Sinkhorn Algorithm as a Special Case of Stochastic Mirror Descent

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Problem 1: Matrix Scaling

Given a matrix $X^0 \in \mathbb{R}^{n \times n}$, find vectors $u, v \in \mathbb{R}^n_+$ such that

 $W \stackrel{\text{def}}{=} \operatorname{diag}(u) X^0 \operatorname{diag}(v)$

is doubly stochastic, i.e. W1 = 1 and $W^{\top}1 = 1$.

Motivation

- Matrix preconditioning for improved linear algebra operations such as solving $X^0w=b$.
- Ranking web page significance: take network connectivity matrix and find the stationary distribution of its doublly-stochastic form
- Estimation of transition probabilities in Markov chains; traffic and transportation planning; network optimization (see [2] for more details).

Sinkhorn Algorithm

Algorithm 1: Sinkhorn Algorithm.

$$\begin{aligned} & \textbf{for } k = 1, \dots \textbf{do} \\ & | X_{i:}^{k+1} = X_{i:}^k / || X_{i:}^k ||_1 \text{ for all } i; \\ & | X_{:j}^{k+2} = X_{:j}^{k+1} / || X_{:j}^{k+1} ||_1 \text{ for all } j; \\ & \textbf{end} \end{aligned}$$

Note that

$$\log X^{k+1} = \log X^k + \operatorname{diag}(u_1^k, \dots, u_n^k) 11^\top, \log X^{k+2} = \log X^{k+1} + 11^\top \operatorname{diag}(v_1^{k+1}, \dots, v_n^{k+1}).$$

This is very helpful for showing the equivalence. Can be trivially generalized to finding W such that $W1=p,\ W^{\top}1=q$ for any $p,q\in\mathbb{R}^d_+$.

[1] Marco Cuturi.

Sinkhorn distances: Lightspeed computation of optimal transport.

In Advances in neural information processing systems, 2013.

- [2] Bahman Kalantari, Isabella Lari, Federica Ricca, and Bruno Simeone.
- On the complexity of general matrix scaling and entropy minimization via the ras algorithm.

 Mathematical Programming, 2008.
- [3] Richard Sinkhorn.

Diagonal equivalence to matrices with prescribed row and column sums.

The American Mathematical Monthly, 1967.

Problem 2: Entropy Regularization

Introduce entropy penalty:

$$\min_{X \in \mathbb{R}^{n \times n}} \sum_{i,j=1}^{n} (C_{ij} X_{ij} + \gamma X_{ij} \log X_{ij})$$
s.t. $X1 = p, X^{\top} 1 = q.$

Linear Programming

Given a matrix $C \in \mathbb{R}^{n \times n}$ and vectors $p, q \in \mathbb{R}^n_+$ such that $\sum_{i=1}^n p_i = \sum_{i=1}^n q_i$ solve

$$\min_{X \in \mathbb{R}^{n \times n}} \sum_{i,j=1}^{n} C_{ij} X_{ij}$$
s.t. $X1 = p, X^{\top} 1 = q, X \geqslant 0.$

Motivation: discrete optimal transport.

Problem 3: Nonsmooth Minimization

Given matrices $A_1, \ldots, A_m \in \mathbb{R}^{n_i \times d}_{++}$ and vectors $b_1, \ldots, b_m \in \mathbb{R}^{n_i}_{++}$ solve

$$\min_{x \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^m \mathcal{KL}(A_i x || b_i).$$

Problem Properties

For $f_i(x) \stackrel{\text{def}}{=} \mathcal{KL}(A_i x || b_i)$ the gradients are given by

$$\nabla f_i(x) = A_i^{\top} \log \frac{A_i x}{b_i},$$

where log and division are taken coordinate-wise. Note f_i is **nonsmooth**.

Main result

Sinkhorn algorithm = Method of Stochastic Bregman projections = Stochastic Mirror Descent.

Bregman Projections

$$\sum_{i,j=1}^{n} (C_{ij}X_{ij} + \gamma X_{ij} \log X_{ij}) = \mathcal{KL}(X||X^0) + \text{const},$$

where $X^0 \stackrel{\text{def}}{=} \exp(-C/\gamma)$.

Let $\omega \colon \mathbb{R}^d \to \mathbb{R}$ be a strictly convex function. The associated **Bregman divergence** is

 $D_{\omega}(x,y) \stackrel{\text{def}}{=} \omega(x) - \omega(y) - \langle \nabla \omega(y), x - y \rangle.$

If $\omega(x) = \sum_{i=1}^{d} x_i (\log x_i - 1)$, then $D_{\omega}(x, y)$ is the Kullback-Leibler divergence,

 $\mathcal{KL}(x||y) \stackrel{\text{def}}{=} \sum_{i=1}^{n} (x_i \log \frac{x_i}{y_i} - x_i + y_i).$

Thus, we are interested in projecting onto the intersection of some sets C_1, \ldots, C_m

$$\min_{x \in \bigcap_{i=1}^m C_i} D_{\omega}(x, x^0).$$

Algorithm 2: Stochastic projections.

for
$$k = 1, ...$$
 do

$$\begin{vmatrix} \operatorname{Sample} i \in \{1, ..., m\}; \\ x^{k+1} = \operatorname{argmin}_{x \in C_i} D_{\omega}(x, x^k); \\ \mathbf{end} \end{vmatrix}$$
end

Algorithm 3: Stochastic Mirror Descent.

for
$$k=1,\ldots$$
 do
$$| \text{Sample } i \in \{1,\ldots,m\}; \\ | \nabla \omega(x^{k+1}) = \nabla \omega(x^k) - \gamma_k \nabla f_i(x^k); \\ \text{end}$$

Intuition

Since $\omega(x) = \sum_{i=1}^{d} x_i (\log x_i - 1)$, $\nabla \omega(x) = \log(x)$. Then, the iterates live in a certain range space,

$$\log(x^{k+1}) \in \log(x^0) + \operatorname{Range}(A^\top),$$

where
$$A = (A_1^\top, \dots, A_m^\top)^\top$$
.

To show equivalence with Problems 1-2, we set x = vec(X), $d = n^2$, $A_1, A_2 \in \{0, 1\}^d$, $A_1x = X1$, $A_2x = X^T1$, $b_1 = p$, $b_2 = q$.

New insight: there is no guarantee for convergence of stochastic mirror descent on that problem, because $\mathcal{KL}(\cdot||b)$ is a nonsmooth function. Moreover, Problem 3 is not constrained, so there is no strong convexity. This is a gap in theory of stochastic mirror descent.