

Data-Driven Conditional Robust Optimization

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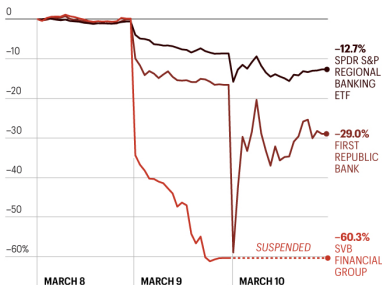
Canada

Motivating example

- Returns of different assets are unknown but may depend on historical returns, economic factors, investor sentiments via social media.
- Portfolio manager can formulate an allocation problem to minimize the value-at-risk (VaR) of the portfolio while preserving an expected return above a given target.

Bank stocks selloff resume

CUMULATIVE PRICE CHANGE SINCE MARCH 8



SOURCE: BLOOMBERG

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Investor News

@newsfilterio

Banks tumble as SVB ignites broader fears about the sector [\\$SIVB \\$FRC \\$ZION \\$SI \\$SBNY](#) newsfilter.io/articles/banks...

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What is contextual stochastic optimization?

- Optimization problems arising in practice almost always involve **unknown parameters** $\xi \in \mathbb{R}^{m_\xi}$
- Oftentimes, there is a relationship between unknown parameters and some observable **contextual data** $\psi \in \mathbb{R}^{m_\psi}$

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- **Contextual Optimization:**
 - Optimizes a policy, $\mathbf{x} : \mathbb{R}^{m_\psi} \rightarrow \mathcal{X}$
 - I.e., action $x \in \mathcal{X}$ is adapted to the observed context ψ
 - **Contextual Stochastic Optimization** problem minimizes the expected cost of running the policy over the joint distribution of (ψ, ξ) :

$$\min_{\mathbf{x}(\cdot)} \mathbb{E}[c(\mathbf{x}(\psi), \xi)] \Leftrightarrow \mathbf{x}^*(\psi) \in \arg \min_{x \in \mathcal{X}} \mathbb{E}[c(x, \xi) | \psi] \text{ a.s.}$$

(see survey Sadana et al. [2024])

What is conditional robust optimization?

- We introduce a novel **Contextual Robust Optimization** paradigm for solving contextual optimization problems in a risk-averse setting:

$$(\text{Robust-CO}) \quad \min_{\mathbf{x}(\cdot)} \max_{\psi \in \mathcal{V}, \xi \in \mathcal{U}(\psi)} c(\mathbf{x}(\psi), \xi)$$

where $\mathcal{U}(\psi)$ is a **conditional uncertainty set** designed to contain with high probability the realization of ξ conditionally on observing ψ .

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- A weak interchangeability property states:

$$\begin{aligned} \mathbf{x}^*(\cdot) \in \arg \min_{\mathbf{x}(\cdot)} \max_{\psi \in \mathcal{V}, \xi \in \mathcal{U}(\psi)} c(\mathbf{x}(\psi), \xi) \\ \Leftrightarrow \mathbf{x}^*(\psi) \in \underbrace{\arg \min_{\mathbf{x} \in \mathcal{X}} \max_{\xi \in \mathcal{U}(\psi)} c(\mathbf{x}, \xi)}_{\text{Conditional Robust Optimization (CRO)}}, \forall \psi \in \mathcal{V} \end{aligned}$$

Desirable coverage properties for $\mathcal{U}(\psi)$

The field of conformal prediction identifies two important properties for conditional uncertainty sets

- Marginal coverage property: $\mathbb{P}(\xi \in \mathcal{U}(\psi)) \geq 1 - \epsilon$
- Conditional coverage property: $\mathbb{P}(\xi \in \mathcal{U}(\psi) | \psi) \geq 1 - \epsilon$ a.s.
- Conditional coverage $\Rightarrow$ Marginal coverage

E.g., target coverage $1 - \epsilon = 90\%$:

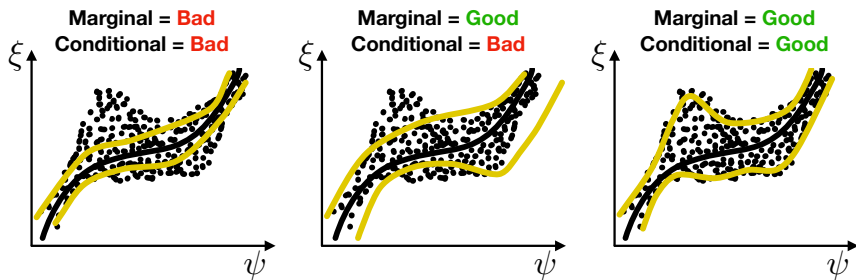


Image from Angelopoulos and Bates, A Gentle Introduction to Conformal Prediction and Distribution-Free Uncertainty Quantification, CoRR, 2021.

Related work in operations research literature

- Contextual Stochastic Optimization:
 - [Hannah et al. \[2010\]](#), [Bertsimas and Kallus \[2020\]](#), ...: Conditional distribution estimation used to formulate and solve the CSO problem.
 - [Donti et al. \[2017\]](#), [Elmachtoub and Grigas \[2022\]](#), ...: End-to-end paradigm applied to solve the data driven CSO problem.
- Distributionally Robust CSO:
 - [Bertsimas et al. \[2022\]](#), [McCord \[2019\]](#), [Wang and Jacquillat \[2020\]](#), [Kannan et al. \[2020\]](#): DRO approaches with ambiguity sets centered at the estimated conditional distribution
- Data-driven Robust Optimization:
 - [Johnstone and Cox \[2021\]](#), [Goerigk and Kurtz \[2023\]](#): learns a “non-contextual” uncertainty set using conformal prediction and NN.
 - [Ohmori \[2021\]](#), [Sun et al. \[2023\]](#), [Blanquero et al. \[2023\]](#): calibrates a set to cover the realizations of a calibrated conditional distribution
 - [Sun et al. \[2023\]](#), [Patel et al. \[2024\]](#) derive contextual sets using conformal prediction
 - [Wang et al. \[2023\]](#) learns a non-contextual set using a task-based obj. with marginal feasibility guarantees

Presentation overview

- ➊ Introduction
- ➋ Deep Data-Driven Robust Optimization (DDDRO)
- ➌ Deep Cluster then Classify (DCC) Algorithms
- ➍ Task-based CRO with Conditional Coverage
- ➎ Concluding Remarks

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Deep Data-Driven Robust Optimization (DDDRO)

- Classic **non-contextual** RO model is written as

$$\min_{x \in \mathcal{X}} \max_{\xi \in \mathcal{U}} c(x, \xi),$$

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- Goerigk and Kurtz [2023] describe the uncertainty set $\mathcal{U}$ in the form,

$$\mathcal{U}(W, R) = \{ \xi \in \mathbb{R}^{m_\xi} : \|f_W(\xi) - \bar{f}_0\| \leq R \},$$

where $f_W : \mathbb{R}^{m_\xi} \rightarrow \mathbb{R}^d$ is a deep neural network (DNN).

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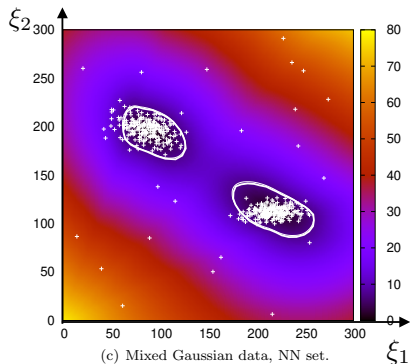
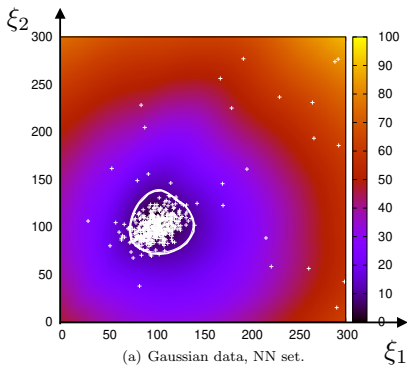
where $f_W : \mathbb{R}^{m_\xi} \rightarrow \mathbb{R}^d$ is a deep neural network (DNN).

