

A Wasserstein Penalty Framework for Stochastic Optimization

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1 Introduction

Consider the stochastic optimization problem

$$\min_{\mathbf{B} \in \mathbb{R}^{m \times n}} \mathbb{E}_{\xi \sim \mathbb{P}} f(\mathbf{B}, \xi),$$

where $\xi \in \Xi$, write $f(\mathbf{B}) = \mathbb{E}f(\mathbf{B}, \xi)$, $\nabla f(\mathbf{B}, \xi) = \nabla_{\mathbf{B}} f(\mathbf{B}, \xi) = \frac{\partial f(\mathbf{B}, \xi)}{\partial \mathbf{B}}$.

Robust optimization has been a very popular topic in the field of optimization.

This article interprets each iteration step in stochastic optimization as a robust decision process.

Algorithm 1 DRO-based Steepest Descent(DROSD)

- 1: Initialize $\mathbf{B}_0 \leftarrow 0$
 - 2: **for** $t = 0, \dots, T - 1$ **do**
 - 3: Compute batch gradients $\mathbf{G}_i \leftarrow \nabla f(\mathbf{B}_t, \xi_{t,i})$ for $i = 1, \dots, N_t$
 - 4: Compute average $\bar{\mathbf{G}}_t \leftarrow \frac{1}{N_t} \sum_{i=1}^{N_t} \mathbf{G}_i$
 - 5: Obtain \mathbf{d}_t by solving a DRO subproblem related to the empirical distribution $\mathbb{P}_{t,N_t} = \sum_{i=1}^{N_t} \delta_{\nabla f(\mathbf{B}_t, \xi_{t,i})}$
 - 6: Update parameters $\mathbf{B}_{t+1} \leftarrow \mathbf{B}_t - \mathbf{d}_t$
 - 7: **end for**
 - 8: **return** \mathbf{B}_T
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Assumption 1 (Lipschitz gradient in \mathbf{B}). *There exists $L \geq 0$ such that for all ξ and all $\mathbf{B}_1, \mathbf{B}_2 \in \mathbb{R}^{m \times n}$,*

$$\|\nabla_{\mathbf{B}} f(\mathbf{B}_1) - \nabla_{\mathbf{B}} f(\mathbf{B}_2)\| \leq L \|\mathbf{B}_1 - \mathbf{B}_2\|_*,$$

where $\|\cdot\|$ is a chosen matrix norm on $\mathbb{R}^{m \times n}$, with dual norm $\|\cdot\|_*$. We will take it to be the nuclear norm in this article, and we will explain why it is optimal to use the nuclear norm. Equivalently, for each fixed ξ , the map $\mathbf{B} \mapsto f(\mathbf{B}, \xi)$ is L -smooth with respect to this norm (the constant L does not depend on ξ).

Algorithm 2 Steepest Descent(DROSD)

- 1: Initialize $\mathbf{B}_0 \leftarrow 0$, $\eta_0 \leftarrow 0$
- 2: **for** $t = 0, \dots, T - 1$ **do**
- 3: Compute batch gradients $\mathbf{G}_i \leftarrow \nabla_{\mathbf{B}} f(\mathbf{B}_t, \xi_{t,i})$ for $i = 1, \dots, N_t$
- 4: Compute average $\bar{\mathbf{G}}_t \leftarrow \frac{1}{N_t} \sum_{i=1}^{N_t} \mathbf{G}_i$
- 5: $\eta_t \leftarrow \beta \eta_{t-1} + (1 - \beta) \|\bar{\mathbf{G}}_t\|$
- 6: $\mathbf{d}_t = \eta_t \frac{\bar{\mathbf{G}}_t}{\|\bar{\mathbf{G}}_t\|}$
- 7: Update parameters $\mathbf{B}_{t+1} \leftarrow \mathbf{B}_t - \mathbf{d}_t$
- 8: **end for**
- 9: **return** \mathbf{B}_T

Algorithm 3 Steepest Descent

- 1: Initialize $\mathbf{B}_0 \leftarrow 0$
- 2: **for** $t = 0, \dots, T - 1$ **do**
- 3: Compute batch gradients $\mathbf{G}_i \leftarrow \nabla_{\mathbf{B}} f(\mathbf{B}_t, \xi_{t,i})$ for $i = 1, \dots, N_t$
- 4: Compute average $\bar{\mathbf{G}}_t \leftarrow \frac{1}{N_t} \sum_{i=1}^{N_t} \mathbf{G}_i$
- 5:

$$\mathbf{d}_t = -\max \left\{ 0, \frac{\|\bar{\mathbf{G}}_t\|_{nuc} - C_t}{2L_w} \right\} U_t V_t^\top,$$
- where
 $U_t \Sigma V_t^\top$ is the thin SVD decomposition of $\bar{\mathbf{G}}_t$.
- 6: Update parameters $\mathbf{B}_{t+1} \leftarrow \mathbf{B}_t - \mathbf{d}_t$
- 7: **end for**
- 8: **return** \mathbf{B}_T

2 Formulation Using Moment Ambiguity Set

For simplicity of notation, we write $f(\mathbf{x}, \xi) = f(\mathbf{B}, \xi)$, where $\mathbf{x} \in \mathbb{R}^{mn}$ is the vectorization of \mathbf{B} .

2.1 Linear Formulation

Consider the robust optimization problem proposed by Delage and Ye [2]:

$$\begin{aligned}\Psi(\mathbf{x}, \Delta\mathbf{x}, \gamma_1, \gamma_2) &= \underset{\mu, f_\xi}{\text{maximize}} \quad \mathbb{E}_{f_\xi}[h(\mathbf{x}, \Delta\mathbf{x}, \xi)] \\ \text{subject to} \quad &\mathbb{E}_{f_\xi}[1] = 1, \quad \mathbb{E}_{f_\xi}[\nabla f(\mathbf{x}, \xi)] = \mu \\ &\mathbb{E}_{f_\xi}[(\nabla f(\mathbf{x}, \xi) - \mu_0)(\nabla f(\mathbf{x}, \xi) - \mu_0)^\top] \preceq \gamma_2 \Sigma_0 \\ &\begin{bmatrix} \Sigma_0 & (\mu - \mu_0) \\ (\mu - \mu_0)^\top & \gamma_1 \end{bmatrix} \succeq 0 \\ &f_\xi(\nabla f(\mathbf{x}, \xi)) \geq 0, \quad \forall \xi \in \mathcal{S},\end{aligned}$$

where we take $h(\mathbf{x}, \Delta\mathbf{x}, \xi) = \Delta\mathbf{x}^T \nabla f(\mathbf{x}, \xi)$.

