Surrogate policies with generalization guarantees for combinatorial optimization problems

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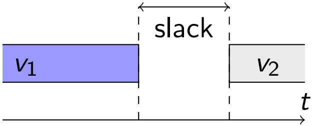
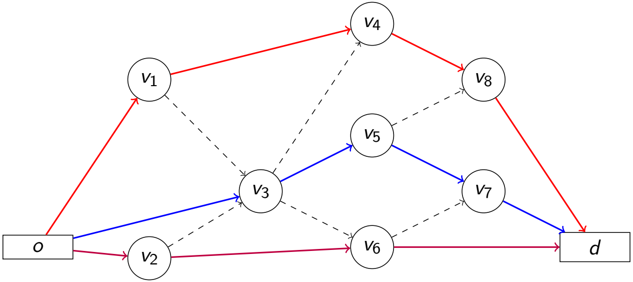
Stochastic Vehicle Scheduling Problem



$$c_p = \text{vehicle cost} + \mathbb{E}(\text{propagated delay cost})$$
$$= c^{\mathrm{veh}} + \frac{1}{|\Omega|}\sum_{\omega\in\Omega}\sum_{v\in P}\xi_v^P(\omega)$$

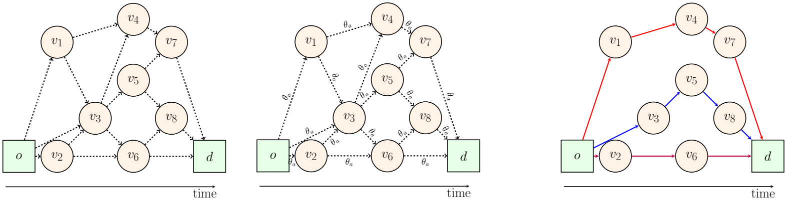
Reduce costs dues to delay propagation along rotations

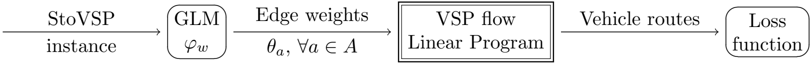


$$\min \sum_{P\in\mathcal{P}} c_P z_y$$
$$\sum_{P\ni v} y_P = 1 \quad \forall v$$
$$y_P \in \{0,1\}$$

Challenge: no more than a single deterministic resolution on industrial instances

Decision aware learning for Stochastic VSP





$$\theta_a = \langle w | \phi(a, x) \rangle$$

Excellent performance on large scale instances[1]

[1] A. P. "Learning to Approximate Industrial Problems by Operations Research Classic Problems". In: *Operations Research* (Apr. 2021), Guillaume Dalle et al. *Learning with Combinatorial Optimization Layers: A Probabilistic Approach*. July 2022. eprint: 2207.13513.

Surrogate policies for combinatorial optimization

Given an instance $\boldsymbol{x}$ in $\mathcal{X}$

$$\min_{\boldsymbol{y} \in \mathcal{Y}(\boldsymbol{x})} f^0(\boldsymbol{y}, \boldsymbol{x})$$

$\mathcal{Y}(x)$ finite but combinatorially large

Policy $\ h : \boldsymbol{x} \in \mathcal{X} \mapsto \boldsymbol{y} \in \mathcal{Y}(\boldsymbol{x})$ in $\mathcal{H}$

Risk with respect to distribution on X

$$\min_{h \in \mathcal{H}} R(h) = \mathbb{E}\Big(f^0\big(h(\boldsymbol{x}), x\big)\Big)$$

Distribution $\mathbb{P}_X$ unknown.

