Contextual Scenario Generation for Two-Stage Stochastic Programming

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Introduction to Two-Stage Stochastic Programs

Two-stage stochastic programs (2SPs) are a widely adopted decision-making tool that are described by the following setting:

- ▶ A 'here-and-now' decision $y \in \mathcal{Y}$ is made, incurring an immediate cost h(y)
- ▶ An uncertain event $\omega \in \Omega$ is then realized, with ω drawn from distribution $\mathbb P$
- ▶ Afterward, the decision maker selects a recourse action $z \in Z(y, \omega)$
- The decision maker optimally reacts to ω, given y, and chooses a recourse action that minimizes the cost q(z, ω), where q represents the recourse cost in scenario ω

$$old y
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 (2SP ABCs)

- For example, a product manufacturer must allocate capacity to machines (y) before knowing product demand (ω)
- Once the product demands are known, they create an optimal production plan (z)
- 2SPs are applied in fields such as logistics, portfolio management, and manufacturing (Ntaimo, 2024)

Introduction to 2SP Problem Setup

The decision maker wishes to solve

$$\min_{\mathbf{y}} h(\mathbf{y}) + \mathbb{Q}(\mathbf{y}) \qquad \text{s.t.} \quad \mathbf{y} \in \mathcal{Y}, \quad \mathbf{y} \in \mathbb{R}^{s_1}$$
(2SP)

where

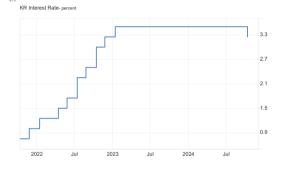
•
$$\mathbb{Q}(\mathbf{y}) = \mathbb{E}_{\mathbb{P}}[Q(\mathbf{y}, \omega)]$$
 is the expected recourse cost

with the optimal recourse cost recourse

$$Q(\boldsymbol{y},\omega) = \min_{\boldsymbol{z}} q(\boldsymbol{z},\omega) \quad \text{s.t.} \quad \boldsymbol{z} \in \mathcal{Z}(\boldsymbol{y},\omega), \quad \boldsymbol{z} \in \mathbb{R}^{s_2} \tag{Stage II}$$

Contextual Stochastic Optimization

- Suppose the decision maker is manufacturing parts for home builders
- The Bank of Korea has lowered interest rates to 3.25%
- ► How does this change our decision **y**?
- Information known to the decision maker at decision time is referred to as context x
- ► The decision maker aims to solve 2SP with costs evaluated using P_{ω|x}



Source: tradingeconomics.com | The Bank of Korea

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Contextual Scenario Generation for 2SP

Problem Setup and an Existing Approach

- ► They do not have access to $\mathbb{P}_{\omega|x}$, and instead only have access to a joint sample (historical data) $S = \{x^{(i)}, \omega^{(i)}\}_{i=1}^{n}$
- There is a contextual stochastic optimization (CSO) zoo (Estes and Richard, 2023)

This suggests the following approach



- A dataset of observations is used to estimate a parametric model.
- Sampling from a parametric model of the conditional scenario distribution yields a large 2SP
- The number of scenarios is reduced and the optimization is performed over the reduced set of scenarios

Contextual Scenario Generation for 2SP

The main idea

The goal is to directly go from x to a small set of scenarios $\zeta_{1...K} = (\zeta_k)_{k=1}^K \in \Omega^K$ by selecting $f: x \mapsto \zeta_{1...K}$ from function class \mathcal{F} (e.g. ReLu networks producing K scenarios)

- By bypassing the scenario generation step, the time between context and decision-making will be decreased while still unlocking the value of stochastic solutions
- The proposed approach is situated in the CSO zoo: major pros consisting of feasibility, decision-time tractability, and value of stochastic solutions

The figure below highlights the proposed approach

Contextual Scenario Generation and Optimization



Maximum Mean Discrepancy Distance

- A Reproducing Kernel Hilbert Space \mathcal{H} (RKHS) with associated positive semi-definite kernel $k: \Omega \times \Omega \rightarrow \mathbb{R}$ is considered
- > The squared maximum mean discrepancy allows us to measure the distance between distributions
- Gretton et al. (2012) showed that the squared maximum mean discrepancy between \mathbb{P}_{η} and \mathbb{P}_{ω} is given by

$$d^2_{\mathcal{G}_{\mathsf{MMD}}}(\mathbb{P}_{\omega},\mathbb{P}_{\eta}) = \mathbb{E}_{(\omega,\omega')\sim\mathbb{P}_{\omega}}[k(\omega,\omega')] + \mathbb{E}_{(\eta,\eta')\sim\mathbb{P}_{\eta}}[k(\eta,\eta')] - 2\mathbb{E}_{\omega\sim\mathbb{P}_{\omega},\eta\sim\mathbb{P}_{\eta}}[k(\omega,\eta)]$$

