A Wasserstein Penalty Framework for Stochastic Optimization

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August 2025

Introduction 1

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, ..., T 1 **do do**
- 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 $\overline{\mathbf{G}}_t \leftarrow \frac{1}{N_t} \sum_{i=1}^{N_t} \mathbf{G}_i$ Obtain \mathbf{d}_t by solving a DRO subproblem related to the empirical distribution $\mathbb{P}_{t,N_t} = \sum_{i=1}^{N_t} \delta_{\nabla f(\mathbf{B}_t,\xi_{t,i})}$
- Update parameters $\mathbf{B}_{t+1} \leftarrow \mathbf{B}_t \mathbf{d}_t$ 6:
- 7: end for
- 8: return \mathbf{B}_T

Assumption 1 (Lipschitz gradient in **B**). There exists $L \geq 0$ such that for all ξ and all $\mathbf{B}_1, \mathbf{B}_2 \in \mathbb{R}^{m \times n}$,

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

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 do
- Compute batch gradients $\mathbf{G}_{i} \leftarrow \nabla_{\mathbf{B}} f(\mathbf{B}_{t}, \xi_{t,i})$ for $i = 1, \dots, N_{t}$ Compute average $\overline{\mathbf{G}}_{t} \leftarrow \frac{1}{N_{t}} \sum_{i=1}^{N_{t}} \mathbf{G}_{i}$ $\eta_{t} \leftarrow \beta \eta_{t-1} + (1-\beta) \|\overline{\mathbf{G}}_{t}\|$ $\mathbf{d}_{t} = \eta_{t} \frac{\mathbf{G}_{t}}{\|\mathbf{G}_{t}\|}$
- 4:
- 6:
- 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, ..., T 1 **do do**
- Compute batch gradients $\mathbf{G}_i \leftarrow \nabla_{\mathbf{B}} f(\mathbf{B}_t, \xi_{t,i})$ for $i = 1, \dots, N_t$
- Compute average $\overline{\mathbf{G}}_t \leftarrow \frac{1}{N_t} \sum_{i=1}^{N_t} \mathbf{G}_i$ 4:

5:

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

where

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

- 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 Delange and Ye [2]:

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

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

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

Proof. In fact, we claim that the maximum is obtained when f_{ξ} is supported at a single point.

Since.

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

we have that

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

Therefore,

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

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,

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

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,

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

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

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

What's more,

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

The only restriction for μ is (6).

$$\Delta \boldsymbol{x}^{T} \boldsymbol{\mu} \leq \Delta \boldsymbol{x}^{T} \boldsymbol{\mu}_{0} + \Delta \boldsymbol{x}^{T} (\boldsymbol{\mu} - \boldsymbol{\mu}_{0})$$

$$= \Delta \boldsymbol{x}^{T} \boldsymbol{\mu}_{0} + (\boldsymbol{\Sigma}_{0}^{1/2} \Delta \boldsymbol{x})^{T} \left(\boldsymbol{\Sigma}_{0}^{\dagger/2} (\boldsymbol{\mu} - \boldsymbol{\mu}_{0}) \right)$$

$$\leq \Delta \boldsymbol{x}^{T} \boldsymbol{\mu}_{0} + \|\boldsymbol{\Sigma}_{0}^{1/2} \Delta \boldsymbol{x}\|_{2} \|\boldsymbol{\Sigma}_{0}^{\dagger/2} (\boldsymbol{\mu} - \boldsymbol{\mu}_{0})\|_{2}$$

$$\leq \Delta \boldsymbol{x}^{T} \boldsymbol{\mu}_{0} + \bar{\boldsymbol{\gamma}} \|\boldsymbol{\Sigma}_{0}^{1/2} \Delta \boldsymbol{x}\|_{2}$$

$$= \Delta \boldsymbol{x}^{T} \boldsymbol{\mu}_{0} + \bar{\boldsymbol{\gamma}} \sqrt{\Delta \boldsymbol{x}^{T} \boldsymbol{\Sigma}_{0} \Delta \boldsymbol{x}},$$

and exact equality holds when

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

Therefore,

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

and the maximum is obtained when f_{ξ} is supported only on one point.

2.2 RELU Formulation 1

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

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

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

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

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

Proof. In fact, we claim that the maximum is obtained when f_{ξ} is supported at a single point.

Since.

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

we have that

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

Therefore,

$$(\mu - \mu_0)(\mu - \mu_0)^T \leq \gamma_2 \Sigma_0. \tag{4}$$

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

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

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,

$$(\mu - \mu_0)(\mu - \mu_0)^T \leq \gamma_1 \Sigma_0. \tag{5}$$

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

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

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

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

The only restriction for μ is (6).

$$\Delta x^{T} \mu \leq \Delta x^{T} \mu_{0} + \Delta x^{T} (\mu - \mu_{0})$$

$$= \Delta x^{T} \mu_{0} + (\Sigma_{0}^{1/2} \Delta x)^{T} \left(\Sigma_{0}^{\dagger/2} (\mu - \mu_{0}) \right)$$

$$\leq \Delta x^{T} \mu_{0} + \|\Sigma_{0}^{1/2} \Delta x\|_{2} \|\Sigma_{0}^{\dagger/2} (\mu - \mu_{0})\|_{2}$$

$$\leq \Delta x^{T} \mu_{0} + \bar{\gamma} \|\Sigma_{0}^{1/2} \Delta x\|_{2}$$

$$= \Delta x^{T} \mu_{0} + \bar{\gamma} \sqrt{\Delta x^{T} \Sigma_{0} \Delta x},$$

and exact equality holds when

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

Therefore,

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

and the maximum is obtained when f_{ξ} is supported only at one point.