Training set $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$

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Parametric hypothesis class $\mathcal{H}$

$$\big\{h_{\boldsymbol{w}} \;:\; \boldsymbol{x} \in \mathcal{X} \mapsto \hat{\boldsymbol{y}}(\psi_{\boldsymbol{w}}(\boldsymbol{x})) \in \mathcal{Y}(\boldsymbol{x}) \,,\; \boldsymbol{w} \in \mathcal{W}\big\}$$

which embeds linear optimization

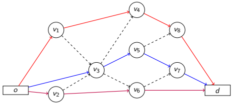
$$\hat{\boldsymbol{y}}(\boldsymbol{\theta}) \in \arg\max_{\boldsymbol{y} \in \mathcal{Y}(\boldsymbol{x})} \langle \boldsymbol{y}, \boldsymbol{\theta} \rangle$$

Learning problem: minimize empirical risk

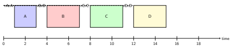
$$\min_{\boldsymbol{w} \in \mathcal{W}} \mathcal{R}_n(h_{\boldsymbol{w}}) = \frac{1}{n} \sum_{i=1}^{n} f^0\big(h_{\boldsymbol{w}}(X_i), X_i\big)$$

$$h_{\boldsymbol{w}} : \xrightarrow[\text{Instance data}]{\boldsymbol{x} \in \mathcal{X}} \boxed{\begin{array}{c}\text{Statistical model}\\ \psi_{\boldsymbol{w}}\end{array}} \xrightarrow[\text{Cost vector}]{\theta \in \mathbb{R}^{d(x)}} \boxed{\begin{array}{c}\text{CO algorithm}\\ \hat{\boldsymbol{y}}(\boldsymbol{\theta}) \in \arg\max_{\boldsymbol{y} \in \mathcal{Y}(\boldsymbol{x})} \langle \boldsymbol{y}, \boldsymbol{\theta} \rangle\end{array}} \xrightarrow[\text{Solution}]{y \in \mathcal{Y}(x)}$$

Stochastic VSP [7]

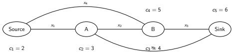


Machine Scheduling [8]

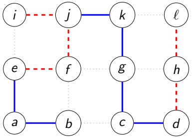


Paths in images [3]

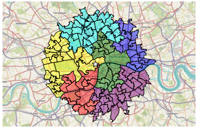
Multiflow network design [4]



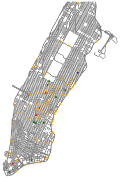
Network Design [3]



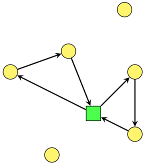
Districting [1]



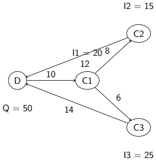
AMoD Fleet [6]



Dynamic Vehicle Routing (*) [2]



Dynamic inventory routing [5]



(*) Winner `https://euro-neurips-vrp-2022.challenges.ortec.com/`

Contextual Stochastic optimization[2]

Unknown distribution $\mathbb{P}$ over (X, ξ)

$\tilde{\boldsymbol{x}} \in \mathcal{X}$ observed context

$\boldsymbol{\xi}$ unobserved noise

$$\min_{h \in \mathcal{H}} \mathbb{E}\left[f^{\mathrm{c}}\left(h(\tilde{X}), \tilde{X}, \xi\right)\right]$$

Training set $\tilde{\boldsymbol{x}}_1, \boldsymbol{\xi}_1, \ldots, \tilde{\boldsymbol{x}}_n, \boldsymbol{\xi}_n$

Optimal policy

$$h^\star : \tilde{\boldsymbol{x}} \longmapsto \underset{\boldsymbol{y} \in \mathcal{Y}(\tilde{\boldsymbol{x}})}{\arg\min}\, \mathbb{E}\left[c\left(h(\tilde{X}), \tilde{X}, \xi\right) \middle| \tilde{X} = \tilde{\boldsymbol{x}}\right]$$

Requires conditional $\mathbb{P}(\xi | X = \boldsymbol{x})$

SAA computationally intractable

[2] Utsav Sadana et al. "A survey of contextual optimization methods for decision-making under uncertainty". In: *European Journal of Operational Research* (2024).

