

Numerical method for approximately optimal solutions of two-stage distributionally robust optimization with marginal constraints

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Two-stage distributionally robust optimization (DRO)

- Two-stage distributionally robust optimization (DRO) problem:

$$\begin{aligned} \phi_{\text{DRO}} := & \underset{\mathbf{a}}{\text{minimize}} \quad \langle \mathbf{c}_1, \mathbf{a} \rangle + \sup_{\mu \in \mathcal{P}_{\mathcal{X}}} \int_{\mathcal{X}} Q(\mathbf{a}, \mathbf{x}) \mu(d\mathbf{x}) \\ & \text{subject to} \quad \mathbf{L}_{\text{in}} \mathbf{a} \leq \mathbf{q}_{\text{in}}, \quad \mathbf{L}_{\text{eq}} \mathbf{a} = \mathbf{q}_{\text{eq}}, \quad \mathbf{a} \in \mathbb{R}^{K_1}. \end{aligned}$$

- First-stage decision variable** $\mathbf{a} \in \mathbb{R}^{K_1}$.
- Uncertain quantity** $\mathbf{x} \in \mathcal{X} := \mathcal{X}_1 \times \cdots \times \mathcal{X}_N \subset \mathbb{R}^N$, where $\mathcal{X}_1, \dots, \mathcal{X}_N$ are compact subsets of \mathbb{R} .
- $\mathcal{P}_{\mathcal{X}} \subseteq \mathcal{P}(\mathcal{X})$ is the **ambiguity set** of probability measures.
- $\langle \mathbf{c}_1, \mathbf{a} \rangle$ is the **first-stage cost**, $Q(\mathbf{a}, \mathbf{x})$ is the **second-stage cost**:

$$\begin{aligned} Q(\mathbf{a}, \mathbf{x}) := & \underset{\mathbf{z}}{\text{minimize}} \quad \langle \mathbf{c}_2, \mathbf{z} \rangle \\ & \text{subject to} \quad \mathbf{A}_{\text{in}} \mathbf{z} \leq \mathbf{V}_{\text{in}} \mathbf{a} + \mathbf{W}_{\text{in}} \mathbf{x} + \mathbf{b}_{\text{in}}, \\ & \quad \mathbf{A}_{\text{eq}} \mathbf{z} = \mathbf{V}_{\text{eq}} \mathbf{a} + \mathbf{W}_{\text{eq}} \mathbf{x} + \mathbf{b}_{\text{eq}}, \\ & \quad \mathbf{z} \in \mathbb{R}^{K_2}. \end{aligned}$$

Two-stage distributionally robust optimization (DRO)

- We consider the case where $\mathcal{P}_{\mathcal{X}}$ is the set of **couplings of fixed marginals** $\mu_1 \in \mathcal{P}(\mathcal{X}_1), \dots, \mu_N \in \mathcal{P}(\mathcal{X}_N)$:

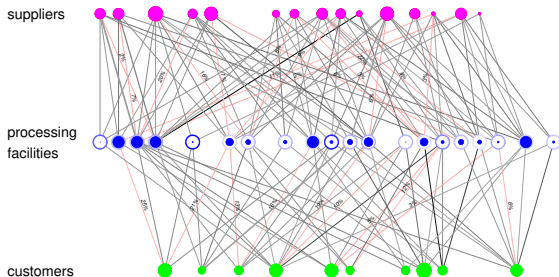
$$\mathcal{P}_{\mathcal{X}} = \Gamma(\mu_1, \dots, \mu_N) := \left\{ \mu \in \mathcal{P}(\mathcal{X}) : \right.$$

the marginal of μ on \mathcal{X}_i is $\mu_i \forall 1 \leq i \leq N \left. \right\}$.

- **Motivation:** there is much less ambiguity about the marginal distributions than the dependence structure (Eckstein, Kupper, and Pohl 2020).