Claim 1. Take $\bar{\gamma} = \min\{\gamma_1, \gamma_2\}$, then

$$\Psi(\mathbf{x}, \Delta\mathbf{x}, \gamma_1, \gamma_2) = \Delta\mathbf{x}^T \mu_0 + \sqrt{\bar{\gamma}} \sqrt{\Delta\mathbf{x}^T \Sigma_0 \Delta\mathbf{x}}.$$

Proof. In fact, we claim that the maximum is obtained when f_ξ is supported at a single point.

Since,

$$(\mu - \mu_0)(\mu - \mu_0)^T + \text{Cov}(\nabla f(\mathbf{x}, \xi)) = \mathbb{E}_{f_\xi}[(\nabla f(\mathbf{x}, \xi) - \mu_0)(\nabla f(\mathbf{x}, \xi) - \mu_0)^\top],$$

we have that

$$(\mu - \mu_0)(\mu - \mu_0)^T \preceq \mathbb{E}_{f_\xi}[(\nabla f(\mathbf{x}, \xi) - \mu_0)(\nabla f(\mathbf{x}, \xi) - \mu_0)^\top].$$

Therefore,

$$(\mu - \mu_0)(\mu - \mu_0)^T \preceq \gamma_2 \Sigma_0. \tag{1}$$

If $\mathbf{y} \in \mathbb{R}^{mn}$ such that $\Sigma_0 \mathbf{y} = 0$, then from (4), we know that $(\mu - \mu_0)^T \mathbf{y} = 0$. Therefore,

$$\mu - \mu_0 \in \text{row } \Sigma_0 = \text{col } \Sigma_0.$$

Since

$$\begin{aligned}&\begin{bmatrix} \Sigma_0 & (\mu - \mu_0) \\ (\mu - \mu_0)^\top & \gamma_1 \end{bmatrix} \succeq 0, \\ &\Sigma_0 - \frac{1}{\gamma_1} (\mu - \mu_0)(\mu - \mu_0)^T \succeq 0.\end{aligned}$$

Therefore,

$$(\mu - \mu_0)(\mu - \mu_0)^T \preceq \gamma_1 \Sigma_0. \tag{2}$$

Combining (1) and (2), we get that

$$(\mu - \mu_0)(\mu - \mu_0)^T \preceq \bar{\gamma} \Sigma_0. \quad (3)$$

What's more,

$$\mathbb{E}_{f_\xi}[h(\mathbf{x}, \Delta \mathbf{x}, \xi)] = \Delta \mathbf{x}^T \mu.$$

The only restriction for μ is (3).

$$\begin{aligned} \Delta \mathbf{x}^T \mu &\leq \Delta \mathbf{x}^T \mu_0 + \Delta \mathbf{x}^T (\mu - \mu_0) \\ &= \Delta \mathbf{x}^T \mu_0 + (\Sigma_0^{1/2} \Delta \mathbf{x})^T (\Sigma_0^{\dagger/2} (\mu - \mu_0)) \\ &\leq \Delta \mathbf{x}^T \mu_0 + \|\Sigma_0^{1/2} \Delta \mathbf{x}\|_2 \|\Sigma_0^{\dagger/2} (\mu - \mu_0)\|_2 \\ &\leq \Delta \mathbf{x}^T \mu_0 + \bar{\gamma} \|\Sigma_0^{1/2} \Delta \mathbf{x}\|_2 \\ &= \Delta \mathbf{x}^T \mu_0 + \bar{\gamma} \sqrt{\Delta \mathbf{x}^T \Sigma_0 \Delta \mathbf{x}}, \end{aligned}$$

and equality holds when

$$\mu = \mu_0 + \frac{\bar{\gamma} \Sigma_0 \Delta \mathbf{x}}{\sqrt{\Delta \mathbf{x}^T \Sigma_0 \Delta \mathbf{x}}}.$$

Therefore,

$$\Psi(\mathbf{x}, \Delta \mathbf{x}, \gamma_1, \gamma_2) = \Delta \mathbf{x}^T \mu_0 + \bar{\gamma} \sqrt{\Delta \mathbf{x}^T \Sigma_0 \Delta \mathbf{x}},$$

and the maximum is obtained when f_ξ is supported only at one point. \square

2.2 RELU Formulation 1

Consider the robust optimization problem proposed by Delage and Ye [2]:

$$\begin{aligned} \Psi(\mathbf{x}, \Delta \mathbf{x}, \gamma_1, \gamma_2) &= \underset{\mu, f_\xi}{\text{maximize}} \quad \mathbb{E}_{f_\xi}[h(\mathbf{x}, \Delta \mathbf{x}, \xi)] \\ \text{subject to} & \quad \mathbb{E}_{f_\xi}[1] = 1, \quad \mathbb{E}_{f_\xi}[\nabla f(\mathbf{x}, \xi)] = \mu \\ & \quad \mathbb{E}_{f_\xi}[(\nabla f(\mathbf{x}, \xi) - \mu_0)(\nabla f(\mathbf{x}, \xi) - \mu_0)^\top] \preceq \gamma_2 \Sigma_0 \\ & \quad \begin{bmatrix} \Sigma_0 & (\mu - \mu_0) \\ (\mu - \mu_0)^\top & \gamma_1 \end{bmatrix} \succeq 0 \\ & \quad f_\xi(\nabla f(\mathbf{x}, \xi)) \geq 0, \quad \forall \xi \in \mathcal{S}, \end{aligned}$$

where we take $h(\mathbf{x}, \Delta \mathbf{x}, \xi) = -\text{RELU}(-\Delta \mathbf{x}^T \nabla f(\mathbf{x}, \xi))$.