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Optimal policy

$$h^{\star} : \tilde{\boldsymbol{x}} \longmapsto \operatorname*{arg\,min}_{\boldsymbol{y} \in \mathcal{Y}(\tilde{\boldsymbol{x}})} \mathbb{E}\Big[c\big(h(\tilde{X}), \tilde{X}, \xi\big) \Big| \tilde{X} = \tilde{\boldsymbol{x}}\Big]$$

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$$h_{\boldsymbol{w}} : \xrightarrow[\text{Context data}]{\tilde{\boldsymbol{x}} \in \mathcal{X}} \boxed{\begin{array}{c}\text{Statistical model} \\ \psi_{\boldsymbol{w}}\end{array}} \xrightarrow[\text{Cost vector}]{\theta \in \mathbb{R}^{d(x)}} \boxed{\begin{array}{c}\text{CO algorithm} \\ \hat{\boldsymbol{y}}(\boldsymbol{\theta}) \in \operatorname*{arg\,max}_{\boldsymbol{y} \in \mathcal{Y}(\tilde{\boldsymbol{x}})} \langle \boldsymbol{y}, \boldsymbol{\theta} \rangle\end{array}} \xrightarrow[\text{Solution}]{y \in \mathcal{Y}(\tilde{\boldsymbol{x}})}$$

Reduction to our setting: $\boldsymbol{x} = (\tilde{\boldsymbol{x}}, \boldsymbol{\xi})$ and $f^{0}(\boldsymbol{y}, \boldsymbol{x}) = f^{c}(\boldsymbol{y}, \tilde{\boldsymbol{x}}, \boldsymbol{\xi})$

Statistical model $\psi_{\boldsymbol{w}}$ relies only on context $\tilde{\boldsymbol{x}}$

[2] Utsav Sadana et al. "A survey of contextual optimization methods for decision-making under uncertainty". In: *European Journal of Operational Research* (2024).

How to train such policies ?

Challenge

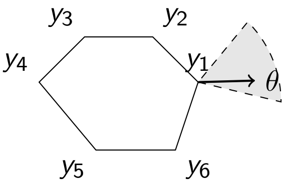
$$\xrightarrow[\text{Cost vector}]{\boldsymbol{\theta} \in \mathbb{R}^{d(x)}} \boxed{\begin{array}{c}\text{CO oracle} \\ \hat{\boldsymbol{y}}(\boldsymbol{\theta}) \in \underset{\boldsymbol{y} \in \mathcal{Y}(\boldsymbol{x})}{\arg\max}\, \boldsymbol{\theta}^\top \boldsymbol{y}\end{array}} \xrightarrow[\text{Solution}]{\boldsymbol{y} \in \mathcal{Y}(\boldsymbol{x})}$$

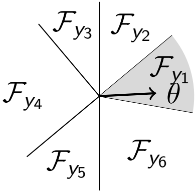
Learning problem

$$\min_{\boldsymbol{w} \in \mathcal{W}} \mathcal{R}_n(h_{\boldsymbol{w}})$$

with

$$\mathcal{R}_n(h_{\boldsymbol{w}}) = \frac{1}{n} \sum_{i=1}^{n} f^0\big(h_{\boldsymbol{w}}(X_i), X_i\big)$$





CO oracle $\hat{\boldsymbol{y}}$ is piecewise constant on the normal fan

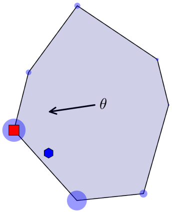
$\nabla_\theta f = 0$ almost everywhere

Perturb linear optimization in empirical risk minimization

Perturb $\boldsymbol{\theta}$ in linear optimization $\max\limits_{\boldsymbol{y}\in\mathcal{Y}(\boldsymbol{x})} \boldsymbol{\theta}^\top \boldsymbol{y}$ to get a smoother regret

$$p_0(\boldsymbol{y}|\boldsymbol{\theta}) = \mathbb{1}\Big(\boldsymbol{y} = \arg\max \boldsymbol{\theta}^\top y\Big)$$

$$p_\lambda(\boldsymbol{y}|\boldsymbol{\theta}) = \mathbb{E}_Z[p_0(\boldsymbol{y}|\boldsymbol{\theta} + \lambda Z(\boldsymbol{x}))]$$



$$\hat{\boldsymbol{y}}(\boldsymbol{\theta}) = \sum_{\boldsymbol{y}\in\mathcal{Y}} p_0(\boldsymbol{y}|\boldsymbol{\theta})\delta_{\boldsymbol{y}}$$

$$f(\hat{\boldsymbol{y}}(\boldsymbol{\theta})) = \sum_{\boldsymbol{y}\in\mathcal{Y}(\boldsymbol{x})} p_0(\boldsymbol{y}|\boldsymbol{\theta}) f(\boldsymbol{y})$$