- Given a dataset $\mathcal{D}_\xi = \{\xi_1, \xi_2 \dots \xi_N\}$, $\mathcal{U}$ is designed by training a NN to minimize the one-class classification loss

$$\min_W \frac{1}{N} \sum_{i=1}^N \|f_W(\xi_i) - \bar{f}_0\|^2,$$

where $\bar{f}_0 := (1/N) \sum_{i \in [N]} f_{W_0}(\xi_i)$ and the radius R is calibrated for $1 - \epsilon$ coverage on the data set.

Illustrative examples



Images from Goerigk and Kurtz. Data-driven robust optimization using deep neural networks. Computers and Operational Research, 151(C), 2023

Solving robust optimization with deep uncertainty sets

- When using piecewise affine activation functions, $\mathcal{U}(W, R)$ can be represented as:

$$\mathcal{U}(W, R) := \left\{ \xi \left| \begin{array}{l} \exists u \in \{0, 1\}^{d \times K \times L}, \zeta \in \mathbb{R}^{d \times L}, \phi \in \mathbb{R}^{d \times L} \\ \sum_{k=1}^K u_j^{k,\ell} = 1, \forall j, \ell \\ \phi^1 = W^1 \xi \\ \zeta_j^\ell = \sum_{k=1}^K u_j^{k,\ell} a_k^\ell \phi_j^\ell + \sum_{k=1}^K u_j^{k,\ell} b_k^\ell, \forall j, \ell \\ \phi^\ell = W^\ell \zeta^{\ell-1}, \forall \ell \geq 2 \\ \sum_{k=1}^K u_j^{k,\ell} \underline{\alpha}_k^\ell \leq \phi_j^\ell \leq \sum_{k=1}^K u_j^{k,\ell} \bar{\alpha}_k^\ell, \forall j, \ell \\ \|\zeta^L - \bar{f}_0\| \leq R \end{array} \right. \right\}$$

- The problem $\max_{\xi \in \mathcal{U}(W, R)} c(x, \xi)$ can therefore be formulated as a mixed-integer second order cone program when $c(x, \xi)$ is linear.

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- The problem $\max_{\xi \in \mathcal{U}(W, R)} c(x, \xi)$ can therefore be formulated as a mixed-integer second order cone program when $c(x, \xi)$ is linear.
- This can be integrated in a cutting plane method for solving the RO:

$$\begin{aligned} & \min_{x \in \mathcal{X}, t} \quad t \\ & \text{subject to} \quad c(x, \xi) \leq t, \forall \xi \in \mathcal{U}' \subset \mathcal{U}(W, R) \end{aligned}$$

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Deep Cluster then Classify (DCC)

- We use $\mathcal{D} := \{(\psi_1, \xi_1), \dots, (\psi_N, \xi_N)\}$ to design data-driven conditional uncertainty sets $\mathcal{U}(\psi)$.
- This approach reduces the side-information ψ to a set of K different clusters and designs customized sets, i.e., $\mathcal{U}(\psi) := \mathcal{U}_{a(\psi)}$
 - $a : \mathbb{R}^{m_\psi} \rightarrow [K]$ is a trained K -class cluster assignment function
 - Each $\mathcal{U}_k$, for $k = 1, \dots, K$, is an uncertainty sets for ξ calibrated on the dataset $\mathcal{D}_\xi^k := \cup_{(\psi, \xi) \in \mathcal{D}: a(\psi)=k} \{\xi\}$ as in Goerigk and Kurtz [2023].

Deep clustering using auto-encoder/decoder networks

We use an auto-encoder and decoder network to identify $a(\cdot)$,

$$\mathcal{L}^1(V, \theta) := \frac{1 - \alpha_K}{N} \sum_{i=1}^N \|g_{V_D}(g_{V_E}(\psi_i)) - \psi_i\|^2 \\ + \frac{\alpha_K}{N} \sum_{i=1}^N \|g_{V_E}(\psi_i) - \theta^{a(\psi_i)}\|^2,$$

where

$$a(\psi) := \underset{k \in [K]}{\operatorname{argmin}} \|g_{V_E}(\psi) - \theta^k\|$$

and V_E and V_D are the network parameters.