Claim 2. Take $\bar{\gamma} = \min\{\gamma_1, \gamma_2\}$, then

$$\Psi(\mathbf{x}, \Delta \mathbf{x}, \gamma_1, \gamma_2) = \min\{0, \Delta \mathbf{x}^T \mu_0 + \sqrt{\bar{\gamma}} \sqrt{\Delta \mathbf{x}^T \Sigma_0 \Delta \mathbf{x}}\}.$$

Proof. In fact, we claim that the maximum is obtained when f_ξ is supported at a single point.

Since

$$(\mu - \mu_0)(\mu - \mu_0)^T + \text{Cov}(\nabla f(\mathbf{x}, \xi)) = \mathbb{E}_{f_\xi}[(\nabla f(\mathbf{x}, \xi) - \mu_0)(\nabla f(\mathbf{x}, \xi) - \mu_0)^\top],$$

we have that

$$(\mu - \mu_0)(\mu - \mu_0)^T \preceq \mathbb{E}_{f_\xi}[(\nabla f(\mathbf{x}, \xi) - \mu_0)(\nabla f(\mathbf{x}, \xi) - \mu_0)^\top].$$

Therefore,

$$(\mu - \mu_0)(\mu - \mu_0)^T \preceq \gamma_2 \Sigma_0. \quad (4)$$

If $\mathbf{y} \in \mathbb{R}^{mn}$ such that $\Sigma_0 \mathbf{y} = 0$, then from (4), we know that $(\mu - \mu_0)^T \mathbf{y} = 0$. Therefore,

$$\mu - \mu_0 \in \text{row } \Sigma_0 = \text{col } \Sigma_0.$$

Since

$$\begin{bmatrix} \Sigma_0 & (\mu - \mu_0) \\ (\mu - \mu_0)^\top & \gamma_1 \end{bmatrix} \succeq 0,$$

$$\Sigma_0 - \frac{1}{\gamma_1}(\mu - \mu_0)(\mu - \mu_0)^T \succeq 0.$$

Therefore,

$$(\mu - \mu_0)(\mu - \mu_0)^T \preceq \gamma_1 \Sigma_0. \quad (5)$$

Combining (4) and (5), we get that

$$(\mu - \mu_0)(\mu - \mu_0)^T \preceq \bar{\gamma} \Sigma_0. \quad (6)$$

What's more, from the concavity of $-\text{RELU}(-\lambda)$,

$$\mathbb{E}_{f_\xi}[h(\mathbf{x}, \Delta \mathbf{x}, \xi)] \leq \min\{0, \mathbb{E}_{f_\xi}(\Delta \mathbf{x}^T \nabla f(\mathbf{x}, \xi))\} = \min\{0, \Delta \mathbf{x}^T \mu\}.$$

The only restriction for μ is (6).

$$\begin{aligned} \Delta \mathbf{x}^T \mu &\leq \Delta \mathbf{x}^T \mu_0 + \Delta \mathbf{x}^T (\mu - \mu_0) \\ &= \Delta \mathbf{x}^T \mu_0 + (\Sigma_0^{1/2} \Delta \mathbf{x})^T (\Sigma_0^{\dagger/2} (\mu - \mu_0)) \\ &\leq \Delta \mathbf{x}^T \mu_0 + \|\Sigma_0^{1/2} \Delta \mathbf{x}\|_2 \|\Sigma_0^{\dagger/2} (\mu - \mu_0)\|_2 \\ &\leq \Delta \mathbf{x}^T \mu_0 + \bar{\gamma} \|\Sigma_0^{1/2} \Delta \mathbf{x}\|_2 \\ &= \Delta \mathbf{x}^T \mu_0 + \bar{\gamma} \sqrt{\Delta \mathbf{x}^T \Sigma_0 \Delta \mathbf{x}}, \end{aligned}$$

and equality holds when

$$\mu = \mu_0 + \frac{\bar{\gamma} \Sigma_0 \Delta \mathbf{x}}{\sqrt{\Delta \mathbf{x}^T \Sigma_0 \Delta \mathbf{x}}}.$$

Therefore,

$$\Psi(\mathbf{x}, \Delta \mathbf{x}, \gamma_1, \gamma_2) = \Delta \mathbf{x}^T \mu_0 + \bar{\gamma} \sqrt{\Delta \mathbf{x}^T \Sigma_0 \Delta \mathbf{x}},$$

and the maximum is obtained when f_ξ is supported only at one point. \square

3 Formulation Using a Second Order Wasserstein Distance Regularization

Fixing an iteration t in Algorithm 1, we solve the following DRO subproblem to obtain d_t :

$$\mathbf{d}_t = \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \sup_{\substack{\mathbb{Q} \in \mathcal{M}(\mathbb{R}^{m \times n}) \\ \mathbb{Q}(\mathbb{R}^{m \times n})=1}} \left\{ \mathbb{E}_{G \sim \mathbb{Q}}[\langle \mathbf{d}, G \rangle] - \frac{1}{2\kappa} W_1^2(\mathbb{P}_{t,N_t}, \mathbb{Q}) \right\}, \quad (\text{P2})$$

where $\langle \mathbf{d}, \mathbf{G} \rangle = \text{trace}(\mathbf{d}^T \mathbf{G})$ and type-p Wasserstein distance $W_p(\mathbb{Q}_1, \mathbb{Q}_2)$ is defined as follows:

Definition 1 (Wasserstein Distance).

$$W_p(\mathbb{Q}_1, \mathbb{Q}_2) = \sqrt[p]{\inf_{\pi \in \Pi(\mathbb{Q}_1, \mathbb{Q}_2)} \int_{\mathbb{R}^m \times \mathbb{R}^m} \|\xi - \xi'\|^p \pi(d\xi, d\xi')},$$

where $\Pi(\mathbb{Q}_1, \mathbb{Q}_2)$ is the collection of distributions on $\mathbb{R}^m \times \mathbb{R}^m$ whose marginal distribution with respect to the first m components is \mathbb{Q}_1 and the marginal distribution with respect to the last m components is \mathbb{Q}_2 .

