AAAI 2023 Optimization with Constraint Learning Lab
Part III: Solution Quality

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Overview

Mathematical Decision Optimization (DO)

Mathematical Decision-Optimization (DO) Model $M(\mathbf{w})$ (*):

$$\begin{aligned} \mathbf{x}^*(\mathbf{w}) \in \arg\min_{\mathbf{x}\in\mathbb{R}^n, \mathbf{y}\in\mathbb{R}^m} \quad & f(\mathbf{x}, \mathbf{y}, \mathbf{w}) \\ \text{s.t.} \quad & \mathbf{g}(\mathbf{x}, \mathbf{y}, \mathbf{w}) \leq \mathbf{0} \\ & \mathbf{y} = \mathbf{h}(\mathbf{x}, \mathbf{w}) \\ & \mathbf{x} \in \Omega(\mathbf{w}) \end{aligned}$$

$\mathbf{w} \in \mathbb{R}^k$ – fixed uncontrollable.
$\Omega(\mathbf{w})$ – polytope (possibly unbounded).

(*) Maragno*, D., Wiberg*, H., Bertsimas, D., Birbil, S. I., Hertog, D. d., and Fajemisin, A. (2021). *Mixed-Integer Optimization with Constraint Learning*.

Mathematical Decision Optimization (DO)

Learned DO Model $\widehat{M}(\mathbf{w})$:

$$
\begin{aligned}
\widehat{\mathbf{x}}(\mathbf{w}) \in \arg\min_{\mathbf{x}\in\mathbb{R}^n,\mathbf{y}\in\mathbb{R}^m} \quad & \widehat{f}(\mathbf{x},\mathbf{y},\mathbf{w}) && \Longleftarrow \text{learn} \\
\text{s.t.} \quad & \mathbf{g}(\mathbf{x},\mathbf{y},\mathbf{w}) \leq \mathbf{0} \\
& \mathbf{y} = \widehat{\mathbf{h}}(\mathbf{x},\mathbf{w}) && \Longleftarrow \text{learn} \\
& \mathbf{x} \in \Omega(\mathbf{w})
\end{aligned}
$$

$\mathbf{w} \in \mathbb{R}^k$ – fixed uncontrollable.
$\Omega(\mathbf{w})$ – polytope (possibly unbounded).

– UN World Food Programme (INFORMS Edelman Award 2021): Food palatability prediction in food basket cost minimization.
– Louisville Metropolitan Sewer District and Tetra Tech (INFORMS Edelman Award 2019 Finalist): Rainfall prediction in wastewater storage maximization.

Solution Quality

What We **Want**:

$$\widehat{\mathbf{x}} = \widehat{\mathbf{x}}(\mathbf{w}), \quad \widehat{\mathbf{y}} = \mathbf{h}(\widehat{\mathbf{x}}, \mathbf{w})$$
$$\mathbf{x} = \mathbf{x}(\mathbf{w}), \quad \mathbf{y} = \mathbf{h}(\mathbf{x}, \mathbf{w})$$

(a) close to optimum

$$f(\widehat{\mathbf{x}}, \widehat{\mathbf{y}}, \mathbf{w}) - f(\mathbf{x}, \mathbf{y}, \mathbf{w}) \leq \epsilon$$

(b) feasible

$$\mathbf{g}(\widehat{\mathbf{x}}, \widehat{\mathbf{y}}, \mathbf{w}) \leq \mathbf{0}$$

Solution Quality

What We **Can**:

known policy: $\mathbf{x}_0 = \mathbf{x}_0(\mathbf{w}), \mathbf{y}_0 = \mathbf{h}(\mathbf{x}_0, \mathbf{w})$

(a) improve upon policy

$$\Pr[f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{w}) - f(\widehat{\mathbf{x}}, \widehat{\mathbf{h}}(\widehat{\mathbf{x}}, \mathbf{w}), \mathbf{w}) \geq \epsilon] \geq (1 - \delta_1)$$

(b) likely feasible

$$\Pr[\mathbf{g}(\widehat{\mathbf{x}}, \widehat{\mathbf{h}}(\widehat{\mathbf{x}}, \mathbf{w}), \mathbf{w}) \leq \mathbf{0}] \geq (1 - \delta_2)$$