- There exists a rich theory associated with RKHSs that lead to some desirable properties (concentration inequalities, generalization guarantees, links to stability theory of 2SPs)
- Specification of k determines the distance

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A Distributional Approach

- Select *f* to minimize a distributional distance between *f*(*x*) and ℙ_{ω|x} ... in expectation over ℙ_x
- Distributional Contextual Scenario Generation (DCSG):

$$\min_{\boldsymbol{f}\in\mathcal{F}}\mathcal{L}_{\mathsf{dist}}(\boldsymbol{f}) := \mathbb{E}_{\boldsymbol{x}\sim\mathbb{P}_{\boldsymbol{x}}}\left[d\left(\mathbb{P}_{\boldsymbol{f}(\boldsymbol{x})},\mathbb{P}_{\omega|\boldsymbol{x}}\right)\right]$$

• where $\mathbb{P}_{f(x)} = \frac{1}{K} \sum_{k=1}^{K} \delta_{f_k(x)}$ denotes an empirical measure associated with the K scenarios f(x)

A Distributional Approach

• Using the squared MMD distance implies $\mathcal{L}_{dist}(f)$ can be written as

$$\mathcal{L}_{\text{dist}}(\boldsymbol{f}) = C + \mathbb{E}_{(\boldsymbol{x},\omega) \sim \mathbb{P}_{\boldsymbol{x},\omega}} \left[\underbrace{\frac{1}{K^2} \sum_{i=1}^{K} \sum_{i'=1}^{K} k(f_i(\boldsymbol{x}), f_{i'}(\boldsymbol{x})) - \frac{2}{K} \sum_{i=1}^{K} k(\omega, f_i(\boldsymbol{x}))}_{:=\ell_{\text{MMD}}(\boldsymbol{f}(\boldsymbol{x}), \omega)} \right],$$

• where $C = \mathbb{E}_{\mathbf{x} \sim \mathbb{P}_{\mathbf{x}}} \mathbb{E}_{(\omega, \omega') \sim \mathbb{P}_{\omega|\mathbf{x}}} [k(\omega, \omega')]$ is a constant with respect to f

yielding an empirical risk minimization:

$$\min_{\boldsymbol{f}\in\mathcal{F}}\mathcal{L}_{\mathsf{MMD}}(\boldsymbol{f})\coloneqq\mathbb{E}_{(\boldsymbol{x},\omega)\sim\mathbb{P}_{\boldsymbol{x},\omega}}\left[\ell_{\mathsf{MMD}}(\boldsymbol{f}(\boldsymbol{x}),\omega)\right]$$

• We select the energy kernel, $k(\omega, \omega') = - \|\omega - \omega'\|_2$ due to its desirable properties. For example

- \blacktriangleright K = 1 reduces to least-squares regression (the first ever contextual approach)
- Considers some of the underlying geometry (Feydy et al., 2019)
- Results L_{dist} being a metric
- Specify the parameterization for **f** and optimize **f** via gradients

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A Problem-driven Approach

• We obtain a first-stage solution by solving (2SP) using $\zeta_{1...K} = f(x)$

$$\mathbf{y}(\zeta_{1...K}) \in \operatorname{proj}_{\mathbf{y}} \operatorname{argmin}_{\mathbf{y},\mathbf{z}_{1},...\mathbf{z}_{K}} h(\mathbf{y}) + \frac{1}{K} \sum_{i=1}^{K} q(\mathbf{z}_{i},\zeta_{i})$$

$$\mathbf{y} \in \mathcal{Y}, \ \mathbf{z}_{i} \in \mathcal{Z}(\mathbf{y},\zeta_{i}) \ \forall i \in \{1,...,K\},$$

$$(\zeta -SAA)$$

• which has an optimal solution set $\mathcal{Y}^*(\zeta_{1...\kappa}) \coloneqq$

$$\left\{ \boldsymbol{y} \in \mathcal{Y} : h(\boldsymbol{y}) + \frac{1}{K} \sum_{i=1}^{K} q(\boldsymbol{z}_i, \zeta_i) \leq v^*(\zeta_{1...K}), \boldsymbol{z}_i \in \mathcal{Z}(\boldsymbol{y}, \zeta_i), \ i \in \{1, \ldots, K\} \right\},\$$

where $v^*(\zeta_{1...\kappa})$ is the optimal objective value of $(\zeta$ -SAA)