Example: supply chain network design

- \mathbf{a} : investment for the processing facilities
- \mathbf{x} : demands of product & failure of edges
- $\langle \mathbf{c}_1, \mathbf{a} \rangle$: investment cost
- $Q(\mathbf{a}, \mathbf{x})$: transportation & processing costs



- Additional examples include: **task scheduling**, **assemble-to-order system**,
...

Contributions

- We develop a **relaxation scheme** for two-stage DRO with marginal constraints such that the relaxation error can be controlled to be **arbitrarily close to 0**.
- We develop a **numerical algorithm** which computes:
 - an **approximately optimal solution** $\hat{\mathbf{a}}$ of ϕ_{DRO} ;
 - **upper bound** $\phi_{\text{DRO}}^{\text{UB}}$ and **lower bound** $\phi_{\text{DRO}}^{\text{LB}}$ such that $\phi_{\text{DRO}}^{\text{LB}} \leq \phi_{\text{DRO}} \leq \phi_{\text{DRO}}^{\text{UB}}$;
 - $\hat{\epsilon} := \phi_{\text{DRO}}^{\text{UB}} - \phi_{\text{DRO}}^{\text{LB}}$ **measuring the sub-optimality** of $\hat{\mathbf{a}}$, where $\hat{\epsilon}$ can be controlled to be **arbitrarily close to 0** by the inputs of the algorithm.
- We perform numerical experiments to demonstrate the proposed algorithm in prominent decision problems including **scheduling**, **assemble-to-order system**, and **supply chain network design**.

Related studies

- Gao and Kleywegt (2017) consider DRO with marginal constraints & Wasserstein distance based constraint.
 - Computation is only tractable when the marginals are discrete and when the second-stage cost is the maximum of finitely many affine functions.
- Chen, Ma, Natarajan, Simchi-Levi, and Yan (2021) deal with a particular class of DRO problem with marginal constraints, most notably appointment scheduling.
 - Focuses on analysing the theoretical computational complexity.
 - No concrete numerical algorithm is provided.
- **Connection with multi-marginal optimal transport (MMOT):**
Carlier, Oberman, Oudet (2015), Pass (2015), Benamou, Carlier, and Nenna (2019), Peyré and Cuturi (2019), Benamou (2021), Neufeld and Xiang (2022), ...

Step 1: Augmentation

- Recall that the two-stage DRO problem

$$\begin{aligned} \phi_{\text{DRO}} := & \underset{\mathbf{a}}{\text{minimize}} \quad \langle \mathbf{c}_1, \mathbf{a} \rangle + \sup_{\mu \in \mathcal{P}_{\mathcal{X}}} \int_{\mathcal{X}} Q(\mathbf{a}, \mathbf{x}) \mu(d\mathbf{x}) \\ & \text{subject to} \quad \mathbf{L}_{\text{in}} \mathbf{a} \leq \mathbf{q}_{\text{in}}, \mathbf{L}_{\text{eq}} \mathbf{a} = \mathbf{q}_{\text{eq}}, \mathbf{a} \in \mathbb{R}^{K_1} \end{aligned}$$

has a **min-max-min** structure.

- To begin, take the dual of the second-stage problem and represent $Q(\mathbf{a}, \mathbf{x}) = \max_{\lambda \in \mathcal{S}_2^*} \{ \langle \mathbf{V}\mathbf{a} + \mathbf{W}\mathbf{x} + \mathbf{b}, \lambda \rangle \}$ for some polytope $\mathcal{S}_2^* \subset \mathbb{R}^{K_2^*}$. This transforms the problem into a **min-max-max** problem.