In the following proofs, we will make use of an important equivalent characterization of Wasserstein distance which is stated below:

Lemma 1 (Kantorovich-Rubinstein[3]).

$$W_1(\mathbb{Q}_1, \mathbb{Q}_2) = \sup_{f \text{ is 1-Lipschitz continuous}} \left(\int_{\mathbb{R}^{m \times n}} f(\xi) \mathbb{Q}_1(d\xi) - \int_{\mathbb{R}^{m \times n}} f(\xi') \mathbb{Q}_2(d\xi') \right).$$

Theorem 1. Problem (P2) is equivalent to

$$\begin{aligned} \mathbf{d}_t &= \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left\{ \mathbb{E}_{\mathbf{G} \sim \mathbb{P}_{t,N_t}}[\langle \mathbf{d}, \mathbf{G} \rangle] + \frac{1}{2} \kappa \|\mathbf{d}\|_*^2 \right\} \\ &= \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left(\langle \mathbf{d}, \bar{\mathbf{G}}_t \rangle + \frac{1}{2} \kappa \|\mathbf{d}\|_*^2 \right), \end{aligned} \quad (\text{D2})$$

where

$$\bar{\mathbf{G}}_t = \frac{1}{N_t} \sum_{i=1}^{N_t} \nabla f(\mathbf{B}_t, \xi_{t,i}).$$

Theorem 2. If $\|\cdot\| = \|\cdot\|_{nuc}$, then the optimal solution of (D2) is

$$\mathbf{d}_t = -\frac{1}{\kappa} \|\bar{\mathbf{G}}_t\|_{nuc} U_t V_t^\top,$$

where

$U_t \Sigma V_t^\top$ is the thin SVD decomposition of $\bar{\mathbf{G}}_t$.

4 Formulation Using p -th Order Wasserstein Distance Regularization ($p \in (1, +\infty)$)

In order to generalize the results in the last section, we study the following optimization problem

$$\mathbf{d}_t = \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \sup_{\substack{\mathbb{Q} \in \mathcal{M}(\mathbb{R}^{m \times n}) \\ \mathbb{Q}(\mathbb{R}^{m \times n})=1}} \left\{ \mathbb{E}_{G \sim \mathbb{Q}}[\langle \mathbf{d}, G \rangle] - \frac{1}{\kappa p} W_1^p(\mathbb{P}_N, \mathbb{Q}) \right\}, \quad (\text{Pp})$$

where $p \in (1, +\infty)$.

Theorem 3. *Problem (Pp) is equivalent to*

$$\begin{aligned} \mathbf{d}_t &= \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left\{ \mathbb{E}_{G \sim \mathbb{P}_{t,N}}[\langle \mathbf{d}, \mathbf{G} \rangle] + \frac{1}{q} \kappa \|\mathbf{d}\|_*^q \right\} \\ &= \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left(\langle \mathbf{d}, \bar{\mathbf{G}}_t \rangle + \frac{1}{q} \kappa \|\mathbf{d}\|_*^q \right), \end{aligned} \quad (\text{Dp})$$

where $\frac{1}{p} + \frac{1}{q} = 1$ and

$$\bar{\mathbf{G}}_t = \frac{1}{N_t} \sum_{i=1}^{N_t} \nabla f(\mathbf{B}_t, \xi_{t,i}).$$

Theorem 4. *If $\|\cdot\| = \|\cdot\|_{nuc}$, the closed-form solution of (Dp) is*

$$\mathbf{d}_t = - \left(\frac{\|\bar{\mathbf{G}}_t\|_{nuc}}{\kappa} \right)^{\frac{1}{q-1}} U_t V_t^\top,$$

where

$U_t \Sigma V_t^\top$ is the thin SVD decomposition of $\bar{\mathbf{G}}_t$.

5 Convergence of MUON beyond Uniform Lipschitz Gradient

Assumption 2 (Wasserstein Lipschitz Gradient). *Denote $\mathbb{P}_{\mathbf{B}}$ as the distribution of $\nabla f(\mathbf{B}, \xi)$. We assume that*

$$W_1(\mathbb{P}_{\mathbf{B}}, \mathbb{P}_{\mathbf{B}'}) \leq L_w \|\mathbf{B} - \mathbf{B}'\|_*, \forall \mathbf{B}, \mathbf{B}'.$$

where W_1 is the type-1 Wasserstein distance.

There exists $C > 0$ such that $W_1(\mathbb{P}_{t,N}, \mathbb{P}_{\mathbf{B}_t}) \leq C$ with high probability. From Assumption 2, we know that $W_1(\mathbb{P}_{\mathbf{B}_t}, \mathbb{P}_{\mathbf{B}}) \leq L_w \|\mathbf{B}_t - \mathbf{B}\|_*$, $\forall \mathbf{B} \in \mathbb{R}^{m \times n}$. Thus, $\forall \mathbf{B} \in \mathbb{R}^{m \times n}$, we have that, with high probability,

$$W_1(\mathbb{P}_{t,N}, \mathbb{P}_{\mathbf{B}}) \leq W_1(\mathbb{P}_{t,N}, \mathbb{P}_{\mathbf{B}_t}) + W_1(\mathbb{P}_{\mathbf{B}_t}, \mathbb{P}_{\mathbf{B}}) \leq C + L_w \|\mathbf{B}_t - \mathbf{B}\|_*.$$

We turn to solve the following subproblem:

$$\mathbf{d}_t = \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \sup_{\mathbf{Q} \in \mathcal{M}(\mathbb{R}^{m \times n}), \mathbf{Q}(\mathbb{R}^{m \times n})=1, W(\mathbb{P}_{t,N_t}, \mathbf{Q}) \leq C + L \|\mathbf{d}\|_*} \mathbb{E}_{\mathbf{G} \sim \mathbf{Q}} [\langle \mathbf{d}, \mathbf{G} \rangle]. \quad (\text{P})$$

Theorem 5. *Problem (P) is equivalent to*

$$\mathbf{d}_t = \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} (\langle \mathbf{d}, \overline{\mathbf{G}}_t \rangle + C \|\mathbf{d}\|_* + L_w \|\mathbf{d}\|_*^2), \quad (\text{D})$$

where

$$\overline{\mathbf{G}}_t = \frac{1}{N} \sum_{i=1}^N \nabla f(\mathbf{B}_t, \xi_{t,i}).$$

Theorem 6. *If $\|\cdot\| = \|\cdot\|_{nuc}$, the closed-form solution of (D) is*

$$\mathbf{d}_t = -\max \left\{ 0, \frac{\|\overline{\mathbf{G}}_t\|_{nuc} - C}{2L_w} \right\} U_t V_t^\top,$$

where

$U_t \Sigma V_t^\top$ is the thin SVD decomposition of $\overline{\mathbf{G}}_t$.