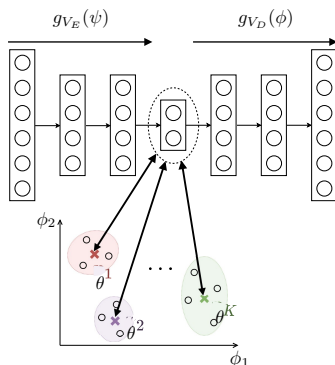


Image adapted from Fard et al. Deep k-means: Jointly clustering with k-means and learning representations. Pattern Recognition Letters, 138:185–192, 2020

Integrated DCC addresses shortcoming of DCC

- 1 DCC fails to tackle the conditional uncertainty set learning problem as a whole
 - Solution: IDCC optimizes V_E , V_D , θ , and $\{W^k\}_{k=1}^K$ jointly using a loss function that trades-off between the objectives used for clustering and each of the K versions of one-class classifiers

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- 2 DCC struggles for cases where clear separation of clusters isn't possible.
 - Solution: IDCC trains a parameterized random assignment policy $\tilde{a}(\psi) \sim \pi(\psi)$:

$$\mathbb{P}(\tilde{a}(\psi) = k) = \pi_k(\psi) := \frac{\exp\{-\beta\|g_V(\psi) - \theta^k\|^2\}}{\sum_{k'=1}^K \exp\{-\beta\|g_V(\psi) - \theta^{k'}\|^2\}}$$

The **random** uncertainty set is $\tilde{\mathcal{U}}(\psi) := \mathcal{U}(W^{\tilde{a}(\psi)}, R^{\tilde{a}(\psi)})$

Experiments

Robust portfolio optimization with market data

- Decision model:

$$x^*(\psi) := \arg \min_{x: \sum_{i=1}^n x_i = 1, x \geq 0} \max_{\xi \in \mathcal{U}(\psi)} -\xi^\top x$$

which captures the need to invest one unit of wealth among the available assets while minimizing risk exposure.

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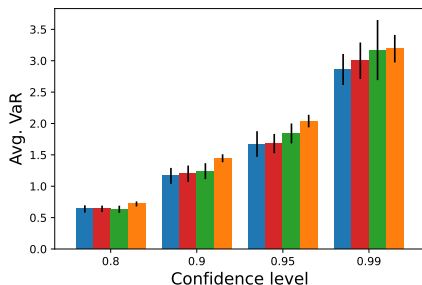
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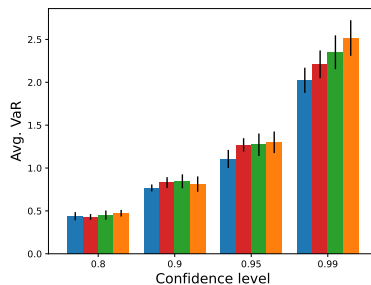
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- Performance metric: out-of-sample VaR of $-\xi^T x(\psi)$

Portfolio optimization: Comparison of avg. VaR across portfolio simulations



(a) 2018



(b) 2019

■ Ellipsoid ■ DDDRO ■ DCC ■ IDCC

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$$\mathbb{P}(\xi \in \mathcal{U}(\psi) | \tilde{a}(\psi) = k) \geq 1 - \epsilon \forall k \quad \checkmark \Rightarrow \mathbb{P}(\xi \in \mathcal{U}(\psi)) \geq 1 - \epsilon \quad \checkmark$$

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- In this next part, we propose **Task-based Conditional Robust Optimization** that promotes **performance** and **conditional coverage**.

Estimate-then-Optimize with continuous adaptation

- We consider a continuously adapted conditional ellipsoidal set:

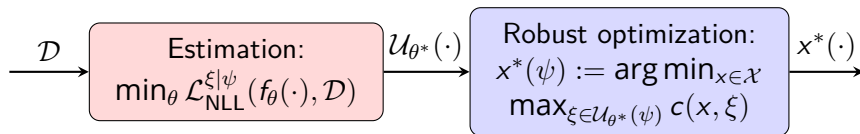
$$\mathcal{U}_\theta(\psi) := \{ \xi \in \mathbb{R}^{m_\xi} : (\xi - \mu_\theta(\psi))^T \Sigma_\theta^{-1}(\psi) (\xi - \mu_\theta(\psi)) \leq R_\theta \},$$