Solution Quality

What We **Can**:

known policy: $\mathbf{x}_0 = \mathbf{x}_0(\mathbf{w}), \mathbf{y}_0 = \mathbf{h}(\mathbf{x}_0, \mathbf{w})$

(a) improve upon policy: Probability of Improvement (PoI)

$$\Pr[f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{w}) - f(\widehat{\mathbf{x}}, \widehat{\mathbf{h}}(\widehat{\mathbf{x}}, \mathbf{w}), \mathbf{w}) \geq \epsilon] \geq (1 - \delta_1)$$

(b) likely feasible: Probability of Constraint Satisfaction (PoCS)

$$\Pr[\mathbf{g}(\widehat{\mathbf{x}}, \widehat{\mathbf{h}}(\widehat{\mathbf{x}}, \mathbf{w}), \mathbf{w}) \leq \mathbf{0}] \geq (1 - \delta_2)$$

PoI and PoCS

Gaussian Process: f as a "random variable".

$$f|D \sim GP$$

$\implies$ Value @ point $(\mathbf{x}, \mathbf{y}, \mathbf{w})$

$$f(\mathbf{x}, \mathbf{y}, \mathbf{w}) \sim \mathcal{N}(\mu_{GP}(\mathbf{x}, \mathbf{y}, \mathbf{w}), \sigma^2_{GP}(\mathbf{x}, \mathbf{y}, \mathbf{w}))$$

$\implies$ Value @ 2 points $(\mathbf{x}', \mathbf{y}', \mathbf{w}'), (\mathbf{x}'', \mathbf{y}'', \mathbf{w}'')$

$$(f(\mathbf{x}', \mathbf{y}', \mathbf{w}'), f(\mathbf{x}'', \mathbf{y}'', \mathbf{w}'')) \sim \mathcal{N}(\boldsymbol{\mu}_{GP}, \boldsymbol{\Sigma}_{GP})$$

$\implies$ PoI and PoCS estimation

Demo: Go to `ocl_lab/POI/poi.ipynb`.

Use Case

World Food Program (WFP) food basket optimization problem.(*)

Model $\widehat{WFP}$ (**):

$$
\begin{array}{llll}
\text{optimal basket} & \widehat{\mathbf{x}} \in \arg\min_{\mathbf{x}\in\mathbb{R}^n, y\in\mathbb{R}} & \mathbf{c}^T\mathbf{x} & \text{minimize cost} \\
& \text{s.t.} & V\mathbf{x} \geq \mathbf{r} & \text{nutritional reqs} \\
& & y \geq t & \text{palatability constraint} \\
& & y = \widehat{h}(\mathbf{x}) & \text{learned palatability} \\
& & \mathbf{x} \in \Omega & \text{non-negativity}
\end{array}
$$

$n = 25$ - number of foods in basket.
$V_{i,j}$ - value of nutrient i in food j; $\mathbf{r}_i$ - nutrient i requirement.

(*) Peters et al. (2021). *The Nutritious Supply Chain: Optimizing Humanitarian Food Assistance.*
(**) Maragno, Wiberg (2021). *OptiCL: Mixed-integer Optimization with Constraint Learning.*

Use Case

Comparing Learned DO Models

Model ($t = 0.5$)	**Objective**	**Palatability**	**PoCS**
OptiCL baseline	3212.5	0.01	0
OptiCL w/ Trust Region	3431	0.55	0.99

Use Case

Objective values (Obj), ground truth palatability (GT), and PoCS of solutions $\widehat{\mathbf{x}}$ for palatability thresholds $t = 0.6, 0.7, 0.75$.

t	OptiCL $\widehat{\mathbf{x}}^*$			OptiCL + TR $\widehat{\mathbf{x}}^*$		
	Obj	GT	PoCS	Obj	GT	PoCS
0.6	3227	0.03	0.0	3446	0.55	0.11
0.7 (I)	3380	0.61	0.0	3531	0.67	0.25
0.7 (II)	3398	0.64	0.0	3542	0.7	0.99
0.75	3492	0.71	0.37	3678	0.65	0.0

	Accuracy	FP	FN
PoCS ≥ 0.8	93.9%	0.36%	5.71%
PoCS ≥ 0.5	94.2%	2.62%	3.21%