5.1 Convergence Rate Analysis Beyond Nuclear Norm

Assumption 3 (Light-tail Distribution). *There exists constants $a > 1$ and $A > 0$ such that*

$$\mathbb{E}_{\mathbf{G} \sim \mathbb{P}_{\mathbf{B}}} [\exp(\|\mathbf{G}\|^a)] \leq A, \forall \mathbf{B} \in \mathbb{R}^{m \times n}.$$

Define the event E_t as $\|\mathbb{E}_{\mathbb{P}_{t,N_t}} \nabla f(\mathbf{B}_t, \xi) - \mathbb{E}_{\mathbf{B}_t} \nabla f(\mathbf{B}_t, \xi)\| \leq C_t\}$, and $\{E_t\}_{t=0}^{+\infty}$ is a collection of independent events.

Theorem 7. *Take $T > 0$, $\delta > 0$. Choose δ_t such that $\delta > \sum_{t=0}^T \delta_t$. Then with probability at least $1 - \delta$, we have that*

$$\frac{1}{T} \sum_{t=0}^{T-1} \|\nabla f(\mathbf{B}_t)\|^2 \leq \frac{8L_w(f(\mathbf{B}_0) - f^*)}{T} + \frac{8}{T} \sum_{t=0}^{T-1} C_t^2, \quad (7)$$

and thus,

$$\min_{0 \leq t < T} \|\nabla f(\mathbf{B}_t)\|^2 \leq \frac{8L_w(f(\mathbf{B}_0) - f^*)}{T} + \frac{8}{T} \sum_{t=0}^{T-1} C_t^2.$$

Remark 1. *Any unitary invariant [4] cross norm [1] $\|\cdot\|$ shares the same C_t . When T is sufficiently large, $\sum_{t=0}^{T-1} C_t^2$ becomes the dominant term of the right-hand side. Thus, the right-hand side is approximately invariant among different norms. From proposition 3.12 of [1], the nuclear norm is the largest cross norm over $\|\cdot\|_2$ and $\|\cdot\|_F$. Therefore, when we use a nuclear norm guided steepest descent, (7) is the strongest and achieves the steepest descent. This is because $\nabla f(\mathbf{B}_t)$ is usually of high rank and $\|\nabla f(\mathbf{B}_t)\|_{nuc} > \|\nabla f(\mathbf{B}_t)\|$ for most unitary invariant cross norms.*

References

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A Rigorous Proofs of the Theorems

We give proofs only for Theorem 3, Theorem 4, Theorem 5, and Theorem 6, since Theorem 1 and Theorem 2 are special cases of Theorem 3 and Theorem 4, respectively.

A.1 Proof of Theorem 3

For convenience, we write $N := N_t, \mathbb{P}_N := \mathbb{P}_{t,N_t}$. Take $\mu = \mathbb{Q} - \mathbb{P}_N$, then $\mu \in \mathcal{M}(\mathbb{R}^{m \times n})$ and $\mu(\mathbb{R}^{m \times n}) = 0$.

$$\begin{aligned} & \sup_{\substack{\mathbb{Q} \in \mathcal{M}_+(\mathbb{R}^{m \times n}) \\ \mathbb{Q}(\mathbb{R}^{m \times n})=1}} \left\{ \mathbb{E}_{\mathbf{G} \sim \mathbb{Q}}[\langle \mathbf{d}, \mathbf{G} \rangle] - \frac{1}{\kappa p} W_1^p(\mathbb{P}_N, \mathbb{Q}) \right\} \\ &= \mathbb{E}_{\mathbf{G} \sim \mathbb{P}_N}[\langle \mathbf{d}, \mathbf{G} \rangle] + \sup_{\substack{\mathbb{Q} \in \mathcal{M}_+(\mathbb{R}^{m \times n}) \\ \mathbb{Q}(\mathbb{R}^{m \times n})=1}} \left\{ \mathbb{E}_{\mathbf{G} \sim \mu}[\langle \mathbf{d}, \mathbf{G} \rangle] - \frac{1}{\kappa p} W_1^p(\mathbb{P}_N, \mathbb{Q}) \right\}. \end{aligned}$$

Consider the normed vector space $Lip(\mathbb{R}^{m \times n})$ with norm $\|\cdot\|_{Lip}$ whose value is the smallest Lipschitz constant of that function. Consider a subset of its dual space $\mathcal{M}(\mathbb{R}^{m \times n})$ that denotes all signed measures on $\mathbb{R}^{m \times n}$, and the dual norm is $\|\cdot\|_{KR}$. Using Hahn Banach theorem, we know that the dual norm of $\|\cdot\|_{KR}$ is also $\|\cdot\|_{Lip}$.

From Theorem 1,

$$\begin{aligned}
W_1(\mathbb{P}_N, \mathbb{Q}) &= \sup_{\|f\|_{Lip}=1} \left(\int_{\mathbb{R}^{m \times n}} f(\xi) \mathbb{P}_N(d\xi) - \int_{\mathbb{R}^{m \times n}} f(\xi') \mathbb{Q}(d\xi') \right) \\
&= \sup_{\|f\|_{Lip}=1} \int_{\mathbb{R}^{m \times n}} f(\xi) \mu(d\xi) = \|\mu\|_{KR}.
\end{aligned}$$

Thus,

$$\begin{aligned}
&\sup_{\substack{\mathbb{Q} \in \mathcal{M}_+(\mathbb{R}^{m \times n}) \\ \mathbb{Q}(\mathbb{R}^{m \times n})=1}} \left\{ \mathbb{E}_{G \sim \mathbb{Q}}[\langle \mathbf{d}, G \rangle] - \frac{1}{\kappa p} W_1^p(\mathbb{P}_N, \mathbb{Q}) \right\} \\
&= \mathbb{E}_{\mathbf{G} \sim \mathbb{P}_N}[\langle \mathbf{d}, \mathbf{G} \rangle] + \sup_{\substack{\mathbb{Q} \in \mathcal{M}_+(\mathbb{R}^{m \times n}) \\ \mathbb{Q}(\mathbb{R}^{m \times n})=1}} \left\{ \mathbb{E}_{G \sim \mu}[\langle \mathbf{d}, G \rangle] - \frac{1}{\kappa p} \|\mu\|_{KR}^p \right\}.
\end{aligned}$$

