Optimization for Machine Learning Discrete Optimization

December 9, 2021 TC2 - Optimisation Université Paris-Saclay



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Course Overview

Date		Торіс
Thu, 4.11.2021	DB	Introduction
Thu, 11.11.2021		no lecture
Thu, 18.11.2021	AA	Continuous Optimization I: differentiability, gradients, convexity, optimality conditions
Thu, 25.11.2021	AA	Continuous Optimization II: constrained optimization, gradient-based algorithms, stochastic gradient [written test / « contrôle continue »]
Thu, 2.12.2021	AA	Continuous Optimization III: stochastic algorithms, derivative-free optimization
Thu, 9.12.2021	DB	Discrete Optimization: greedy algorithms, branch&bound, dynamic programming
Thu 16.12.2021	DB	Written exam
		! always 13h30 till 16h00

Concrete Information About Exam

Written exam

- multiple choice, typically 4 answers each (1-4 answers correct)
- closed book (nothing allowed but pen) \rightarrow easier questions \odot
- next Thursday (Dec. 16) @ 1:30pm
- 1.5 hours

 Back to some examples of optimization problems in Machine Learning ...

- Classification
 - Is there a cat on the picture?



Yes / No

- Classification
 - Is there a cat on the picture?



Yes

- Classification
 - Is there a cat on the picture?



Yes

- Classification
 - Is there a cat on the picture?



No

Labelled data / training sets



Given a set of examples $\{(x^1, y^1), \ldots, (x^n, y^n)\}$ with x^i the features and y^i labels/targets

Given a set of examples $\{(x^1, y^1), \ldots, (x^n, y^n)\}$ with x^i the features and y^i labels/targets

Find a mapping $h: x \in X \to y \in \mathbb{R}$ that will assign the "correct" target to each input New image (not in the training set) $h\left(\begin{array}{c} & & \\$

Hypothesis: linear model

$$x_0 = 1 h_w(x) = w_0 + w_1 x_1 + \ldots + w_{d-1} x_{d-1} = \langle w, x \rangle$$

Find $h_w(x)$ via solving the minimization problem



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Generalization: Parametrization of the Hypothesis

Linear:
$$h_w(x) = \langle w, x \rangle = \sum_{i=0}^{d-1} w_i x_i$$



Polynomial:
$$h_w(x) = \sum_{i,j=0}^{d-1} w_{i,j} x_i x_j$$





Neural network:

Start from the linear regression problem:

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n (h_w(x^i) - y^i)^2$$

Let $y_h := h_w(x)$

Loss function:
$$l : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_+$$

 $(y_h, y) \to l(y_h, y)$

For linear regression $l(y_h, y) = (y_h - y)^2$

Training (optimization) problem:

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n l(h_w(x^i), y^i)$$

Generalization: Different loss functions

Quadratic loss:
$$l(y_h, y) = (y_h - y)^2$$



Binary loss:
$$l(y_h, y) = \begin{cases} 0 \text{ if } y_h = y \\ 1 \text{ if } y_h \neq y \end{cases}$$

Hinge loss:
$$l(y_h, y) = \max\{0, 1 - y_h y\}$$



Very often it is not possible to solve analytically the equation $\nabla f(x) = 0$ and we have to resort to an iterative algorithm (or numerical optimization algorithm) that will generate a sequence of points $\{x_k : k \ge 0\}$ that should converge to $\operatorname{argmin}_x f(x)$

Optimization algorithm:

input $f, \nabla f, (\nabla^2 f)$ initialize $k = 0, x_0$ [other state variables] while not happy do update x_k k = k + 1end-do return x_k, k

Goal: $\lim_{k \to \infty} f(x_k) = \min_x f(x)$ $\lim_{k \to \infty} ||x_k - x^*|| = 0$ Depending on the information the algorithm is using to create a new point (or iterate) we distinguish

Zero-order's algorithms: only use f (no gradients, ...). Those methods are also called derivative-free optimization algorithms. Used when gradient or Hessian are difficult to compute, or when the functions are not differentiable.