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- Given a data set $\mathcal{D} = \{(\psi_1, \xi_1), (\psi_2, \xi_2) \dots (\psi_N, \xi_N)\}$, an estimate-then-optimize (ETO) approach takes the form:



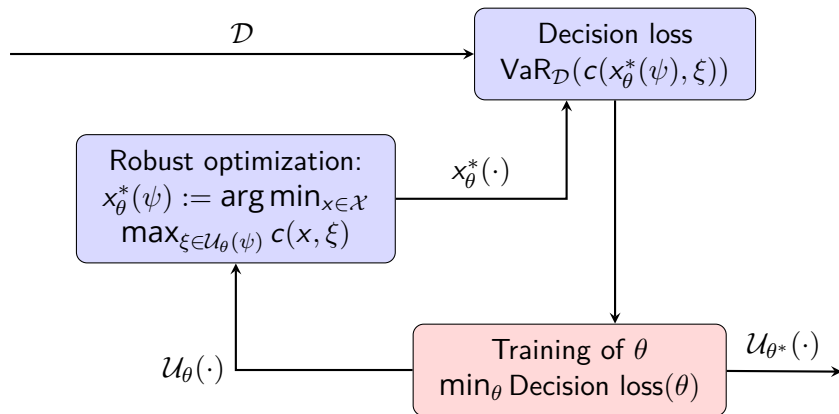
where $\mathcal{L}_{\text{NLL}}^{\xi|\psi}$ is the negative log likelihood for a conditional Gaussian density estimator (see Barratt and Boyd [2021]):

$$\xi \sim f_\theta(\psi) := \mathcal{N}(\mu_\theta(\psi), \Sigma_\theta(\psi))$$

and R_θ s.t. $\mathbb{P}_{\mathcal{D}}(\xi \in \mathcal{U}_\theta(\psi)) = 1 - \epsilon$

(Single) Task-based Set (TbS) training

A task-based approach learns the estimator by trying to minimize the decision loss, e.g. the portfolio risk based on VaR



Decision loss relaxation and derivatives

- Decision loss $\text{VaR}_{\mathcal{D}}(c(x_{\theta}^*(\psi), \xi))$ suffers from multiple local optima.



Figure 3: Simulation-based trade risk profile

Image from Mausser and Rosen, *Beyond VaR: from measuring risk to managing risk*, CIFE, 1999.

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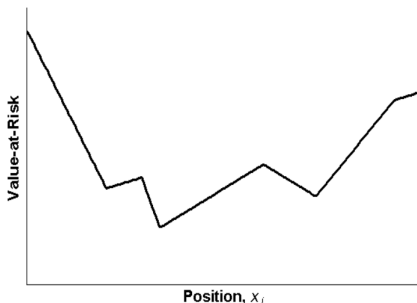


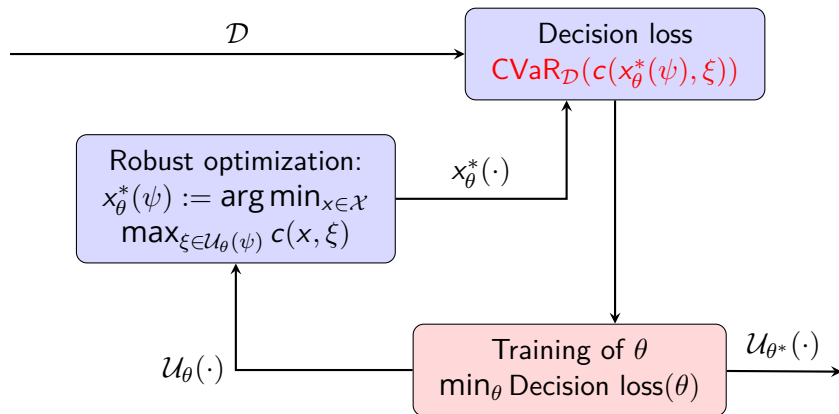
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- We therefore replace it with upper bound $\text{CVaR}_{\mathcal{D}}(c(x_{\theta}^*(\psi), \xi))$.

$$\frac{\partial \text{CVaR}_{i \sim N}(y_i)}{\partial y_i} = v_i(y) \text{ with } v(y) \in \underset{v \in \mathbb{R}_+^M: \mathbb{1}^T v = 1, v \leq ((1-\alpha)N)^{-1}}{\text{argmax}} v^T y$$

Decision loss relaxation and derivatives



Robust optimization reformulation and derivatives

- We assume that $c(x, \xi)$ is convex in x and concave in ξ , while $\mathcal{X}$ is a convex set.