Step 1: Augmentation

- Next, to combine the two maximization steps, we augment $Q(\cdot, \cdot)$ and $\Gamma(\mu_1, \dots, \mu_N)$:

$$Q_{\text{aug}}(\mathbf{a}, \mathbf{x}, \boldsymbol{\lambda}) := \langle \mathbf{V}\mathbf{a} + \mathbf{W}\mathbf{x} + \mathbf{b}, \boldsymbol{\lambda} \rangle \quad \forall \mathbf{a}, \forall \mathbf{x}, \forall \boldsymbol{\lambda},$$

$$\Gamma_{\text{aug}}(\mu_1, \dots, \mu_N) := \left\{ \mu_{\text{aug}} \in \mathcal{P}(\mathcal{X} \times \mathcal{S}_2^*) : \right.$$

the marginal of μ_{aug} on \mathcal{X}_i is $\mu_i \forall 1 \leq i \leq N \left. \right\}$.

Lemma (Augmentation)

The following equality holds:

$$\begin{aligned} \phi_{\text{DRO}} = & \underset{\mathbf{a}}{\text{minimize}} \quad \langle \mathbf{c}_1, \mathbf{a} \rangle + \sup_{\mu_{\text{aug}} \in \Gamma_{\text{aug}}(\mu_1, \dots, \mu_N)} \int_{\mathcal{X} \times \mathcal{S}_2^*} Q_{\text{aug}}(\mathbf{a}, \mathbf{x}, \boldsymbol{\lambda}) \mu_{\text{aug}}(d\mathbf{x}, d\boldsymbol{\lambda}) \\ & \text{subject to} \quad \mathbf{L}_{\text{in}} \mathbf{a} \leq \mathbf{q}_{\text{in}}, \quad \mathbf{L}_{\text{eq}} \mathbf{a} = \mathbf{q}_{\text{eq}}, \quad \mathbf{a} \in \mathbb{R}^{K_1}. \end{aligned}$$

Step 2: Relaxation

- Relax the marginal constraints into **finitely many linear constraints**.
 - Fixing a marginal can be seen as having infinitely many linear constraints.
- Augmented couplings are replaced by a **moment set**:

Definition (Moment set (Neufeld and X. 2022))

For $i = 1, \dots, N$, $[\mu_i]_{\mathcal{G}_i}$ is called a moment set centered at μ_i characterized by functions $\mathcal{G}_i \subset \mathcal{L}^1(\mathcal{X}_i, \mu_i)$: $\nu_i \in [\mu_i]_{\mathcal{G}_i} \Leftrightarrow \int_{\mathcal{X}_i} \mathbf{g}_i d\mu_i = \int_{\mathcal{X}_i} \mathbf{g}_i d\nu_i \forall \mathbf{g}_i \in \mathcal{G}_i$.
Moreover,

$$\Gamma_{\text{aug}}([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N}) := \left\{ \mu_{\text{aug}} \in \Gamma_{\text{aug}}(\nu_1, \dots, \nu_N) : \nu_i \in [\mu_i]_{\mathcal{G}_i} \forall 1 \leq i \leq N \right\}.$$

- Relaxed two-stage DRO problem:**

$$\begin{aligned} & \underset{\mathbf{a}}{\text{minimize}} && \langle \mathbf{c}_1, \mathbf{a} \rangle + \sup_{\mu_{\text{aug}} \in \Gamma_{\text{aug}}([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N})} \int_{\mathbf{x} \times \mathcal{S}_2^*} Q_{\text{aug}}(\mathbf{a}, \mathbf{x}, \lambda) \mu_{\text{aug}}(d\mathbf{x}, d\lambda) \\ & \text{subject to} && \mathbf{L}_{\text{in}} \mathbf{a} \leq \mathbf{q}_{\text{in}}, \mathbf{L}_{\text{eq}} \mathbf{a} = \mathbf{q}_{\text{eq}}, \mathbf{a} \in \mathbb{R}^{K_1}. \end{aligned}$$

