_{k}^{\mathrm{ex}}(x-x^{k}) \\ \mathrm{s.t.} \qquad G_{\mathrm{L}}(x;x^{k}) = 0,$$

with $B_k^{\text{ex}} = \nabla_x^2 \mathcal{L}(x^k, \lambda^k).$

Obtain new iterate x^+ and new multiplier $\lambda_{\rm QP}^+$ and iterate

$$\begin{array}{rcl} x^{k+1} & = & x^+ \\ \lambda^{k+1} & = & \lambda^+_{\rm QP} \end{array}$$

Can be called Sequential Quadratic Programming (SQP) with exact Hessian and full steps







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Regard again NLP with both, equalities and inequalities:

$$\min_{x} F(x) \text{ s.t. } \begin{cases} G(x) = 0, \\ H(x) \ge 0. \end{cases}$$

Introduce Lagrangian function

$$\mathcal{L}(x,\lambda,\mu) = F(x) - \lambda^{\top} G(x) - \mu^{\top} H(x)$$



THEOREM(Karush-Kuhn-Tucker (KKT) conditions) For an optimal solution x^* exist multipliers λ^* and μ^* such that

$$\begin{aligned} \nabla_{x}\mathcal{L}(x^{*},\lambda^{*},\mu^{*}) &= 0, \\ G(x^{*}) &= 0, \\ H(x^{*}) &\geq 0, \\ \mu^{*} &\geq 0, \\ H(x^{*})^{\top}\mu^{*} &= 0, \end{aligned}$$

These contain nonsmooth conditions (the last three) which are called "complementarity conditions". This system cannot be solved by Newton's Method. But still with SQP...



By linearizing all functions within the KKT Conditions, and setting $\lambda^+ = \lambda^k + \Delta \lambda$ and $\mu^+ = \mu^k + \Delta \mu$, we obtain the KKT conditions of the following Quadratic Program (QP):

$$\begin{split} \min_{x} \quad \nabla F(x^{k})^{\top} \Delta x &+ \frac{1}{2} \Delta x^{\top} B_{k}^{\mathrm{ex}} \Delta x \\ \mathrm{s.t.} \quad \left\{ \begin{array}{ll} G(x^{k}) + \nabla G(x^{k})^{\top} \Delta x &= 0, \\ H(x^{k}) + \nabla H(x^{k})^{\top} \Delta x &\geq 0, \end{array} \right. \end{split}$$

with

$$B_k^{\text{ex}} = \nabla_x^2 \mathcal{L}(x^k, \lambda^k, \mu^k)$$

and its solution delivers

$$\Delta x^k, \quad \lambda_{\rm QP}^+, \quad \mu_{\rm QP}^+$$



In each SQP iteration, solve the following QP:

$$\begin{split} \min_{x} & F_{\mathrm{L}}(x;x^{k}) + \frac{1}{2}(x-x^{k})^{\top}B_{k}^{\mathrm{ex}}(x-x^{k}) \\ \mathrm{s.t.} & \begin{cases} G_{\mathrm{L}}(x;x^{k}) &= 0, \\ H_{\mathrm{L}}(x;x^{k}) &\geq 0, \end{cases} \end{cases}$$

with

$$B_k^{\text{ex}} = \nabla_x^2 \mathcal{L}(x^k, \lambda^k, \mu^k)$$

and QP solution delivers new iterate

$$x^{k+1}, \quad \lambda^{k+1}, \quad \mu^{k+1}$$

In special case of least squares objectives

$$F(x) = \frac{1}{2} \|R(x)\|_2^2$$

can approximate Hessian $\nabla^2_x \mathcal{L}(x^k,\lambda^k,\mu^k)$ by cheaper and always semidefinite matrix

 $B_k^{\rm GN} = \nabla R(x) \nabla R(x)^\top.$

Need no multipliers to compute B_k^{GN} . Obtain convex QP subproblem:

$$\begin{split} \min_{\Delta x} & R(x^k)^\top \nabla R(x^k)^\top \Delta x + \frac{1}{2} \Delta x^\top B_k^{\text{GN}} \Delta x \\ \text{s.t.} & G(x^k) + \nabla G(x^k)^\top \Delta x = 0, \\ & H(x^k) + \nabla H(x^k)^\top \Delta x \ge 0, \end{split}$$



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s.t.
$$\begin{array}{l} G(x^k) + \nabla G(x^k)^\top \Delta x &= 0, \\ H(x^k) + \nabla H(x^k)^\top \Delta x &\geq 0, \end{array}$$