Robust optimization reformulation and derivatives

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- Using Fenchel duality, one can follow Ben-Tal et al. [2015] to reformulate the robust optimization problem as:

$$x_{\theta}^*(\psi) := \arg \min_{x \in \mathcal{X}} \max_{\xi \in \mathcal{U}_{\theta}(\psi)} c(x, \xi) = \arg \min_{v, x \in \mathcal{X}} \underbrace{\delta^*(v | \mathcal{U}_{\theta}(\psi)) - c_*(x, v)}_{f(x, v, \mathcal{U}_{\theta}(\psi))}$$

where the support function

$$\delta^*(v | \mathcal{U}_{\theta}(\psi)) := \sup_{\xi \in \mathcal{U}_{\theta}(\psi)} \xi^T v = \mu^T v + \sqrt{v^T \Sigma v}$$

while the partial concave conjugate function is defined as

$$c_*(x, v) := \inf_{\xi} v^T \xi - c(x, \xi)$$

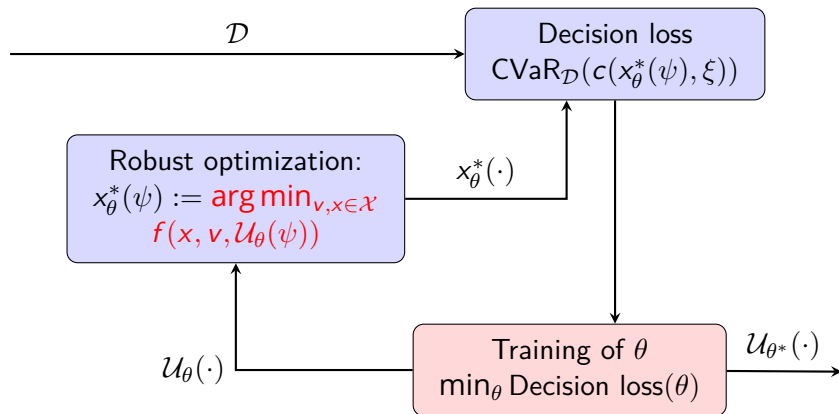
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- The derivatives of $x_{\theta}^*(\psi) := \arg \min_{v, x \in \mathcal{X}} f(x, v, \mathcal{U}_{\theta}(\psi))$ w.r.t. θ can be obtained using implicit differentiation (see Blondel et al. [2022])

Robust optimization reformulation and derivatives



Comparative study with GMM environment

- $(\psi, \xi) \in \mathbb{R}^2 \times \mathbb{R}^2$ drawn from a joint Gaussian mixture model with two modes
- Data: 600 points for training, 400 for validation, 1000 for test
- Targeted confidence level of 90%
- Average is calculated over 10 runs

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	ETO-ACPS	ETO-DbS	TbS	
Avg. CVaR	1.69 ± 0.05	1.64 ± 0.07	1.03 ± 0.10	
Avg. VaR	1.12 ± 0.04	1.07 ± 0.02	0.72 ± 0.07	
Avg. marginal cov.	$91\% \pm 1.4\%$	$85\% \pm 7.8\%$	$23\% \pm 6.1\%$	

Second-task: Conditional coverage

Lemma

An uncertainty set $\mathcal{U}_\theta(\psi)$ has an a.s. conditional coverage of $1 - \epsilon$ if and only if

$$\mathcal{L}_{CC}(\theta) := \mathbb{E}[(\mathbb{P}(\xi \in \mathcal{U}_\theta(\psi)|\psi) - (1 - \epsilon))^2] = 0$$

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$\mathcal{L}_{CC}(\theta)$ can be approximated using:

$$\hat{\mathcal{L}}_{CC}(\theta) := \mathbb{E}_{\mathcal{D}}[(g_{\phi^*(\theta)}(\psi) - (1 - \epsilon))^2]$$

where $g_{\phi^*(\theta)}(\psi) \approx \mathbb{P}(\xi \in \mathcal{U}_\theta(\psi)|\psi)$ is obtained using logistic regression of membership variable $y(\psi, \xi; \theta) := \mathbb{1}\{\xi \in \mathcal{U}_\theta(\psi)\}$ on ψ .