A Problem-driven Approach

- Select *f* such that the 2SP solutions on *f*(*x*) produce the highest quality set of optimal (ζ-SAA) solutions 𝒱^{*}(*f*(*x*)) according to ℙ_{ω|x}
- We measure the quality of the optimal solution set \(\mathcal{Y}^*(f(x))\) by the best possible two-stage performance among solutions in \(\mathcal{Y}^*(f(x))\). This corresponds to

$$\boldsymbol{f}(\boldsymbol{x}) \in \operatorname*{argmin}_{\zeta_{1}, \dots, \zeta_{K}} \min_{\boldsymbol{y} \in \mathcal{Y}^{*}(\zeta_{1} \dots \kappa)} \quad \boldsymbol{h}(\boldsymbol{y}) + \mathbb{E}_{\omega \sim \mathbb{P}_{\omega \mid \boldsymbol{x}}} \left[Q\left(\boldsymbol{y}, \omega\right) \right]$$

holding (almost surely) with respect to \mathbb{P}_{x} .

► Relaxing the constraint that all y ∈ 𝔅^{*}(ζ_{1...κ}) must be the same in every ω, yields the following

$$\min_{\boldsymbol{f}\in\mathcal{F}} \quad \mathbb{E}_{(\boldsymbol{x},\omega)\sim\mathbb{P}_{\boldsymbol{x},\omega}} \left[\min_{\boldsymbol{y}\in\mathcal{Y}^*(\boldsymbol{f}(\boldsymbol{x}))} h(\boldsymbol{y}) + Q(\boldsymbol{y},\omega) \right]$$
(Opt-PCSG')

Suggesting the following loss function

$$\ell_{\mathsf{opt}}(\zeta_{1...\kappa},\omega) \coloneqq \min_{\boldsymbol{y} \in \mathcal{Y}^*(\zeta_{1...\kappa})} h(\boldsymbol{y}) + Q\left(\boldsymbol{y},\omega\right)$$

Evaluating the Optimistic Loss

Evaluating $\ell_{opt}(\zeta_{1...K}, \omega)$ is equivalent to solving

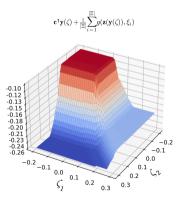
$$\ell_{opt}(\zeta_{1...K},\omega) = \min_{\mathbf{y},\mathbf{z},\mathbf{z}_{1},...\mathbf{z}_{K}} \quad h(\mathbf{y}) + q(\mathbf{z},\omega)$$
(Opt-Search)
s.t.
$$h(\mathbf{y}) + \frac{1}{K} \sum_{i=1}^{K} q(\mathbf{z}_{i},\zeta_{i}) \leq v^{*}(\zeta_{1...K})$$
(1)
$$\mathbf{y} \in \mathcal{Y}, \ \mathbf{z} \in \mathcal{Z}(\mathbf{y},\omega), \ \mathbf{z}_{i} \in \mathcal{Z}(\mathbf{y},\zeta_{i}), \ \forall i \in \{1,\ldots,K\}.$$

- In addition to linear programs and convex programs with multiple solutions, the optimistic approach is generally amenable to mixed-integer programs (MIP) with convex relaxations
- If (Opt-Search) is difficult to solve, we can settle for a feasible solution by solving (ζ-SAA) and (Stage II) (easy for 2SP)
- (Opt-Search) reduces to solving (ζ-SAA) and (Stage II) when (ζ-SAA) exhibits unique solutions

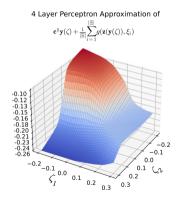
Gradient Sparsity

Solving Opt-PCSG' via gradient-based methods is not easy since the gradients of the objective with respect to the surrogate scenarios are sparse.

Ex. K = 1, unique solutions, n = 1, $\boldsymbol{f} = (\zeta_1, \zeta_2)^T$



(a) The loss plotted against two components of the surrogate scenario ζ .



(b) Approximating the loss surface with a neural network has a smoothing effect.