While

$$\sup_{\substack{\mathbb{Q} \in \mathcal{M}_+(\mathbb{R}^{m \times n}) \\ \mathbb{Q}(\mathbb{R}^{m \times n})=1}} \left\{ \mathbb{E}_{G \sim \mu}[\langle \mathbf{d}, G \rangle] - \frac{1}{\kappa p} \|\mu\|_{KR}^p \right\}$$

is just the conjugate function of $\frac{1}{\kappa p} \|\cdot\|_{KR}^p$ which equals $\frac{\kappa}{q} \|\cdot\|_{Lip}^q$, where $\frac{1}{p} + \frac{1}{q} = 1$. We also know that $\frac{\kappa}{q} \|\langle \mathbf{d}, \cdot \rangle\|_{Lip}^q = \frac{\kappa}{q} \|\mathbf{d}\|_{op}^q$.

Therefore, we have shown that

$$\begin{aligned}
&\sup_{\substack{\mathbb{Q} \in \mathcal{M}_+(\mathbb{R}^{m \times n}) \\ \mathbb{Q}(\mathbb{R}^{m \times n})=1}} \left\{ \mathbb{E}_{G \sim \mathbb{Q}}[\langle \mathbf{d}, G \rangle] - \frac{1}{\kappa p} W_1^p(\mathbb{P}_N, \mathbb{Q}) \right\} \\
&= \mathbb{E}_{G \sim \mathbb{P}_N}[\langle \mathbf{d}, G \rangle] + \frac{\kappa}{q} \|\mathbf{d}\|_{op}^q.
\end{aligned}$$

□

B Proof of Theorem 4

Assume that $\mathbf{d} = c\mathbf{M}$, where $\|\mathbf{M}\|_{op} = 1$. We solve the optimization problem

$$\min_{c \geq 0, \mathbf{M} \in \mathbb{R}^{m \times n}} \left(c \langle \mathbf{M}, \bar{G}_t \rangle + \frac{1}{q} \kappa c^q \right).$$

By Neumann's Inequality,

$$\min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \langle \mathbf{M}, \bar{G}_t \rangle = -\|\bar{G}_t\|_{nuc}.$$

The minimal value is achieved if and only if $\mathbf{M} = -U_t V_t^T$. When the minimal value is achieved, it suffices to minimize

$$-c\|\bar{G}_t\|_{nuc} + \frac{1}{q}\kappa c^q,$$

and the optimal value of c is naturally given by $(\frac{\|\bar{G}_t\|_{nuc}}{\kappa})^{1/(q-1)}$. \square

C Proof of Theorem 5

For simplicity, write $N = N_t$, $\mathbb{P}_N = \mathbb{P}_{t,N_t}$. We follow the notations in [5], taking $X = (\mathcal{M}(\mathbb{R}^{m \times n}))^N$ to be the space of N -tuples of signed finite measures on $\mathbb{R}^{m \times n}$. Take C as a convex conic subset of X which contains all nonnegative measures. Take $Y = \mathbb{R}^{N+1}$ and $K = \mathbb{R}_{\leq 0} \times \{0\}^N$.

Therefore, $X^* = \mathcal{L}^\infty(\mathbb{R}^{m \times n})$, $C^* = \{f \in C : f \geq 0\}$, $Y^* = \mathbb{R}^{N+1}$, $K^* = \mathbb{R}_{\leq 0} \times \mathbb{R}^N$. We also take $b = (-(C + L\|\mathbf{d}\|_*), -1, \dots, -1)^T \in \mathbb{R}^{N+1}$.

There exists a nonnegative measure π on $\mathbb{R}^{m \times n} \times \mathbb{R}^{m \times n}$ whose marginal distribution for the first m components is \mathbb{P}_N and the marginal distribution for the second m components is \mathbb{Q} , such that

$$\mathbb{E}_{(\xi, \xi') \sim \pi} \|\xi - \xi'\| = W(\mathbb{P}_N, \mathbb{Q}).$$

We denote

$$\mathbf{q} = (\mathbb{Q}^1, \mathbb{Q}^2, \dots, \mathbb{Q}^N)^T \in X.$$

The first stage of problem (P)

$$\sup_{W(\mathbb{P}_N, \mathbb{Q}) \leq C + L\|\mathbf{d}\|_*} \mathbb{E}_{\mathbb{Q}}[\langle \mathbf{d}, \nabla_{\mathbf{B}} f_{\mathbf{x}}(\mathbf{B}) \rangle]$$

is equivalent to

$$\begin{cases} \sup_{\Pi \in M(\mathbb{R}^{m \times n}, \mathbb{R}^{m \times n})} & \int_{\mathbb{R}^{m \times n}} \langle \mathbf{d}, \mathbf{G} \rangle \Pi(dG, \mathbb{R}^{m \times n}), \\ \text{s.t.} & \frac{1}{N} \sum_{i=1}^N \int_{\mathbb{R}^{m \times n}} \|\mathbf{G} - \mathbf{G}_i\| \mathbb{Q}^i(dG) \leq C + L\|\mathbf{d}\|_{op}, \\ & \int_{\mathbb{R}^{m \times n}} \mathbb{Q}^i(dG) = 1, \end{cases} \quad (8)$$

We write $\mathbf{G} = \nabla_{\mathbf{B}} f_{\mathbf{x}}(\mathbf{B})$, $\mathbf{G}_i = \nabla_{\mathbf{B}} f_{\mathbf{x}_i}(\mathbf{B})$, $c = (\frac{1}{N} \langle \mathbf{d}, \mathbf{G} \rangle)_{i=1}^N$, $A\mathbf{q} = (A^0\mathbf{q}, A^1\mathbf{q}, \dots, A^N\mathbf{q})^T$, where $A^i\mathbf{q} = \int_{\mathbb{R}^{m \times n}} \mathbb{Q}^i(dG)$, $A^0\mathbf{q} = \frac{1}{N} \sum_{i=1}^N \int_{\mathbb{R}^{m \times n}} \|G - G_i\| \mathbb{Q}^i(dG)$.