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$$\mathcal{L}_{CC}(\theta) := \mathbb{E}[(\mathbb{P}(\xi \in \mathcal{U}_\theta(\psi)|\psi) - (1 - \epsilon))^2] = 0$$

$\mathcal{L}_{CC}(\theta)$ can be approximated using:

$$\hat{\mathcal{L}}_{CC}(\theta) := \mathbb{E}_{\mathcal{D}}[(g_{\phi^*(\theta)}(\psi) - (1 - \epsilon))^2]$$

where $g_{\phi^*(\theta)}(\psi) \approx \mathbb{P}(\xi \in \mathcal{U}_\theta(\psi)|\psi)$ is obtained using logistic regression of membership variable $y(\psi, \xi; \theta) := \mathbb{1}\{\xi \in \mathcal{U}_\theta(\psi)\}$ on ψ .

- I.e., letting the augmented data set

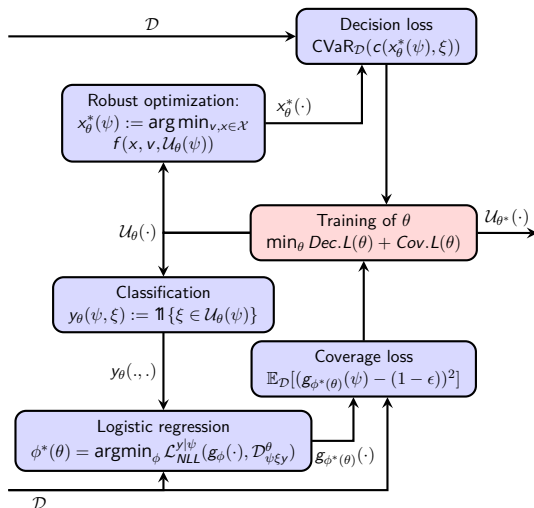
$$\mathcal{D}_{\psi\xi y}^\theta := \{(\psi_1, \xi_1, y(\psi_1, \xi_1; \theta)), \dots, (\psi_N, \xi_N, y(\psi_N, \xi_N; \theta))\},$$

one solves $\phi^*(\theta) \in \operatorname{argmin}_{\phi} \mathcal{L}_{NLL}^{y|\psi}(g_{\phi}(\cdot), \mathcal{D}_{\psi\xi y}^\theta)$ with

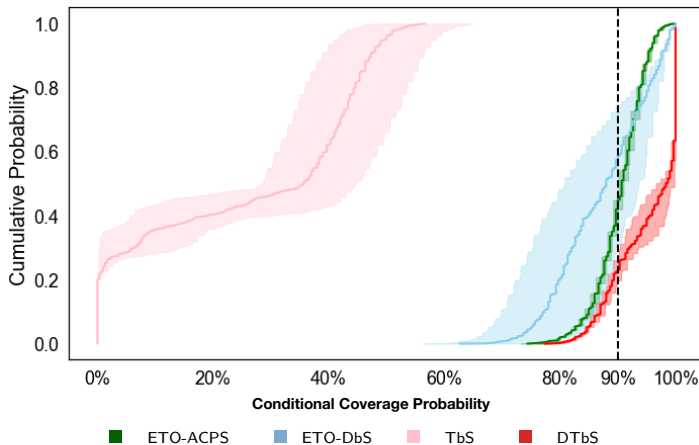
$$g_{\phi}(\psi) := \frac{1}{1 + \exp^{\phi^T \psi + \phi_0}}$$

Double Task-based Set (DTbS) training

We train $\mathcal{U}_\theta(\psi)$ using the two tasks: produce good decision + produce good conditional coverage:



Comparative study with GMM environment



(See uncertainty set animation ([url](#)))