Step 3: Dualization

- Let $\mathcal{G}_i = \{g_{i,1}, \dots, g_{i,m_i}\}$ for $i = 1, \dots, N$ and let $m := \sum_{i=1}^N m_i$.
 - $\mathbf{g}(x_1, \dots, x_N) := (g_{1,1}(x_1), \dots, g_{N,m_N}(x_N))^T \quad \forall (x_1, \dots, x_N) \in \mathcal{X}$.
 - $\mathbf{v} := \left(\int_{\mathcal{X}_1} g_{1,1} d\mu_1, \dots, \int_{\mathcal{X}_N} g_{N,m_N} d\mu_N \right)^T$.
- Replacing the relaxed inner maximization problem by its dual yields the following linear semi-infinite programming (LSIP) problem:

$$\underset{\mathbf{a}, y_0, \mathbf{y}}{\text{minimize}} \quad \langle \mathbf{c}_1, \mathbf{a} \rangle + y_0 + \langle \mathbf{v}, \mathbf{y} \rangle$$

$$\text{subject to} \quad y_0 + \langle \mathbf{g}(\mathbf{x}), \mathbf{y} \rangle - \langle \mathbf{V}^T \boldsymbol{\lambda}, \mathbf{a} \rangle \geq \langle \mathbf{W}\mathbf{x} + \mathbf{b}, \boldsymbol{\lambda} \rangle$$

$$\forall \mathbf{x} \in \mathcal{X}, \forall \boldsymbol{\lambda} \in \mathcal{S}_2^*, \quad (\text{LSIP})$$

$$\mathbf{L}_{\text{in}} \mathbf{a} \leq \mathbf{q}_{\text{in}}, \quad \mathbf{L}_{\text{eq}} \mathbf{a} = \mathbf{q}_{\text{eq}},$$

$$\mathbf{a} \in \mathbb{R}^{K_1}, \quad y_0 \in \mathbb{R}, \quad \mathbf{y} \in \mathbb{R}^m.$$

- Each approximately optimal solution $(\hat{\mathbf{a}}, \hat{y}_0, \hat{\mathbf{y}})$ of (LSIP) provides:
 - an **approximately optimal solution** $\hat{\mathbf{a}}$ of the DRO problem,
 - an **upper bound** $\langle \mathbf{c}_1, \hat{\mathbf{a}} \rangle + \hat{y}_0 + \langle \mathbf{v}, \hat{\mathbf{y}} \rangle$ for ϕ_{DRO} (with controlled quality).

Step 4: Bounding from below

- The problem (LSIP) admits the following dual:

$$\begin{aligned}
 & \underset{\xi_{\text{in}}, \xi_{\text{eq}}, \mu_{\text{aug}}}{\text{maximize}} && \langle \mathbf{q}_{\text{in}}, \xi_{\text{in}} \rangle + \langle \mathbf{q}_{\text{eq}}, \xi_{\text{eq}} \rangle + \int_{\mathcal{X} \times \mathcal{S}_2^*} \langle \mathbf{W}\mathbf{x} + \mathbf{b}, \lambda \rangle \mu_{\text{aug}}(\mathrm{d}\mathbf{x}, \mathrm{d}\lambda) \\
 & \text{subject to} && \mathbf{L}_{\text{in}}^{\text{T}} \xi_{\text{in}} + \mathbf{L}_{\text{eq}}^{\text{T}} \xi_{\text{eq}} - \mathbf{V}^{\text{T}} \left(\int_{\mathcal{X} \times \mathcal{S}_2^*} \lambda \mu_{\text{aug}}(\mathrm{d}\mathbf{x}, \mathrm{d}\lambda) \right) = \mathbf{c}_1, \quad (\text{LSIP}^*) \\
 & && \xi_{\text{in}} \leq \mathbf{0}, \quad \mu_{\text{aug}} \in \Gamma_{\text{aug}}([\mu_1]_{\mathcal{G}_1}, \dots, [\mu_N]_{\mathcal{G}_N}), \\
 & && \xi_{\text{in}} \in \mathbb{R}^{n_{\text{in}}}, \quad \xi_{\text{eq}} \in \mathbb{R}^{n_{\text{eq}}}, \quad \mu_{\text{aug}} \in \mathcal{P}(\mathcal{X} \times \mathcal{S}_2^*).
 \end{aligned}$$