Neural Network Approximation

We propose a neural architecture inspired by Patel et al. (2022)'s architecture, to model ℓ_{opt}

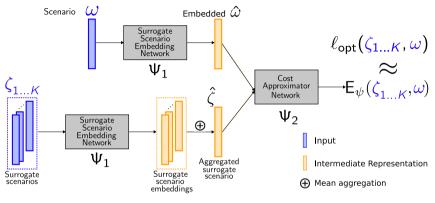


Figure: Loss-Net Architecture

How to train? \rightarrow use f_{MMD} to generate dataset from contextual observations $\{\mathbf{x}^{(i)}, \zeta_{1...K}^{(i)}\}_{i=1}^{n}$ with $\zeta_{1...K}^{(i)} = f_{\text{MMD}}(\mathbf{x}) \rightarrow$ fit E_{ψ} with $\{(\zeta_{1...K}^{(i)}, \omega^{(i)}), \ell_{\text{opt}}(\zeta_{1...K}^{(i)}, \omega^{(i)})\}_{i=1}^{n}$

Replacing the Loss with the Approximate Loss

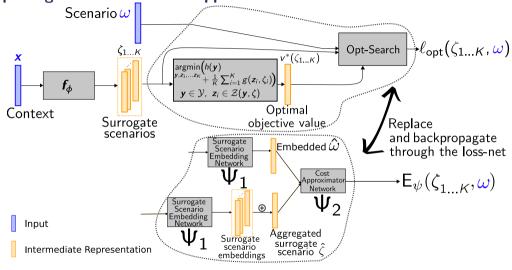


Figure: Replace the true downstream loss with the task-net approximated loss

With MMD Regularization

- Optimizing the approximate task-loss con produce *f*, such that ζ⁽ⁱ⁾_{1...K} = *f*(*x*⁽ⁱ⁾), *i* = 1, ..., *n* are 'far' from ζ⁽ⁱ⁾_{1...K} originally used to train the loss approximator
- \blacktriangleright Idea: regularize the approximate task loss by the MMD loss to select \pmb{f}_ϕ

$$\min_{\phi} \quad \frac{1}{n} \sum_{i=1}^{n} \hat{E}(\boldsymbol{f}_{\phi}(\boldsymbol{x}^{(i)}), \omega^{(i)}) + \lambda \ell_{\mathsf{MMD}}(\boldsymbol{f}_{\phi}(\boldsymbol{x}^{(i)}), \omega^{(i)}), \quad (\mathsf{Static-PCSG})$$

> This approach with K = 1 is equivalent to Zharmagambetov et al. (2024)'s approach

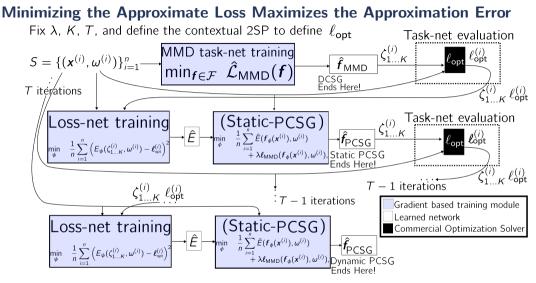


Figure: The relationship between the DCSG, Static-PCSG and Dynamic-PCSG approaches

Contextual Newsvendor Problem

- ► Each day, a newsvendor purchases y newspapers at unit-cost c with a budget constraint: y ≤ u
- The vendor sells as many papers as possible at a unit price q and can return unsold papers at a salvage price r < c</p>
- Contextual information x, such as day of the week, weather, and previous sales, is observed before purchasing
- Demand ω is unknown at the time of purchase, after which the newsvendor optimally sells z and salvages w papers
- ► They wish to solve: $\min_{y} cy + \mathbb{E}_{\omega \sim \mathbb{P}_{\omega|x}} [Q(y, \omega)]$ s.t. $y \in [0, u]$ where $Q(y, \omega) = \min_{z \ge 0, w \ge 0} -qz rw$ s.t. $z \le \omega, z + w \le y$