First-order algorithms: use f and ∇f . Standard algorithms when f is differentiable, convex.

Second-order algorithms: use f, ∇f and $\nabla^2 f$. When we can have an "easy" access to the Hessian matrix.

descent direction



Generic algorithm:

choose an initial point x_0 , k = 0while not happy

choose a descent direction d_k

line-search: choose a step-size σ_k

$$x_{k+1} = x_k + \sigma_k d_k$$
$$k = k+1$$

Line search: 1-d minimization along the descent direction $\sigma \rightarrow f(x_k + \sigma d_k)$

Descent direction: direction such that for σ small enough

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

When are we "happy", i.e. when do we stop the algorithm?

when gradient norm becomes small

 $\|\nabla f(x_k)\| \le \epsilon$

when step-size becomes small

$$\|x_{k+1} - x_k\| \le \epsilon$$

when progress in f becomes small

$$\frac{|f(x_{k+1}) - f(x_k)|}{|f(x_k)|} \le \epsilon$$

Take as descent direction the Newton step:

$$d_k = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

The Newton's direction minimizes the best locally quadratic approximation of f. Indeed, by Taylor's expansion we can approximate f locally in x by

$$g(h) = f(x) + \nabla f(x)^{\top} h + \frac{1}{2} h^{\top} \nabla^2 f(x) h$$
$$\approx f(x+h)$$

Minimizing g with respect to h yields:

$$h = -[\nabla^2 f(x)]^{-1} \nabla f(x)$$

In quasi-Newton's methods, the Newton direction is approximated by using solely first order information (gradient)

Key idea: successive iterates x_k , x_{k+1} and gradients $\nabla f(x_k)$ yield second order information

$$q_k \approx \nabla^2 f(x_{k+1}) p_k$$

$$p_k = x_{k+1} - x_k, \ q_k = \nabla f(x_{k+1}) - \nabla f(x_k)$$

BFGS algorithm:

 B_k approximation of Hessian matrix

$$d_{k} = -B_{k}^{-1} \nabla f(x_{k})$$

$$x_{k+1} = x_{k} + \sigma_{k} d_{k} \text{ (find } \sigma_{k} \text{ via line-search)}$$

$$y_{k} = \nabla f(x_{k+1}) - \nabla f(x_{k})$$

$$B_{k+1} = B_{k} + \frac{y_{k} y_{k}^{\top}}{y_{k}^{\top} \sigma_{k} d_{k}} - \frac{B_{k} d_{k} d_{k}^{\top} B_{k}}{d_{k}^{\top} B_{k} d_{k}}$$

efficient update to compute the inverse of B_k

Considered as the state-of-the-art quasi-Newton's algorithm. Implemented in all (good) optimization toolboxes

Gradient Descent - Simple Theoretical Analysis

Theorem[Linear convergence of gradient descent] Assume $f : \mathbb{R}^d \to \mathbb{R}$ is twice continuously differentiable, convex and for all $x, \mu I_d \preccurlyeq \nabla^2 f(x) \preccurlyeq LI_d$ with $\mu > 0$. Let x^* be the unique global minimum of f. The gradient descent algorithm with fixed step-size $\sigma_t = \frac{1}{L}$ satisfies

$$||x_{k+1} - x^*||^2 \le \left(1 - \frac{\mu}{L}\right) ||x_k - x^*||^2$$

That is the algorithm converges geometrically (also called linearly):

$$||x_k - x^*||^2 \le \left(1 - \frac{\mu}{L}\right)^k ||x_0 - x^*||^2$$

algorithm slower and slower with increasing condition number

In comparison, convergence of Newton's method is quadratic:

$$||x_{k+1} - x^*|| \le c ||x_k - x^*||^2 \text{ with } c < 1$$
$$||x_{k+1} - x^*||^2 \le c^2 (||x_k - x^*||^2)^2 \text{ with } c < 1$$

We now come back to our training optimization problem

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^n \underbrace{l(h_w(x^i), y^i)}_{f_i(w)}$$

the f_i can include a regularization term

Gradient descent update:

$$w_{k+1} = w_k - \sigma_k \frac{1}{n} \sum_{i=1}^n \nabla f_i(w_k)$$

Problem: each iteration requires to compute a gradient $\nabla f_i(w)$ for each data point. We don't want to do that when n is large (quite typical).