- For each approximately optimal solution $(\hat{\xi}_{\text{in}}, \hat{\xi}_{\text{eq}}, \hat{\mu}_{\text{aug}})$ of (LSIP^{*}):
 - if $\tilde{\mu}_{\text{aug}} \in \Gamma_{\text{aug}}(\mu_1, \dots, \mu_N)$ satisfies

$$\mathbf{L}_{\text{in}}^{\text{T}} \hat{\xi}_{\text{in}} + \mathbf{L}_{\text{eq}}^{\text{T}} \hat{\xi}_{\text{eq}} - \mathbf{V}^{\text{T}} \left(\int_{\mathcal{X} \times \mathcal{S}_2^*} \lambda \tilde{\mu}_{\text{aug}}(\mathrm{d}\mathbf{x}, \mathrm{d}\lambda) \right) = \mathbf{c}_1,$$

then $\langle \mathbf{q}_{\text{in}}, \hat{\xi}_{\text{in}} \rangle + \langle \mathbf{q}_{\text{eq}}, \hat{\xi}_{\text{eq}} \rangle + \int_{\mathcal{X} \times \mathcal{S}_2^*} \langle \mathbf{W}\mathbf{x} + \mathbf{b}, \lambda \rangle \tilde{\mu}_{\text{aug}}(\mathrm{d}\mathbf{x}, \mathrm{d}\lambda)$ is a **lower bound** for ϕ_{DRO} (with controlled quality).

Step 4: Bounding from below

Definition (Partial reassembly)

Let $\bar{\mathcal{X}}_i := \mathcal{X}_i$ for $i = 1, \dots, N$. $\tilde{\mu}_{\text{aug}}$ is called a partial reassembly of $\hat{\mu}_{\text{aug}} \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \mathcal{S}_2^*)$ with the marginals μ_1, \dots, μ_N if there exists a probability measure $\gamma \in \mathcal{P}(\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N \times \mathcal{S}_2^*)$ such that:

- 1 the marginal of γ on $\mathcal{X}_1 \times \dots \times \mathcal{X}_N \times \mathcal{S}_2^*$ is $\hat{\mu}_{\text{aug}}$;
- 2 for $i = 1, \dots, N$, the marginal $\gamma_i \in \Gamma(\hat{\mu}_i, \mu_i)$ of γ on $\mathcal{X}_i \times \bar{\mathcal{X}}_i$ satisfies $\int_{\mathcal{X}_i \times \bar{\mathcal{X}}_i} |x - y| \gamma_i(\mathrm{d}x, \mathrm{d}y) = W_1(\hat{\mu}_i, \mu_i)$;
- 3 the marginal of γ on $\bar{\mathcal{X}}_1 \times \dots \times \bar{\mathcal{X}}_N \times \mathcal{S}_2^*$ is $\tilde{\mu}_{\text{aug}}$.

The set of *partial reassemblies* is denoted by

$$R_{\text{part}}(\hat{\mu}_{\text{aug}}; \mu_1, \dots, \mu_N) \subset \Gamma_{\text{aug}}(\mu_1, \dots, \mu_N).$$

- **Idea:** morphing $\hat{\mu}_{\text{aug}}$ in an “optimal” way to turn its marginals on $\mathcal{X}_1, \dots, \mathcal{X}_N$ into μ_1, \dots, μ_N while leaving its marginal on \mathcal{S}_2^* unchanged.
- One can construct a partial reassembly using Sklar’s theorem from copula theory.