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 :

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

where $\langle \mathbf{d}, \mathbf{G} \rangle = \operatorname{trace}(\mathbf{d}^T \mathbf{G})$ 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 later proofs, we will make use of an important equivalent characterization of Wasserstein distance which is stated below:

Theorem 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 2. Problem (P2) is equivalent to

$$\mathbf{d}_{t} = \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left\{ \mathbb{E}_{\mathbf{G} \sim \mathbb{P}_{t, N_{t}}} [\langle \mathbf{d}, \mathbf{G} \rangle] + \frac{1}{2} \kappa \|\mathbf{d}\|_{*}^{2} \right\}$$

$$= \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left(\langle \mathbf{d}, \overline{\mathbf{G}}_{t} \rangle + \frac{1}{2} \kappa \|\mathbf{d}\|_{*}^{2} \right),$$
(D2)

where

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

Theorem 3. If $\|\cdot\| = \|\cdot\|_{nuc}$, then the optimal solution of (D2) is

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

where

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

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

In order to generalize the results in the last section, we require that

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

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

Theorem 4. Problem (Pp) is equivalent to

$$\mathbf{d}_{t} = \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left\{ \mathbb{E}_{G \sim \mathbb{P}_{t, N_{t}}} [\langle \mathbf{d}, \mathbf{G} \rangle] + \frac{1}{q} \kappa \|\mathbf{d}\|_{*}^{q} \right\}$$

$$= \arg \min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left(\langle \mathbf{d}, \overline{\mathbf{G}}_{t} \rangle + \frac{1}{q} \kappa \|\mathbf{d}\|_{*}^{q} \right),$$
(Dp)

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

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

Theorem 5. If $\|\cdot\| = \|\cdot\|_{nuc}$, the closed-form solution of (Dp) is

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

where

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

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,

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

We turn to solve the following subproblem:

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

Theorem 6. Problem (P) is equivalent to

$$\mathbf{d}_{t} = \arg\min_{\mathbf{d} \in \mathbb{R}^{m \times n}} \left(\langle \mathbf{d}, \overline{\mathbf{G}}_{t} \rangle + C \|\mathbf{d}\|_{*} + L_{w} \|\mathbf{d}\|_{*}^{2} \right), \tag{D}$$

where

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

Theorem 7. 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 a uniform constant a > 1 and A > 0 such that

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

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

Theorem 8. 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

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

and thus.

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

Remark 1. Any unitary invariant [4] cross norm [1] $\|\cdot\|$ shares the same C_t , and 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 $\|\cdot\|_2$. Therefore, when we use a nuclear norm guided steepest descent, (7) is the strongest and the descent is better than when other norms are used because $\nabla f(\mathbf{B}_t)$ are usually of high rank and $\|\nabla f(\mathbf{B}_t)\|_{nuc} > \|\nabla f(\mathbf{B}_t)\|$ for most other unitary invariant cross norms.

References

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A Rigorous Proofs of the Theorems

We give proofs only for Theorem 4, Theorem 5, Theorem 6, and Theorem 7, since Theorem 2 and Theorem 3 are special cases of Theorem 4 and Theorem 5, respectively.

A.1 Proof of Theorem 4

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 $\mu(\mathbb{R}^{m \times n}) = 0$.

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

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,

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

Thus,

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

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

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 to $\frac{\kappa}{q}\|\cdot\|_{Lip}^q$, 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 end up with the conclusion in the theorem.

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

$$= \mathbb{E}_{G\sim\mathbb{P}_{N}}[\langle \mathbf{d},G\rangle] + \frac{\kappa}{q} \|\mathbf{d}\|_{op}^{q}.$$

Proof of Theorem 5 \mathbf{B}

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

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

By Neumann's Inequality,

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

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

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

and the optimal c is $(\frac{\|\overline{G}_t\|_{nuc}}{\kappa})^{1/(q-1)}$ naturally.

C Proof of Theorem 6

For simplicity, write $N=N_t$, $\mathbb{P}_N=\mathbb{P}_{t,N_t}$. We follow the notations in [5], take $X=(\mathcal{M}(\mathbb{R}^{m\times n}))^N$ 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 $K=\mathbb{R}_{<0}\times\{0\}^N$.

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 $b = (-(C + L\|\mathbf{d}\|_*), -1, \ldots, -1)^T \in \mathbb{R}^{N+1}$.