Experimental Setup

- **Distribution of contextual information:** Context x follows a 2D normal distribution, mapped to demand distribution $\mathbb{P}_{\omega|x}$ over 200 points via a random neural network f_{Random} . Demand has mean 15.1 and std. deviation 0.25
- Sample: n = 500 samples of (x, ω); models MMD (DCSG), Static, and Dynamic trained on this set
- Model Architectures: f_{ϕ} is a fully connected ReLU network, selected via a random search optimizing $\hat{\mathcal{L}}_{MMD}$ on a 20% hold-out set. Loss network E_{ψ} architecture is selected similarly
- **Evaluation:** Models tested on $i = 1, ..., n_{val} = 100$ out-of-sample $\mathbf{x}_{val}^{(i)}$ and their associated $\mathbb{P}_{\omega | \mathbf{x}_{val}^{(i)}}$. First-stage solution evaluated using 2SP objective, considering surrogate scenarios $\zeta_{1...K}^{(i)} = \mathbf{f}(\mathbf{x}^{(i)})$ (full process repeated 20 times)
- Comparison Metric: True 2SP Objectives v⁽ⁱ⁾_{MMD}, v⁽ⁱ⁾_{Static}, v⁽ⁱ⁾_{Dynamic}, and optimal newsvendor solution v⁽ⁱ⁾_{2SP} computed per validation observation

Two Benchmaks

The Expected Value Solution

- Determined by considering the newsvendor problem with a single scenario given by $\mathbb{E}[\omega|\mathbf{x}]$
- In practice, the conditional mean is not known, so this is a benchmark that cannot be implemented

Analytical Contextual Solution

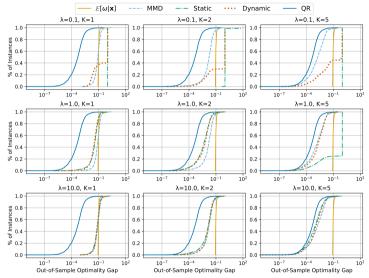
The optimal solution to the newsvendor is

$$y^* = \begin{cases} 0 & \text{if } \frac{q-c}{q-r} < F_{\mathbb{P}}(0), \\ u & \text{if } \frac{q-c}{q-r} > F_{\mathbb{P}}(u), \\ F_{\mathbb{P}}^{-1}\left(\frac{q-c}{q-r}\right) & \text{otherwise.} \end{cases}$$

where $F_{\mathbb{P}}$ is the cumulative density according to \mathbb{P} and $F_{\mathbb{P}}^{-1}(\alpha)$ is the α quantile of F.

► suggesting a quantile estimation approach to obtain a linear model $F_{\mathbb{P}_{\omega|x}}^{-1}\left(\frac{q-c}{q-r}\right) = \beta^{\mathsf{T}}x$, from the training sample (Liu et al., 2022)

Out of Sample Gap – Cumulative Distribution Functions



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Takeaways and Conclusion

- ▶ The proposed approach is able to unlock the value of stochastic solutions
- Although, it is not as performant as problem-specific analytic approaches, it is competitive in certain settings
- Regularization is critically important for the problem-driven approach
- Refining the loss approximation tends to improve performance

We perform similar exercises for other 2SPs from manufacturing and finance and demonstrate computational and performance benifets.

Summary: A generic framework for generating scenarios contextually that is performant and computationally tractable

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Thank you! I look forward to your questions

Contextual Scenario Generation for 2SP – Distributional

Select $f: x \mapsto \zeta_{1...K}$ from a vector-valued function class \mathcal{F} such that the distributional distance between the empirical distribution supported on f(x) and $\mathbb{P}_{\omega|x}$ is minimized in expectation over \mathbb{P}_x .

- F: hypothesis set for the task mapping, parametrized via feed-forward fully connected ReLu networks.
- Approach: Distributional Contextual Scenario Generation (DCSG)

$$\min_{\boldsymbol{f}\in\mathcal{F}}\mathcal{L}_{\text{dist}}(\boldsymbol{f}) := \mathbb{E}_{\boldsymbol{x}\sim\mathbb{P}_{\boldsymbol{x}}}\left[d\left(\mathbb{P}_{\boldsymbol{f}(\boldsymbol{x})},\mathbb{P}_{\omega|\boldsymbol{x}}\right)\right] \tag{DCSG}$$

- ▶ $\mathbb{P}_{f(x)} = \frac{1}{K} \sum_{\zeta \in f(x)}^{K} \delta_{\zeta}$: empirical measure associated with f(x).
- $d(\cdot, \cdot)$: measure of distance between the distributions.