The gradient of $f(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(w)$ is approximated by the gradient of a single data function $f_i(w)$ at each iteration

 $\nabla f(w) \approx \nabla f_i(w)$ for j chosen at random

Stochastic gradient descent update:

sample
$$j \in \{1, \dots, n\}$$

 $w_{k+1} = w_k - \sigma_k \nabla f_i(w_k)$

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Integer Programming

- variables are integers
- simplest example:
 optimization in {0, 1}ⁿ

Combinatorial Optimization

- Search space not necessarily anymore a subset of \mathbb{R}^n
- for example, optimization on graphs

ML example:

hyperparameter tuning with algorithm parts being present $(x_i = 1)$ or not $(x_i = 0)$ *ML example:* structure optimization of neural networks

Discrete vs. Continuous Optimization

Important Differences/Observations

- finite search space \rightarrow still: enumeration impracticable
- discrete neighborhood, sometimes not even clear how to define
- gradient inexistent \rightarrow follow locally best neighbor?
- different neighborhoods, different definition of local optimum!

example later

- partial evaluations common for discrete problems
- blackbox vs. greybox vs. whitebox

...meaning that solvers for discrete problems are typically more specialized

Overview Discrete Optimization

Algorithms for discrete problems:

- often highly problem-specific
- but some general concepts are repeatedly used:
 - greedy algorithms
 - branch and bound
 - dynamic programming
 - randomized search heuristics [not in this lecture]

Motivation for this Last Part of the Lecture:

- get an idea of the most common algorithm design principles
- we cannot
 - go into details and present many examples of algorithms

...but for a few

analyze algorithms theoretically with respect to their runtime

Greedy Algorithms

From Wikipedia:

"A greedy algorithm is an algorithm that follows the problem solving *heuristic* of making the locally optimal choice at each stage with the hope of finding a global optimum."

• Note: typically greedy algorithms do not find the global optimum

Lecture Outline Greedy Algorithms

What we will see:

- Example 1: Money Change problem
- **2** Example 2: ϵ -Greedy Algorithm for Multi-Armed Bandits

Change-making problem

- Given n coins of distinct values w₁=1, w₂, ..., w_n and a total change W (where w₁, ..., w_n, and W are integers).
- Minimize the total amount of coins Σx_i such that $\Sigma w_i x_i = W$ and where x_i is the number of times, coin i is given back as change.

Greedy Algorithm

Unless total change not reached:

add the largest coin which is not larger than the remaining amount to the change

Note: only optimal for standard coin sets, not for arbitrary ones!

Related Problem:

finishing darts (from 501 to 0 with 9 darts)

Example 2: Multi-Armed Bandits

- generic problem of resource allocation
- classic reinforcement learning problem showing the exploration—exploitation tradeoff dilemma



Yamaguch

i先生

Example 2: Multi-Armed Bandits



- *K* single-arm bandits with a lever
- Each bandit has a fixed but unknown probability distribution \mathcal{R}_i attached to it with a mean μ_i
- At each time step t, we decide to pull a lever (i) and get a reward r_t according to R_i
- Overall, we want to maximize the sum of the rewards
- The regret after T steps is defined as $\rho = T \mu_{max} \sum_{t=1}^{T} r_t$
Exploration vs. Exploitation: The ϵ -Greedy Algorithm

Exploration: pull new levers (or underexplored ones) to get better estimates on the expected rewards

Exploitation: pull the arm, we think is the best arm

...the latter being the greedy approach here

The *ε*-Greedy Algorithm

- With probability $1-\epsilon$: pull the lever, we think is best
- With probability ϵ : pull a random lever (uniformly)

To be decided (not discussed further here):

How to estimate the probabilities (e.g. pulling each lever once at first) How to choose ϵ (constant vs. decreasing over time)

constant ϵ gives linear regret

Branch and Bound

- Basically enumerates the entire search space
- But uses clever strategies to avoid enumerations in bad areas







when can we actually avoid evaluating all solutions?



