

Final Project for “Convex Optimization”

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1 Algorithms for large-scale Optimal Transport

1. Consider the standard form of LP

$$(1.1) \quad \begin{aligned} \min_{\pi \in \mathbb{R}^{m \times n}} \quad & \sum_{i=1}^m \sum_{j=1}^n c_{ij} \pi_{ij} \\ \text{s.t.} \quad & \sum_{j=1}^n \pi_{ij} = \mu_i, \quad \forall i = 1, \dots, m, \\ & \sum_{i=1}^m \pi_{ij} = \nu_j, \quad \forall j = 1, \dots, n, \\ & \pi_{ij} \geq 0. \end{aligned}$$

- (a) Solve (1.1) by calling mosek and gurobi **directly** in Matlab or python. The package “CVX” is **not allowed** to use here. Compare the performance between the simplex methods and interior point methods.
- (b) Write down and implement a first-order method, for example, the alternating direction method of multipliers.
- (c) Test problems:
 - Generate some random data c , μ and ν .
 - Find or construct the data sets in the references:
 - Jörn Schrieber, Dominic Schuhmacher, Carsten Gottschlich, DOTmark – A Benchmark for Discrete Optimal Transport.
 - Samuel Gerber, Mauro Maggioni, Multiscale Strategies for Computing Optimal Transport.

2. Read the reference:

- Gabriel Peyre, Marco Cuturi, Computational Optimal Transport, <https://arxiv.org/abs/1803.00567>.
some slides on optimal transport can be found at <https://optimaltransport.github.io/slides/>
- Ernest K. Ryu, Yongxin Chen, Wuchen Li, Stanley Osher, Vector and Matrix Optimal Mass Transport: Theory, Algorithm, and Applications, <https://arxiv.org/abs/1712.10279>

- (a) Find one of the most important optimization problems from the above references. Write down the background and formulation clearly.
- (b) Write and implement an algorithm for the optimization problem in 2(a) from the chosen reference. Try to reproduce the numerical results in that reference.
- (c) Try to write down and implement an algorithm covered in this course for the optimization problem in 2(a). This algorithm should be different from the one in 2(b).

3. Requirement:

- (a) Compare the efficiency (cpu time) and accuracy (checking optimality condition) of different methods.
- (b) Prepare a report including
 - detailed answers to each question
 - numerical results and their interpretation
- (c) Pack all of your codes in one file named as “proj2-name-ID.zip” and send it to TA: pkuopt@163.com
- (d) If you get significant help from others on one routine, write down the source of references at the beginning of this routine.

2 Algorithms and analysis for shallow neural network

Let $f(\theta; x_i)$ be the output of a neural network and $\sigma(x)$ be one of the following element-wise activation function

$$(2.1) \quad \text{Relu}(x) = \max(0, x),$$

$$(2.2) \quad \text{Sigmoid}(x) = \frac{1}{1 + \exp(-x)},$$

$$(2.3) \quad \text{Tanh}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}.$$

For a given data set $\{\{x_i, y_i\}_{i=1}^N\}$, consider the supervised learning problem:

$$(2.4) \quad \min_{\theta} h(\theta) = \sum_{i=1}^N L(y_i, f(\theta; x_i)),$$

where L is the following loss functions

$$(2.5) \quad \ell_2 \text{ loss} : L(y_i, f(\theta; x_i)) = \frac{1}{2} \|y_i - f(\theta; x_i)\|_2^2.$$

In the following questions, the activation and loss function can be any of their combinations.

1. Consider the two-layer feed-forward neural network

$$f(\theta; x) := f_{W,v}(x) = \frac{1}{\sqrt{m}} v^\top \sigma(Wx),$$

where $x_i \in \mathbb{R}^d$ is the input data, $W \in \mathbb{R}^{m \times d}$, $v \in \mathbb{R}^m$ are weight matrix. The parameters are concatenated into one column vector $\theta = [\text{vec}(W)^\top, v^\top]^\top$, where $\text{vec}(W)$ transforms the matrix W into a vector by stacking all the columns of W one underneath the other.

- (a) Compute the gradient (or subgradient) of $h(\theta)$ with respect to θ and estimate its Lipschitz constant.
- (b) Compute the Hessian of $h(\theta)$ with respect to θ if it is available and estimate the upper and lower bound of its eigenvalues.
- (c) Will the function $h(\theta)$ be strongly convex in a small neighbourhood of the global optimal solution? Either try numerical experiments on a few small examples or try to establish certain theoretical results.
- (d) Suppose that **the gradient descent method** with certain line search schemes or **or certain stepsize strategies** is applied to solve (2.4). Write down the method and the corresponding convergence results from **a few literatures** or the classic textbooks on nonlinear programming such as
 - “Numerical Optimization”, Jorge Nocedal and Stephen Wright, Springer
 - “Optimization Theory and Methods”, Wenyu Sun, Ya-Xiang Yuan

Is it possible that this method converges to a global optimal solution of (2.4)? Either try numerical experiments on a few examples or try to establish certain theoretical results.

- (e) Suppose that **the stochastic gradient method** is applied to solve (2.4). Write down the method and the corresponding convergence results from a few literatures. Is it possible that this method converges to a global optimal solution of (2.4)? Either try numerical experiments on a few examples or try to establish certain theoretical results.
- (f) Suppose that **the KFAC method** is applied to solve (2.4)
 - Optimizing Neural Networks with Kronecker-factored Approximate Curvature, James Martens, Roger Grosse, <https://arxiv.org/abs/1503.05671>

Write down the method and the corresponding convergence results from a few literatures. Is it possible that this method converges to a global optimal solution of (2.4)? Either try numerical experiments on a few examples or try to establish certain theoretical results.

2. Requirement:

- (a) Test problems:
 - random examples created by yourself.
 - MNIST or Cifar-10.
 - **You can consider the experiment setup in the following paper:**
 - Fine-grained analysis of optimization and generalization for overparameterized two-layer neural networks, Arora, Sanjeev, Simon S. Du, Wei Hu, Zhiyuan Li, and Ruosong Wang, <https://arxiv.org/abs/1901.08584>
- (b) Requirements on numerical experiments:
 - **Specify the weight initialization schemes chosen in your experiments.**
 - **Write all the prerequisites and the usage of your codes in detail.**
- (c) Prepare a report including:
 - detailed answers to each question.
 - numerical results and their interpretation if there are numerical experiments.
- (d) Pack all of your codes in one file named as “proj2-name-ID.zip” and send it to TA: pkupt@163.com

- (e) If you get significant help from others on one routine, write down the source of references at the beginning of this routine.