$Z(\boldsymbol{x}) \sim RU$ where U uniform on the sphere, R random scalar indep. of U

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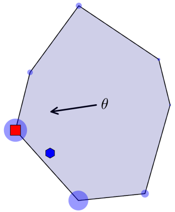

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$Z(\boldsymbol{x}) \sim RU$ where U uniform on the sphere, R random scalar indep. of U

Replace $\min_{\boldsymbol{w}\in\mathcal{W}} \mathcal{R}_n(h_{\boldsymbol{w}})$

$$\mathcal{R}_n(h_{\boldsymbol{w}}) = \frac{1}{n}\sum_{i=1}^n f^0\Big(\hat{\boldsymbol{y}}\big(\psi_{\boldsymbol{w}}(X_i)\big), X_i\Big)$$

by $\min_{\boldsymbol{w}\in\mathcal{W}} \mathcal{R}_{n\lambda}(h_{\boldsymbol{w}})$

$$\mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}}) = \frac{1}{n}\sum_{i=1}^n \mathbb{E}_Z\Big\{\big[f^0(\hat{\boldsymbol{y}}(\psi_{\boldsymbol{w}}(X_i) + \lambda Z(X_i)), X_i)\big]\Big\}$$

Which guarantees can we obtain for the policy returned by our learning algorithm ?

$$\min_{\boldsymbol{w}\in\mathcal{W}} \mathcal{R}_{n\lambda}(h_{\boldsymbol{w}}) \quad \text{with} \quad \mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}}) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{E}_Z\Big\{\big[f^0(\hat{\boldsymbol{y}}(\psi_{\boldsymbol{w}}(X_i)+\lambda Z(X_i)), X_i)\big]\Big\}$$

Risks and estimators

$$\bar{\mathcal{R}} = \mathbb{E}\Big[\min_{\boldsymbol{y}\in\mathcal{Y}(x)} f^0(\boldsymbol{y}, X)\Big]$$

$$\mathcal{R}_t(h_{\boldsymbol{w}}) = \mathbb{E}_{X,Z}\big[f^0(\hat{\boldsymbol{y}}(\psi_{\boldsymbol{w}}(X) + tZ(X)), X)\big]$$

$$\mathcal{R}_{n,t}(h_{\boldsymbol{w}}) = \frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_Z\Big[f^0(\hat{\boldsymbol{y}}(\psi_{\boldsymbol{w}}(X_i) + tZ(X_i)), X_i)\Big]$$

$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}\in\mathcal{W}} \mathcal{R}_0(h_{\boldsymbol{w}})$		opt. pol
$\boldsymbol{w}_{n,\lambda} = \arg\min_{\boldsymbol{w}\in\mathcal{W}} \mathcal{R}_{n\lambda}(h_{\boldsymbol{w}})$		learn. opt.
$\boldsymbol{w}_{n,\lambda}^{\mathrm{alg}}$:	learning algorithm	result

$$\begin{aligned}
0 \le \mathcal{R}_0(h_{\boldsymbol{w}_{n,\lambda}^{\mathrm{alg}}}) - \bar{\mathcal{R}} = {} & \underbrace{\mathcal{R}_0(h_{\boldsymbol{w}_{M,n,\lambda}}) - \mathcal{R}_\lambda(h_{\boldsymbol{w}_{M,n,\lambda}})}_{\text{Pert. bias Theorem}} + \underbrace{\mathcal{R}_\lambda(h_{\boldsymbol{w}_{M,n,\lambda}}) - \mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}_{M,n,\lambda}})}_{\text{Emp. process Theorem}} \\
& + \underbrace{\mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}_{M,n,\lambda}}) - \mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}_{n,\lambda}})}_{\text{K-SoS alg. Theorem}} + \underbrace{\mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}_{n,\lambda}}) - \mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}^\star})}_{\le 0} \\
& + \underbrace{\mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}^\star}) - \mathcal{R}_\lambda(h_{\boldsymbol{w}^\star})}_{\text{Emp. process Theorem}} + \underbrace{\mathcal{R}_\lambda(h_{\boldsymbol{w}^\star}) - \mathcal{R}_0(h_{\boldsymbol{w}^\star})}_{\text{Pert. bias Theorem}} \\
& + \underbrace{\mathcal{R}_0(h_{\boldsymbol{w}^\star}) - \bar{\mathcal{R}}}_{\text{Model bias.}}
\end{aligned}$$