There exists a nonnegative measure π on $\mathbb{R}^{m \times n} \times \mathbb{R}^{m \times n}$ whose marginal

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 problem of (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

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

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 $A^i \mathbf{q} = \int_{\mathbb{R}^{m \times n}} \mathbb{Q}^i (dG)$, $A^0 \mathbf{q} = \frac{1}{N} \sum_{i=1}^N \int_{\mathbb{R}^{m \times n}} \|G - G_i\| \mathbb{Q}^i (dG)$. The (8) is equivalent to

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

We now turn to look at its dual problem:

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

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

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

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

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

(11) is equivalent to that

$$-s^{i} \geq \frac{1}{N} \sup_{\mathbf{G}} (\langle \mathbf{d}, \mathbf{G} \rangle + \lambda \| \mathbf{G} - \mathbf{G}_{i} \|)$$

$$= \frac{1}{N} \sup_{\mathbf{G}} (\langle \mathbf{d}, \mathbf{G} - \mathbf{G}_{i} \rangle - |\lambda| \| \mathbf{G} - \mathbf{G}_{i} \|) + \frac{\langle \mathbf{d}, \mathbf{G}_{i} \rangle}{N}$$

$$= \frac{1}{N} (|\lambda| \| \cdot \|)^{*}(\mathbf{d}) + \frac{\langle \mathbf{d}, G_{i} \rangle}{N}$$

$$= \frac{\langle \mathbf{d}, \mathbf{G}_{i} \rangle}{N} + \begin{cases} 0, \|\mathbf{d}\|_{*} \leq -\lambda, \\ +\infty, \text{ otherwise.} \end{cases}$$

Notice 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], notice that $A(C) = \mathbb{R}^{N+1}_{\geq 0}, \ A(C) - K = \mathbb{R}^{N+1}_{\geq 0}, \ -b \in \operatorname{int}(A(C) - K).$

D Proof of Theorem 7

The methodology is very similar to the proof of Theorem 5. We repeat the proof here for completeness.

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

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

By Neumann's Inequality,

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

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

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

and the minimal value is $\frac{\max\{0, \|G_t\|_{nuc} - C\}}{2L}$ naturally.

E Proof of Lemma 1

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

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

is of rank one.

F Proof of Theorem 8

Lemma 1. If event E_t happens, then $\forall \mathbf{d} \in \mathbb{R}^{m \times n}$,

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

Proof. By the mean-value problem, 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,

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

Lemma 2. On the event E_t , if $\mathbf{B}_{t+1} = \mathbf{B}_t + \mathbf{d}_t$, then

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

Proof. Since

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

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

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

Lemma 3.

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

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

$$\langle \mathbf{d}, \overline{\mathbf{G}}_{t} - \nabla f(\mathbf{B}_{t}) \rangle = \int_{\mathbb{R}^{m \times n}} \langle \mathbf{d}, \mathbf{G} \rangle \mathbb{P}_{t, N_{t}}(\mathbf{dG}) - \int_{\mathbb{R}^{m \times n}} \langle \mathbf{d}, \mathbf{G} \rangle \mathbb{P}_{\mathbf{B}_{t}}(\mathbf{dG})$$

$$\leq W(\mathbb{P}_{t, N_{t}}, \mathbb{P}_{\mathbf{B}_{t}})$$

$$< C_{t}.$$

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

Lemma 4. If $x, y \ge 0$, then $(x - y)_+^2 \ge \frac{1}{2}x^2 - y^2$.

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 $x^2 - 2xy + y^2 \ge \frac{1}{2}x^2 - y^2$. Rearranging terms gives $\frac{1}{2}x^2 - 2xy + 2y^2 \ge 0$. Multiplying through by 2 yields $x^2 - 4xy + 4y^2 \ge 0$, or $(x-2y)^2 \ge 0$. 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 $0 \ge \frac{1}{2}x^2-y^2$, or $y^2 \ge \frac{1}{2}x^2$. Since x < y and both are non-negative, $y^2 > x^2 \ge \frac{1}{2}x^2$, so the inequality holds strictly.

Lemma 5.

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

Proof.

$$f(\mathbf{B}_{t} + \mathbf{d}_{t}) - f(\mathbf{B}_{t}) \leq -\frac{(\|\overline{\mathbf{G}}_{t}\| - C_{t})_{+}^{2}}{4L_{w}} \leq -\frac{(\|\nabla f(\mathbf{B}_{t})\| - 2C_{t})_{+}^{2}}{4L_{w}}$$

$$\leq -\frac{\frac{1}{2}\|\nabla f(\mathbf{B}_{t})\|^{2} - 4C_{t}^{2}}{4L_{w}}$$

$$= -\frac{1}{8L_{w}}\|\nabla f(\mathbf{B}_{t})\|^{2} + \frac{1}{L_{w}}C_{t}^{2}.$$

Now Theorem 8 follows by taking the summation of (12) from 0 to T-1, dividing both sides by T, and rearranging.