Then (8) is equivalent to

$$\begin{cases} \sup_{\mathbb{Q} \in C} \langle c, \mathbf{q} \rangle, \\ \text{s.t.} \quad A\mathbf{q} + b \in K. \end{cases} \quad (9)$$

We now turn to look at its dual problem:

$$\begin{cases} \sup_{y^* \in K^*} \langle b, y^* \rangle, \\ \text{s.t.} \quad A^*y^* + c \in C^*. \end{cases} \quad (10)$$

Assume that $y^* = (\lambda, s_1, s_2, \dots, s_N)$, then

$$\begin{aligned}
\langle y^*, A\mathbf{q} \rangle &= \frac{\lambda}{N} \sum_{i=1}^N \int_{\mathbb{R}^{m \times n}} \|\mathbf{G} - \mathbf{G}_i\| \mathbb{Q}^i(dG) + \sum_{i=1}^N s^i \int_{\mathbb{R}^{m \times n}} \mathbb{Q}^i(dG) \\
&= \int_{\mathbb{R}^{m \times n}} \sum_{i=1}^N \left(\frac{\lambda}{N} \|\mathbf{G} - \mathbf{G}_i\| + s^i \right) \mathbb{Q}^i(dG) \\
&= \langle A^*y^*, x \rangle.
\end{aligned}$$

Hence, $A^*y^* = (\frac{\lambda}{N} \|\mathbf{G} - \mathbf{G}_i\| + s^i)_{i=1}^N$. Since $A^*y^* + c \in C^*$,

$$0 \geq A^*y^* + c = \left(\frac{\lambda}{N} \|\mathbf{G} - \mathbf{G}_i\| + s^i + \frac{1}{N} \langle \mathbf{d}, \mathbf{G} \rangle \right), \forall i. \quad (11)$$

(11) is equivalent to that

$$\begin{aligned}
-s^i &\geq \frac{1}{N} \sup_{\mathbf{G}} (\langle \mathbf{d}, \mathbf{G} \rangle + \lambda \|\mathbf{G} - \mathbf{G}_i\|) \\
&= \frac{1}{N} \sup_{\mathbf{G}} (\langle \mathbf{d}, \mathbf{G} - \mathbf{G}_i \rangle - |\lambda| \|\mathbf{G} - \mathbf{G}_i\|) + \frac{\langle \mathbf{d}, \mathbf{G}_i \rangle}{N} \\
&= \frac{1}{N} (|\lambda| \|\cdot\|)^*(\mathbf{d}) + \frac{\langle \mathbf{d}, \mathbf{G}_i \rangle}{N} \\
&= \frac{\langle \mathbf{d}, \mathbf{G}_i \rangle}{N} + \begin{cases} 0, \|\mathbf{d}\|_* \leq -\lambda, \\ +\infty, \text{otherwise.} \end{cases}
\end{aligned}$$

It follows that $\langle c, \mathbf{q} \rangle = -\lambda(C + L\|\mathbf{d}\|) - \sum_{i=1}^N s^i$. To minimize this, take $-\lambda = \|\mathbf{d}\|_*$ and $-s^i = \frac{\langle \mathbf{d}, \mathbf{G}_i \rangle}{N}$.
(10) is now written as

$$\min_{\mathbf{d}} \frac{1}{N} \sum_{i=1}^N \langle \mathbf{d}, \mathbf{G}_i \rangle + (C + L\|\mathbf{d}\|_*) \|\mathbf{d}\|_*.$$

To show strong duality in Proposition 3.4 of [4], we observe that $A(C) = \mathbb{R}_{\geq 0}^{N+1}$, $A(C) - K = \mathbb{R}_{\geq 0}^{N+1}$, $-b \in \text{int}(A(C) - K)$. \square

D Proof of Theorem 6

The methodology is very similar to the proof of Theorem 4. We repeat the proof here for completeness.

Assume that $\mathbf{d} = c\mathbf{M}$, where $\|\mathbf{M}\|_{op} = 1$, then our goal is:

$$\min_{c \geq 0, \mathbf{M} \in \mathbb{R}^{m \times n}} (c \langle \mathbf{M}, \overline{\mathbf{G}}_t \rangle + Cc + Lc^2).$$

By Neumann's Inequality,

$$\min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \langle \mathbf{M}, \bar{\mathbf{G}}_t \rangle = -\|\bar{\mathbf{G}}_t\|_{nuc}.$$

The minimal value is achieved if and only if $\mathbf{M} = -U_t V_t^T$. When the minimal value is achieved, it suffices to minimize

$$(C - \|\mathbf{G}_t\|_{nuc})c + Lc^2, c \geq 0.$$

and the optimal value of c is naturally given by $\frac{\max\{0, \|\mathbf{G}_t\|_{nuc} - C\}}{2L}$. \square

E Proof of Lemma 2

Take any $\xi \in \Xi$, $\mathbf{B} \in \mathbb{R}^{m \times n}$,

$$\nabla f(\mathbf{B}, \xi) = \frac{\partial f(\mathbf{B}, \xi)}{\partial \mathbf{B}} = \frac{\partial f(\mathbf{B}, \xi)}{\partial \mathbf{a}^l} \mathbf{h}^{l-1^T},$$

is of rank one. \square

F Proof of Theorem 7

Lemma 2. *If event E_t happens, then $\forall \mathbf{d} \in \mathbb{R}^{m \times n}$,*

$$f(\mathbf{B}_t + \mathbf{d}) - f(\mathbf{B}_t) \leq \sup_{W(\mathbb{P}_{t,N_t}, \mathbb{Q}) \leq C_t + L_w \|\mathbf{d}\|_*} \mathbb{E}_{\mathbb{Q}} \langle \mathbf{d}, \mathbf{G} \rangle.$$