How do we get Upper and Lower Bounds?

We assume again maximization here...

• A feasible solution gives us a lower bound

the optimum will be at least as good as a solution, we know

- Hence, fast (non-exact) algorithms such as greedy can give us lower bounds
- For upper bounds, we can relax the problem

for example, by removing constraints

An Example: Branch&Bound for the KP



Dake

()

KP: How to Branch?



! order of variables plays an important role optimally, the subproblems don't overlap

KP: How to Bound?



Maximization, so LB by greedy approach for example:

Choose items in decreasing profit/weight ratio until knapsack full

UB by relaxation of constraints (on the variables here): Use greedy algorithm and pack add. item partially if there is space ...this variable can be used to branch next

Dynamic Programming

Wikipedia:

"[...] **dynamic programming** is a method for solving a complex problem by breaking it down into a collection of simpler subproblems."

But that's not all:

- dynamic programming also makes sure that the subproblems are not solved too often but only once by keeping the solutions of simpler subproblems in memory ("trading space vs. time")
- it is an exact method, i.e. in comparison to the greedy approach, it always solves a problem to optimality

Optimal Substructure

A solution can be constructed efficiently from optimal solutions of sub-problems

Overlapping Subproblems

Wikipedia: "[...] a problem is said to have **overlapping subproblems** if the problem can be broken down into subproblems which are reused several times or a recursive algorithm for the problem solves the same subproblem over and over rather than always generating new subproblems."

Main Idea Behind Dynamic Programming

Main idea: solve larger subproblems by breaking them down to smaller, easier subproblems in a recursive manner

Typical Algorithm Design:

- decompose the problem into subproblems and think about how to solve a larger problem with the solutions of its subproblems
- specify how you compute the value of a larger problem recursively with the help of the optimal values of its subproblems ("Bellman equation")
- Solution bottom-up solving of the subproblems (i.e. computing their optimal value), starting from the smallest by using the Bellman equality and a table structure to store the optimal values
- eventually construct the final solution (can be omitted if only the value of an optimal solution is sought)

Example: The Knapsack Problem (KP)

Knapsack Problem





Dake

0

What are Good Subproblem Definitions for the KP?

Consider the following subproblems:

- 1) P(i): optimal profit when packing exactly *i* items
- 2) P(i): optimal profit when packing at most *i* items
- 3) P(i, j): optimal profit when allowing to pack the first *i* items into a knapsack of size *j*

Which one allows us to solve larger subproblems from the solutions of smaller ones?

Which value are we actually interest in, when trying to solve the problem?

Opt. Substructure and Overlapping Subproblems

Consider the following subproblem:

P(i, j): optimal profit when allowing to pack the first *i* items into a knapsack of size *j*

Optimal Substructure

The optimal choice of whether taking item *i* or not can be made easily for a knapsack of weight *j* if we know the optimal choice for items $1 \dots i - 1$:

$$P(i,j) = \begin{cases} 0 & \text{if } i = 0 \text{ or } j = 0\\ P(i-1,j) & \text{if } w_i > j\\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$$

Overlapping Subproblems

a recursive implementation of the Bellman equation is simple, but the P(i, j) might need to be computed more than once!