Controlling the approximation error

Theorem (Approximation of two-stage DRO with marginal constraints)

Suppose that:

- 1 for $i = 1, \dots, N$, \mathcal{G}_i contains only continuous functions;
- 2 $(\hat{\mathbf{a}}, \hat{\mathbf{y}}_0, \hat{\mathbf{y}})$ is an ϵ -optimal solution of (LSIP) for $\epsilon > 0$;
- 3 $(\hat{\xi}_{\text{in}}, \hat{\xi}_{\text{eq}}, \hat{\mu}_{\text{aug}})$ is an ϵ^* -optimal solution of (LSIP*) for $\epsilon^* > 0$;
- 4 $\tilde{\mu}_{\text{aug}} \in R_{\text{part}}(\hat{\mu}_{\text{aug}}; \mu_1, \dots, \mu_N)$;
- 5 $\phi_{\text{DRO}}^{\text{UB}} := \langle \mathbf{c}_1, \hat{\mathbf{a}} \rangle + \hat{\mathbf{y}}_0 + \langle \mathbf{v}, \hat{\mathbf{y}} \rangle$;
- 6 $\phi_{\text{DRO}}^{\text{LB}} := \langle \mathbf{q}_{\text{in}}, \hat{\xi}_{\text{in}} \rangle + \langle \mathbf{q}_{\text{eq}}, \hat{\xi}_{\text{eq}} \rangle + \int_{\mathcal{X} \times \mathcal{S}_2^*} \langle \mathbf{W}\mathbf{x} + \mathbf{b}, \boldsymbol{\lambda} \rangle \tilde{\mu}_{\text{aug}}(d\mathbf{x}, d\boldsymbol{\lambda})$;
- 7 $\tilde{\epsilon} := \epsilon + \epsilon^* + \left(\sum_{i=1}^N \sup_{\nu_i \in [\mu_i]_{\mathcal{G}_i}} \{W_1(\mu_i, \nu_i)\} \right) \sup_{\boldsymbol{\lambda} \in \mathcal{S}_2^*} \{ \|\mathbf{W}^T \boldsymbol{\lambda}\|_{\infty} \}$.

Then,

- $\phi_{\text{DRO}}^{\text{LB}} \leq \phi_{\text{DRO}} \leq \phi_{\text{DRO}}^{\text{UB}}$ with $\phi_{\text{DRO}}^{\text{UB}} - \phi_{\text{DRO}}^{\text{LB}} \leq \tilde{\epsilon}$;
- $\hat{\mathbf{a}}$ is an $\hat{\epsilon}$ -optimal solution of the two-stage DRO problem, where $\hat{\epsilon} := \phi_{\text{DRO}}^{\text{UB}} - \phi_{\text{DRO}}^{\text{LB}} \leq \tilde{\epsilon}$.

Practical questions

- **Question 1:** for any $\epsilon > 0$, can we obtain ϵ -optimal solutions of (LSIP) and (LSIP*)?
 - **Answer 1:** yes, we develop a suitable **cutting-plane algorithm** (inspired by Conceptual Algorithm 11.4.1 of Goberna and López (1998)) to obtain ϵ -optimal solutions of (LSIP) and (LSIP*).
- **Question 2:** can we numerically evaluate an integral with respect to a $\tilde{\mu}_{\text{aug}} \in R_{\text{part}}(\hat{\mu}_{\text{aug}}; \mu_1, \dots, \mu_N)$?
 - **Answer 2:** yes, using the copula theory, we develop an algorithm to **explicitly construct a partial reassembly** and **efficiently generate independent random samples** from it.
- **Question 3:** can we control $\sup_{\nu_i \in [\mu_i]_{\mathcal{G}_i}} \{W_1(\mu_i, \nu_i)\}$ to be arbitrarily close to 0 for $i = 1, \dots, N$?
 - **Answer 3:** yes, for any $\epsilon_i > 0$ we can **explicitly construct** a finite collection \mathcal{G}_i of continuous piece-wise affine functions with $\sup_{\nu_i \in [\mu_i]_{\mathcal{G}_i}} \{W_1(\mu_i, \nu_i)\} \leq \epsilon_i$.

