

Optimization Algorithms

Introduction

Marc Toussaint Technical University of Berlin Winter 2024/25

Learning & Intelligent Systems Lab

Applications

time = 2/78



argmin.lis.tu-berlin.de

Research

- Intersection of AI & Robotics
- Combining learning and reasoning
- physical reasoning, task-and-motion planning (logic-geometric programming)
- reinforcement learning, perception-based policies, reactive control/learning
- driven by robotics problems

Why is Optimization interesting?



$$\delta \int_{t_0}^{t_1} L(q(t), \dot{q}(t), t) \ dt = 0$$

Principle of Least Action



Introduction -4/22



Native state

protein folding



Introduction -5/22

$$\min_{\beta} \|\beta\|^2 \quad \text{s.t.} \quad y_i(\phi(x_i)^\top \beta) \ge 1, \ i = 1, \dots, n$$

support vector machine



Introduction - 6/22

$$\min_{f \in \mathcal{H}} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$

loss minimization (e.g., NNs)



Introduction – 7/22

$$\min_{u,x} \int_0^T f(x(t), u(t)) \ dt \quad \text{s.t.} \quad \dot{x} = f(x, u), \ g(x(t)) \le 0, \ h(x(T)) = 0$$

optimal control



Introduction - 8/22





construction statics



Introduction -9/22



"Logic Geometric Programming" Introduction - 10/22

Why is Optimization interesting?

- Optimality principles are a means of scientific and engineering description
- It is often easier to describe a thing (natural or artifical) via an optimality priciple than directly
- Almost any scientific field uses optimality principles to describe nature & artifacts
 - Physics, Chemistry, Biology, Mechanics, ...
 - Operations research, scheduling, ...
 - Computer Vision, Speach Recognition, Machine Learning, Robotics, AI, ...
- Endless applications

Teaching optimization

- Optimization includes largely different approaches/formalisms:
 - Standard continuous, convex or non-linear optimization
 - Discrete Optimization
 - Global Optimization
 - Stochastic Optimization, Evolutionary Algorithms, Swarm optimization, etc

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- This lecture focusses on continuous, convex or non-linear optimization

Optimization Problems

• Generic optimization problem, also called Mathematical Program:

Let $x \in \mathbb{R}^n, f: \mathbb{R}^n \to \mathbb{R}, g: \mathbb{R}^n \to \mathbb{R}^m, h: \mathbb{R}^n \to \mathbb{R}^l$. Find

 $\min_{x} f(x)$ s.t. $g(x) \le 0, h(x) = 0$

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$$\min_{x} f(x)$$
 s.t. $g(x) \le 0, h(x) = 0$

- **Blackbox**: only f(x) can be evaluated
- **Gradient**: $\nabla f(x)$ can be evaluated
- Gauss-Newton type: $f(x) = \phi(x)^\top \phi(x)$ and $\nabla\!\phi(x)$ can be evaluated
- Stochastic Gradient: only "samples of $\nabla f(x)$ " can be evaluated efficiently
- **2nd order**: $\nabla^2 f(x)$ can be evaluated
- Approximate methods:
 - Use samples of f(x) to approximate $\nabla f(x)$ locally
 - Use samples of $\nabla \! f(x)$ to approximate $\nabla^2 f(x)$ locally

Planned Outline

- Part 1: Downhill algorithms for unconstrained optimization:
 - gradient descent, backtracking line search, Wolfe conditions, convergence properties
 - covariant gradients, Newton, quasi-Newton methods, (L)BFGS
- Part 2: Algorithms for constrained optimization:
 - KKT conditions, Lagrangian
 - Log-barrier, Augmented Lagrangian, primal-dual Newton
 - SQP
- Part 3: Extended topics (subject to change):
 - Stochastic gradient methods
 - Global optimization
 - stochastic search, evolutionary algorithms
 - maybe this year: ADMM & NLP Reformulations

References

- Maths for Intelligent Systems script on ISIS page
- Boyd and Vandenberghe: *Convex Optimization*. http://www.stanford.edu/~boyd/cvxbook/
- Nocedal & Wright: *Numerical Optimization* www.bioinfo.org.cn/~wangchao/maa/Numerical_Optimization.pdf

(this course won't of course cover all this - just for reference)



Organization



- 6 LPs (180h, 12h/w, 15 weeks)
- Lectures, weekly, in person
- Exercise Sheets & Coding Assignments:
 - Weekly exercise sheets, mostly analytic problems, discussed in the tutorials
 - Hand-in coding assignments, every ~ 3 weeks: Submit your optimization algorithms/problems via git \rightarrow are numerically evaluated/graded
- ISIS as central webpage
- Contact:
 - Tutors: Sayantan Auddy <auddy@tu-berlin.de>, Cornelius Braun, Hongyou Zhou
 - Office (grades/etc): Ilaria Cicchetti-Nilsson <office@lis.ut-berlin.de>

Assignments & Exam

- Voting System for the exercise sheets:
 - Before attending the tutorial, students mark in an ISIS questionnaire which exercises they have worked on
 - Students are randomly selected to present their solutions (no need for correct solutions just something to present and discuss)
 - When not attending: upload pdf notes/solutions on ISIS

• Exam prerequisites:

- at least 50% votes in the exercises, and
- at least 50% points in the hand-in coding assignments

(If you fulfilled these prerequisites last year, you don't have to redo them.)

• The written exam will be about analytical problems, determines final grade (no



Registration

- Registration for the exam in Moses will open in January
- To gain the exam prerequisites you'll have to register for the coding exercises (will be organized in the second/third week), and submit your votes on the exercise sheets
- There is no further registration for this course necessary

Prerequisites

- Module description:
 - Good knowledge in linear algebra and calculus
 - \rightarrow Specifically, the 'Maths for Intelligent Systems Script' up to Chapter 3.
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 - Do you have intuition about basic linear algebra? (Fig. 2 and Sec. 3.6)
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- Coding:
 - Numeric coding in Python (numpy)
 - Familiarity with git will help

Module description (Moses 41016)

• Learning Outcomes

- The students will be able to develop and apply optimization algorithms.
- They can formulate real-world problems appropriately as mathematical programs.
- They have a detailed understanding of the different categories of optimization problems, and methods to approach them.
- They have a basic understanding of the theory behind and properties of optimization algorithms.
- They have an overview of and experience with existing optimization software and are able to apply them to solve optimization problems.

Content

- The course is on continuous optimization problems, with focus on non-linear mathematical programming (constrained optimization).
- Part 1 introduces efficient downhill algorithms in the unconstrained case: ...
- Part 2 will introduce efficient algorithms for constrained optimization: ...
- Part 3 will cover extended topics (global optimization, stochastic gradient, stochastich search) ...
- Prerequisites
 - Good knowledge in linear algebra and calculus
 - Basic programming knowledge in Python

Module description (Moses 41016)

- Grading
 - graded, written exam, English (120min)
- This module is used in the following module lists:
 - Computational Engineering Science (Informationstechnik im Maschinenwesen) (Master of Science)
 - Computer Engineering (Master of Science)
 - Computer Science (Informatik) (Master of Science)
 - Elektrotechnik (Master of Science)
 - ICT Innovation (Master of Science)
 - Medieninformatik (Master of Science)
 - Physikalische Ingenieurwissenschaft (Master of Science)