To circumvent solving the subproblems more than once, we can store their results (in a matrix for example)...



best achievable profit with items 1...i and a knapsack of size j

Example instance with 5 items with weights and profits (5,4), (7,10), (2,3), (4,5), and (3,3). Weight restriction is W=11.



knapsack weight

initialization: P(i,j) = 0 if i = 0 or j = 0

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for
$$i = 1$$
 to n :
for $j = 1$ to W :

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$$

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	P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
ns	0	0	0	0	0	0	0	0	0	0	0	0	0
iter	1	0	0										
I.	2	0											
	3	0											
•	4	0											
	5	0											

knapsack weight

for i = 1 to n: for j = 1 to W: $P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$

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ns	0	0	0	0	0	0	0	0	0	0	0	0	0
iter	1	0	0	0									
I.	2	0											
	3	0											
♦	4	0											
	5	0											

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ns	0	0	0	0	0	0	1 0	0	0	0	0	0	0
iter	1	0	0	0	0	0	4						
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	3	0											
+	4	0											
	5	0											

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iter	1	0	0	0	0	0	4	4					
I.	2	0				$+p_{1}($	= 4)						
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	3	0											
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iter	1	0 🔺	0	0	0	0	4	4	↑ 4	4	4	4	4
Ι	2	0	0	0	0	0	4	4	-10				
	3	0					$+p_{2}($	= 10)					
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knapsack weight

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Example instance with 5 items with weights and profits (5,4), (7,10), (2,3), (4,5), and (3,3). Weight restriction is W = 11.

	P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
ns	0	0	0	0	0	0	0	0	0	0	0	0	0
iter	1	0	0	0	0	0	4	4	4	4	4	4	4
Ι	2	0	0	0	0	0	† 4	4	10	10	10	10	10
	3	0	0	3	3	3	4						
♦	4	0			$+p_3($	- 5)							
	5	0											

knapsack weight

for i = 1 to n: for j = 1 to W: $P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$

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ns	0	0	0	0	0	0	0	0	0	0	0	0	0
iter	1	0	0	0	0	0	4	4	4	4	4	4	4
I	2	0	0	0	0	0	4	↑ 4	10	10	10	10	10
	3	0	0	3	3	3	4	4					
+	4	0				$\pm p_3$	(- 3)						
	5	0											

knapsack weight

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Hems items item i	P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
	0	0	0	0	0	0	0	0	0	0	0	0	0
	1	0	0	0	0	0	4	4	4	4	4	4	4
	2	0	0	0	0	0	4	4	1 0	10	10	10	10
	3	0	0	3	3	3	4	4	10	etc.			
	4	0					$+p_3($	_ 5)					
	5	0											

knapsack weight

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	P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
ns	0	0	0	0	0	0	0	0	0	0	0	0	0
llter	1	0	0	0	0	0	4	4	4	4	4	4	4
	2	0	0	0	0	0	4	4	10	10	10	10	10
	3	0	0	3	3	3	4	4	10	10	13	13	13
ŧ	4	0	0	3	3	5	5	8	10	10	13	13	15
	5	0	0	3	3	5	6	8	10	10	13	13	15

knapsack weight

for i = 1 to n:

for
$$j = 1$$
 to W :

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$$

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	P(i,j)	0	1	2	3	4	5	6	7	8	9	10	11
ns	0	0	0	0	0	0	0	0	0	0	0	0	0
llter	1	0	0	0	0	0	4	4	4	4	4	4	4
	2	0	0	0	0	0	4	4	10	10	10	10	10
	3	0	0	3	3	3	4	4	10	10	13	13	13
ŧ	4	0	0	3	3	5	5	8	10	10	13	13	15
	5	0	0	3	3	5	6	8	10	10	13	13	15

knapsack weight

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Dynamic Programming Approach to the KP

Question: How to obtain the actual packing?

Answer: we just need to remember where the max came from!

P(i,j) \mathbf{O} items x_1 $x_2 = 1$ $x_3^{10} = \mathbf{0}^{10}$ 13 <u>x</u>4 <u>1</u>3₁ $x_{5} = 0$

knapsack weight ------

for i = 1 to n:

for
$$j = 1$$
 to W :

$$P(i,j) = \begin{cases} P(i-1,j) & \text{if } w_i > j \\ \max\{P(i-1,j), p_i + P(i-1,j-w_i)\} & \text{if } w_i \le j \end{cases}$$

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