Contextual Scenario Generation for 2SP – Problem Driven

Propose a problem-driven contextual scenario Generation approach (PCSG), that aims to select f such that the 2SP solution defined on f minimizes the 2SP objective evaluated using $\mathbb{P}_{\omega|x}$

$$\min_{\boldsymbol{f} \in \mathcal{F}} \quad \mathbb{E}_{(\boldsymbol{x},\omega) \sim \mathbb{P}_{\boldsymbol{x},\omega}} \left[h(\boldsymbol{y}\left(\boldsymbol{f}(\boldsymbol{x})\right)) + Q\left(\boldsymbol{y}\left(\boldsymbol{f}(\boldsymbol{x})\right),\omega\right) \right]$$

$$s.t. \quad \boldsymbol{y}\left(\boldsymbol{f}(\boldsymbol{x})\right) \in \operatorname{proj}_{\boldsymbol{y}} \operatorname{argmin}_{\boldsymbol{y},\boldsymbol{z}_{1},\ldots,\boldsymbol{z}_{K} \in \mathcal{Y} \times \mathcal{Z}(\boldsymbol{y},\boldsymbol{f}(\boldsymbol{x}))} h(\boldsymbol{y}) + \frac{1}{\mathcal{K}} \sum_{i=1}^{\mathcal{K}} q(\boldsymbol{z}_{i},\boldsymbol{f}_{i}(\boldsymbol{x})) \quad (a.s.)$$

$$(PCSG)$$

Contextual Scenario Generation for 2SP – The Zoo

Estes and Richard (2023) provide an insightful segmentation of contextual methods for stochastic optimization.

Conditional-density-estimation-then-optimize

• Estimate $\mathbb{P}_{\omega|x}$ then solve 2SP \rightarrow does not directly address computational considerations

Direct-solution-prediction

Form a mapping $g : x \mapsto y$, from function class \mathcal{G} to solve $\min_{g \in \mathcal{G}} \mathbb{E}_{(x,\omega) \sim \mathbb{P}_{x,\omega}} [h(g(x)) + Q(g(x), \omega)] \rightarrow \text{necessitates problem-specific approaches due to feasibility considerations}$

Predict-then-optimize

- Solve $\min_{\mathbf{y}, \mathbf{z} \in \mathbb{R}^{s_1 \times s_2}} h(\mathbf{y}) + q(\mathbf{z}, \tilde{\omega})$ s.t $\mathbf{y} \in \mathcal{Y}, \ \mathbf{z} \in \mathcal{Z}(\mathbf{y}, \tilde{\omega})$ where $\tilde{\omega} = \mathbf{h}(\mathbf{x}) \in \Omega$ is a scenario predicted by a learned \mathbf{h} in some hypothesis class \mathcal{H}
- ▶ Naive predict-then-optimize: select h via standard statistical approaches \rightarrow does not consider downstream costs
- Smart predict-then-optimize: select h such that the resulting solutions to perform well according to $\mathbb{E}_{(x,\omega)\sim\mathbb{P}_{x,\omega}}[h(y)+Q(y,\omega)] \rightarrow$ typically problem-specific, suffers from vanishing gradients, resulting solutions do not hedge against uncertainty (by nature of being a point predictor)

Contextual Scenario Generation for 2SP – The Zoo

The proposed approach is related to the aforementioned areas as follows: **Conditional-density-estimation-then-optimize**

Addresses computational concerns by approximating P_{w|x} by a distribution supported on K scenarios

Direct-solution-prediction

(2SP) defined on K discrete scenarios preserves first-stage feasibility. The proposed approach makes minimal assumptions regarding problem structure

Predict-then-optimize

Using a distribution supported on K scenarios results in solutions with more optionality. Furthermore, the loss network, tailored to 2SPs makes addresses the issues of gradients

Contextual Scenario Generation for 2SP – Experimental Results

- A joint sample n = 500 is obtained as the decision maker's historical data
- ► The proposed methods are trained on the joint sample and evaluated out-of-sample using n_{eval} true conditional distributions P_{ω|x}
- This process is repeated 20 times to ensure reproducibility
- Example: Table 1 shows a contextual version of Higle and Sen (1996)'s CEP1 2SP, comparing methods across K

		$\mathbb{E}[\omega \mathbf{x}]$	MMD	Static				Dynamic			
	$\tilde{\lambda}$	-	-	0.01	0.1	1	10	0.01	0.1	1	10
	1	11.6%	0.0%	29.8%	0.2%	0.0%	0.1%	55.7%	2.1%	0.4%	0.3%
K	2 5	0.2% 0.1%	15.1% 13.9%	5.4% 0.3%	4.9% 7.9%	10.0% 11.5%	12.6% 14.2%	18.9% 17.0%	9.2% 13.2%	10.1% 9.9%	$13.8\% \\ 11.9\%$

Table: (CEP1) Fraction of instances where each method has the lowest out-of-sample 2SP cost. The regularizaton is set such that $\lambda = \text{DCSR}$ Objective * $\tilde{\lambda}$

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