Numerical algorithm

- Putting these pieces together, we develop a numerical algorithm, whose properties are summarized as follows.

Theorem (Properties of the proposed algorithm)

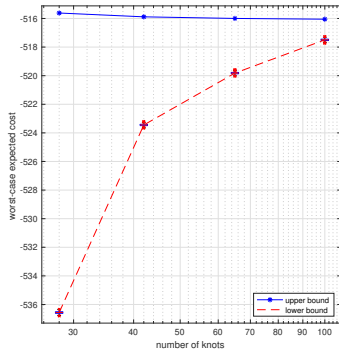
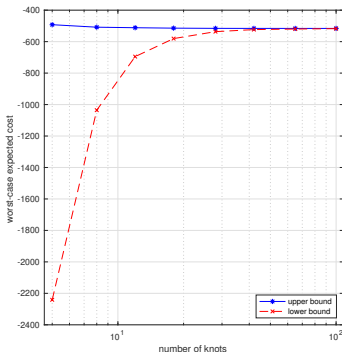
Under suitable conditions, for any $\tilde{\epsilon} > 0$, there exists inputs to the proposed algorithm such that it produces the outputs: $\hat{\mathbf{a}}$, $\phi_{\text{DRO}}^{\text{LB}}$, $\phi_{\text{DRO}}^{\text{UB}}$ such that

- $\phi_{\text{DRO}}^{\text{LB}} \leq \phi_{\text{DRO}} \leq \phi_{\text{DRO}}^{\text{UB}}$;
- $\hat{\mathbf{a}}$ is an $\hat{\epsilon}$ -optimizer of the two-stage DRO problem, where $\hat{\epsilon} := \phi_{\text{DRO}}^{\text{UB}} - \phi_{\text{DRO}}^{\text{LB}} \leq \tilde{\epsilon}$.

- Remark:** the sub-optimality measure $\hat{\epsilon}$ can be computed, and it is often **much less conservative** than its theoretical upper bound $\tilde{\epsilon}$.

Convergence of the bounds

- When appropriately chosen continuous piece-wise affine functions are incrementally added to $(\mathcal{G}_i)_{i=1:N}$, the difference between the upper bound $\phi_{\text{DRO}}^{\text{UB}}$ and the lower bound $\phi_{\text{DRO}}^{\text{LB}}$ goes to 0.

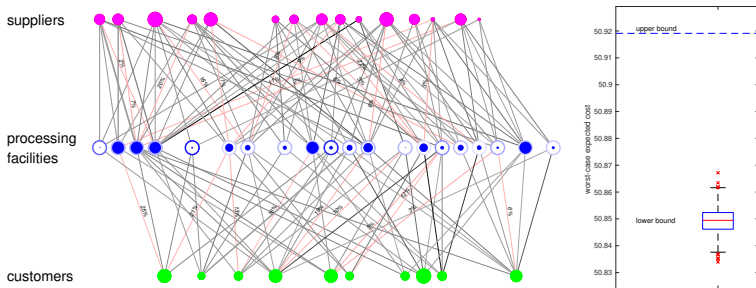


Numerical example: supply chain network design

Settings:

- We consider 15 suppliers, 20 processing facilities, 10 customers, 150 edges with 25 susceptible to failure. ($N = 10 + 25$, $K_1 = 170$, $K_2 = 150$);
- $\mathcal{X}_1 = \mathcal{X}_2 = \dots = \mathcal{X}_{10} = [0, 2]$, $\mathcal{X}_{11} = \mathcal{X}_{12} = \dots = \mathcal{X}_{35} = \{0, 1\}$.
- μ_1, \dots, μ_{10} are mixture of truncated normal distributions.
- Parameters in the model are randomly generated.

Result:



The difference between the upper bound and the lower bound is ~ 0.07 .

References

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