Comparative study with GMM environment

- $(\psi, \xi) \in \mathbb{R}^2 \times \mathbb{R}^2$ drawn from a joint Gaussian mixture model with two modes
- Data: 600 points for training, 400 for validation, 1000 for test
- Targeted confidence level of 90%
- Average is calculated over 10 runs

	ETO-ACPS	ETO-DbS	TbS	
Avg. CVaR	1.69 ± 0.05	1.64 ± 0.07	1.03 ± 0.10	
Avg. VaR	1.12 ± 0.04	1.07 ± 0.02	0.72 ± 0.07	
Avg. marginal cov.	$91\% \pm 1.4\%$	$85\% \pm 7.8\%$	$23\% \pm 6.1\%$	

Comparative study with GMM environment

- $(\psi, \xi) \in \mathbb{R}^2 \times \mathbb{R}^2$ drawn from a joint Gaussian mixture model with two modes
- Data: 600 points for training, 400 for validation, 1000 for test
- Targeted confidence level of 90%
- Average is calculated over 10 runs

	ETO-ACPS	ETO-DbS	TbS	!! DTbS !!
Avg. CVaR	1.69 ± 0.05	1.64 ± 0.07	1.03 ± 0.10	1.08 ± 0.13
Avg. VaR	1.12 ± 0.04	1.07 ± 0.02	0.72 ± 0.07	0.75 ± 0.10
Avg. marginal cov.	$91\% \pm 1.4\%$	$85\% \pm 7.8\%$	$23\% \pm 6.1\%$	$92\% \pm 1.5\%$

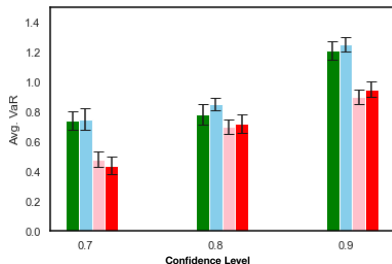
Portfolio optimization with market data

- Contextual info: Trading volume, volatility index (VIX), 10-year treasury yield index (TNX), oil index (CLF), S&P 500 (GSPC), gold price (GC=F), Dow Jones (DJI).
- Market data from Yahoo! Finance: 70 different stocks during period from 01/01/2012 to 31/12/2019 (2017-2019 reserved for test).
- Target confidence level of 70%, 80%, or 90%

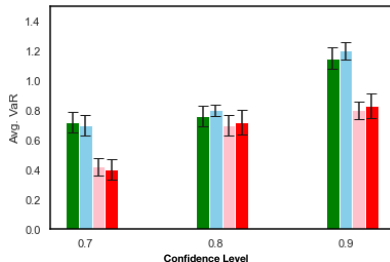
Model	Marginal coverage					
	2018			2019		
	70%	80%	90%	70%	80%	90%
ETO-ACPS	68%	78%	87%	71%	78%	89%
ETO-DbS	59%	75%	87%	61%	76%	86%
TbS	23%	24%	29%	26%	30%	32%
DTbS	71%	80%	93%	69%	78%	92%

Portfolio optimization with market data

- Contextual info: Trading volume, volatility index (VIX), 10-year treasury yield index (TNX), oil index (CLF), S&P 500 (GSPC), gold price (GC=F), Dow Jones (DJI).
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(a) 2018



(b) 2019

■ ETO-ACPS

■ ETO-DbS

■ TbS

■ DTbS

Outline

- 1 Introduction
- 2 Deep Data-Driven Robust Optimization (DDDRO)
- 3 Deep Cluster then Classify (DCC) Algorithms
- 4 Task-based CRO with Conditional Coverage
- 5 Concluding Remarks

Concluding remarks

- We introduced a new contextual robust optimization approach for solving risk averse contextual optimization problems.
- In CRO, deep neural networks can be used to:
 - Represent richly structured uncertainty sets, e.g. DDDRO, IDCC
 - Adapt uncertainty set continuously to covariates, e.g. ETO-ACPS,..., DTbS.
- Two types of training procedures: “Estimate-then-optimize” vs. “Task-based”
- Two types of training objectives:
 - Statistical performance: achieving the right marginal/conditional coverage
 - Decision performance: producing decisions that achieve low VaR/CVaR

Thank you

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