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

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Overview

1. Decision Optimization
2. Solution Quality
3. PoI and PoCS
4. Use Case

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 $\widehat{M}(\mathbf{w})$:

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

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

– UN World Food Programme (INFORMS Edelman Award 2021): Food palatibility 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

$$f(\widehat{\mathbf{x}}^*, \widehat{\mathbf{y}}^*, \mathbf{w}) - f(\mathbf{x}^*, \mathbf{y}^*, \mathbf{w}) \le \epsilon$$

(b) feasible

$$\mathbf{g}(\widehat{\mathbf{x}}^*, \widehat{\mathbf{y}}^*, \mathbf{w}) \le \mathbf{0}$$

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".

$$f|D \sim GP$$

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

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

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

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

$\Longrightarrow$ PoI and PoCS estimation

Hands-on 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**	**Platibility**	**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 scores (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%