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Need no multipliers to compute B_k^{GN} . Obtain convex QP subproblem:

$$\begin{split} \min_{x} & \frac{1}{2} \| R_{\mathrm{L}}(x;x^{k}) \|_{2}^{2} \\ \mathrm{s.t.} & G_{\mathrm{L}}(x;x^{k}) = 0, \\ H_{\mathrm{L}}(x;x^{k}) \geq 0, \end{split}$$





Constrained Least-Squares Problem

$$\min_{x} \quad \frac{1}{2} \|R(x)\|_{2}^{2}$$

s.t.
$$\begin{array}{l} G(x) &= 0, \\ H(x) &\geq 0, \end{array}$$

Constrained Gauss-Newton Subproblem

$$\begin{aligned} x^{k+1} &= \arg \min_{x} \quad \frac{1}{2} \| R_{\mathrm{L}}(x;x^{k}) \|_{2}^{2} \\ \text{s.t.} \quad \begin{array}{l} G_{\mathrm{L}}(x;x^{k}) &= 0, \\ H_{\mathrm{L}}(x;x^{k}) &\geq 0, \end{array} \end{aligned}$$

Linear convergence, i.e.

$$|x^{k+1} - x^*|| \le \kappa ||x^k - x^*||$$

```
Contraction rate \kappa < 1 small if ||R(x^*)||_2^2 small.
```

[Bock 1987]





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For an equality constrained QP

$$\min_{x} g^{\top} x + \frac{1}{2} x^{\top} A x \text{ s.t.} \quad b + B x = 0,$$

the solution (x, λ) is just solution of one linear system:

$$\begin{array}{rcl} g & +Ax & -B^{\top}\lambda & = & 0, \\ b & +Bx & = & 0, \end{array}$$

In case of inequalities, two variants exist:

- Active Set Methods (similar to simplex for LP, not explained here)
- Interior Point Methods (next slide)



For notational convenience, regard inequality constrained QP in following form

$$\min_{x} g^{\top} x + \frac{1}{2} x^{\top} A x \text{ s.t.} \quad \begin{array}{c} b + B x &= 0, \\ x &\geq 0, \end{array}$$

Idea: replace inequalities by barrier function $-\tau \log(x_i)$, let τ go to zero.

Convex Barrier Subproblem in IP Method

$$\min_{x} g^{\top} x + \frac{1}{2} x^{\top} A x - \tau \sum_{i} \log(x_{i}) \text{ s.t. } b + B x = 0,$$

Solve each $\tau\text{-}\mathsf{problem}$ with Newton-type method for equality constrained optimization. Can show

- error goes to zero for $\tau \to 0$
- if τ is reduced each time by a constant factor, and each new problem is initialized at old solution, the number of Newton iterations is bounded (polynomial complexity)

Nonlinear Systems in Interior Point Methods

Optimality conditions for

Convex Barrier Subproblem in IP Method

$$\min_{x} g^{\top} x + \frac{1}{2} x^{\top} A x - \tau \sum_{i} \log(x_i) \quad \text{s.t.} \quad b + B x = 0,$$

can be shown to be equivalent to system in variables (x,λ,μ)

$$g + Ax - B^{\top}\lambda - \mu = 0,$$

$$b + Bx = 0,$$

$$x_i\mu_i = \tau, \quad i = 1, \dots, n.$$

Only last condition is nonlinear, it replaces the last KKT condition. The system can be solved by Newton's method, e.g. in QP solver HPIPM for fast MPC.

Note: IP method can also directly address nonlinear programs, e.g. in NLP solver IPOPT.

Summary



- Optimization problems can be:
 - unconstrained or constrained
 - convex or non-convex
 - linear or non-linear
 - differentiable or non-smooth
 - continuous or (mixed-)integer
 - finite or infinite dimensional
 - ▶ ...
- Important classes are
 - linear programs (LP)
 - quadratic programs (QP)
 - nonlinear programs (NLP)
- Newton-type algorithms linearize nonlinear functions and solve convex subproblems

General NLP

 $\min_{\substack{x \in \mathbb{R}^{n_x}}} F(x)$ s.t. G(x) = 0 $H(x) \ge 0$

For least-squares: $F(x) = ||R(x)||_2^2$ get

Gauss-Newton QP subproblem

 $\min_{\substack{x \in \mathbb{R}^{n_x}}} \|R_{\mathrm{L}}(x; \bar{x})\|_2^2$ s.t. $G_{\mathrm{L}}(x; \bar{x}) = 0$ $H_{\mathrm{L}}(x; \bar{x}) \ge 0$



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