Proof. By the mean-value theorem, there exists $\theta \in (0, 1)$, such that

$$f(\mathbf{B}_t + \mathbf{d}) - f(\mathbf{B}_t) = \langle \nabla f(\mathbf{B}_t + \theta \mathbf{d}), \mathbf{d} \rangle = \mathbb{E}_{\mathbf{G} \sim \mathbb{P}_{\mathbf{B}_t + \theta \mathbf{d}}} \langle \mathbf{G}, \mathbf{d} \rangle.$$

Since

$$W(\mathbb{P}_{\mathbf{B}_t + \theta \mathbf{d}}, \mathbb{P}_{t,N_t}) \leq W(\mathbb{P}_{\mathbf{B}_t + \theta \mathbf{d}}, \mathbb{P}_{\mathbf{B}_t}) + W(\mathbb{P}_{t,N_t}, \mathbb{P}_{\mathbf{B}_t}) \leq L_w \|\mathbf{d}\|_* + C_t,$$

we have that,

$$f(\mathbf{B}_t + \mathbf{d}) - f(\mathbf{B}_t) = \mathbb{E}_{\mathbf{G} \sim \mathbb{P}_{\mathbf{B}_t + \theta \mathbf{d}}} \langle \mathbf{G}, \mathbf{d} \rangle \leq \sup_{W(\mathbb{P}_{t,N_t}, \mathbb{Q}) \leq C_t + L_w \|\mathbf{d}\|_*} \mathbb{E}_{\mathbb{Q}} \langle \mathbf{d}, \mathbf{G} \rangle.$$

\square

Lemma 3. *On the event E_t , if $\mathbf{B}_{t+1} = \mathbf{B}_t + \mathbf{d}_t$, then*

$$f(\mathbf{B}_{t+1}) - f(\mathbf{B}_t) \leq -\frac{(\|\bar{\mathbf{G}}_t\| - C_t)_+^2}{4L_w}.$$

Proof. We observe that

$$f(\mathbf{B}_t + \mathbf{d}_t) - f(\mathbf{B}_t) \leq \sup_{W(\mathbb{P}_{t,N_t}, \mathbb{Q}) \leq C_t + L_w \|\mathbf{d}\|_*} \mathbb{E}_{\mathbb{Q}} \langle \mathbf{d}_t, \mathbf{G} \rangle = \langle \mathbf{d}_t, \overline{\mathbf{G}}_t \rangle + C_t \|\mathbf{d}_t\|_* + L_w \|\mathbf{d}_t\|_*^2.$$

Since \mathbf{d}_t is taken to be the infimum of the right-hand side,

$$f(\mathbf{B}_t + \mathbf{d}_t) - f(\mathbf{B}_t) \leq \inf_{c \geq 0} c(-\|\overline{\mathbf{G}}_t\| + C_t) + L_w c^2 = -\frac{(\|\overline{\mathbf{G}}_t\| - C_t)_+^2}{4L_w}.$$

□

Lemma 4.

$$\|\overline{\mathbf{G}}_t - \nabla f(\mathbf{B}_t)\| \leq C_t.$$

Proof. Take arbitrary $\mathbf{d} \in \mathbb{R}^{m \times n}$, $\|\mathbf{d}\|_* = 1$, we have by Theorem 1 that

$$\begin{aligned} \langle \mathbf{d}, \overline{\mathbf{G}}_t - \nabla f(\mathbf{B}_t) \rangle &= \int_{\mathbb{R}^{m \times n}} \langle \mathbf{d}, \mathbf{G} \rangle \mathbb{P}_{t,N_t}(\mathbf{d}\mathbf{G}) - \int_{\mathbb{R}^{m \times n}} \langle \mathbf{d}, \mathbf{G} \rangle \mathbb{P}_{\mathbf{B}_t}(\mathbf{d}\mathbf{G}) \\ &\leq W(\mathbb{P}_{t,N_t}, \mathbb{P}_{\mathbf{B}_t}) \\ &\leq C_t. \end{aligned}$$

Therefore, $\|\overline{\mathbf{G}}_t - \nabla f(\mathbf{B}_t)\| \leq C_t$. □

Lemma 5. If $x, y \geq 0$, then $(x - y)_+^2 \geq \frac{1}{2}x^2 - y^2$.

Proof. Case 1: $x \geq y$,

In this case, $(x - y)_+ = x - y$, so the left side is $(x - y)^2 = x^2 - 2xy + y^2$. The inequality becomes $x^2 - 2xy + y^2 \geq \frac{1}{2}x^2 - y^2$. Rearranging terms gives $\frac{1}{2}x^2 - 2xy + 2y^2 \geq 0$. Multiplying through by 2 yields $x^2 - 4xy + 4y^2 \geq 0$, or $(x - 2y)^2 \geq 0$. This is always true, with equality when $x = 2y$.

Case 2: $x < y$,

In this case, $(x - y)_+ = 0$, so the left side is 0. The inequality becomes $0 \geq \frac{1}{2}x^2 - y^2$, or $y^2 \geq \frac{1}{2}x^2$. Since $x < y$ and both are non-negative, $y^2 > x^2 \geq \frac{1}{2}x^2$. The inequality holds strictly. □

Lemma 6.

$$f(\mathbf{B}_t + \mathbf{d}_t) - f(\mathbf{B}_t) \leq -\frac{1}{8L_w} \|\nabla f(\mathbf{B}_t)\|^2 + \frac{1}{L_w} C_t^2. \quad (12)$$

Proof.

$$\begin{aligned} f(\mathbf{B}_t + \mathbf{d}_t) - f(\mathbf{B}_t) &\leq -\frac{(\|\overline{\mathbf{G}}_t\| - C_t)_+^2}{4L_w} \leq -\frac{(\|\nabla f(\mathbf{B}_t)\| - 2C_t)_+^2}{4L_w} \\ &\leq -\frac{\frac{1}{2}\|\nabla f(\mathbf{B}_t)\|^2 - 4C_t^2}{4L_w} \\ &= -\frac{1}{8L_w} \|\nabla f(\mathbf{B}_t)\|^2 + \frac{1}{L_w} C_t^2. \end{aligned}$$

□

Now Theorem 7 follows by taking the summation of (12) from 0 to $T - 1$, dividing both sides by T , and rearranging.