Theorem Aubin-Frankowski, De Castro, P., and Rudi, 2024+

Let $0 \geq 0$ and $\lambda > 0$ be such that $\lambda \geq 0$. Let $\tau \in (0,1)$. Under conditions detailed later, there exists a constant $C > 0$ that depends only on ε, τ and f^0 such that for any $\boldsymbol{w} \in \mathcal{W}$ and $n \geq 1$, one has

$$|\mathcal{R}_0(h_{\boldsymbol{w}}) - \mathcal{R}_\lambda(h_{\boldsymbol{w}})| = C\lambda^\tau \mathrm{polylog}(\lambda) \quad \text{(Perturbation bias Theorem)}$$

$$|\mathcal{R}_\lambda(h_{\boldsymbol{w}}) - \mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}})| = \mathcal{O}_{\mathbb{P}}\left(\frac{1}{\lambda\sqrt{n}}\right) \quad \text{(Empirical process Theorem)}$$

and, for $h_{\boldsymbol{w}_{n,\lambda}}$ given by the kernel Sum-of-Squares estimate solution to $\min_{\boldsymbol{w}\in\mathcal{W}} \mathcal{R}_{n,\lambda}$,

$$|\mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}_{M,n,\lambda}}) - \mathcal{R}_{n,\lambda}(h_{\boldsymbol{w}_{n,\lambda}})| = \mathcal{O}_{\mathbb{P}}\left(\frac{1}{\lambda^{s-\frac{d}{2}}}\right) \quad \text{(K-SoS Theorem)}$$

where $\mathrm{polylog}(\lambda)$ is a polynomial logarithm term and $s > d/2$ is some tuning parameter on the order of regularity of the admissible functions.

Large data regime

The theorem yields the following bound

$$0 \leq \mathcal{R}_0(h_{\boldsymbol{w}_{n,\lambda}^{\mathrm{alg}}}) - \bar{\mathcal{R}} \leq C\lambda^{\tau}\mathrm{polylog}(\lambda) + \mathcal{O}_{\mathbb{P}}\left(\frac{1}{\lambda\sqrt{n}}\right) + \mathcal{O}_{\mathbb{P}}\left(\frac{1}{\lambda^{s-\frac{d}{2}}}\right) + \mathcal{R}_0(h_{\boldsymbol{w}^\star}) - \bar{\mathcal{R}}$$

Optimizing over λ, we get

$$\mathcal{R}_0(h_{\boldsymbol{w}_{n,\lambda}^{\mathrm{alg}}}) - \bar{\mathcal{R}} \underset{n\to\infty}{\longrightarrow} \mathcal{R}_0(h_{\boldsymbol{w}^\star}) - \bar{\mathcal{R}}$$

Contextual stochastic optimization

$$\min_{h \in \mathcal{H}} \mathbb{E}_{X,\xi}\Big[f^{\mathrm{c}}\big(h(\tilde{X}), \tilde{X}, \xi\big)\Big]$$

SAA learning of our policy

$$\min_{\boldsymbol{w}} \sum_{i=1}^{n} \mathbb{E}_{Z}\Big[f^{\mathrm{c}}\big(h_{\boldsymbol{w}}(\tilde{\boldsymbol{x}}_i), \tilde{\boldsymbol{x}}_i, \boldsymbol{\xi}_i\big)\Big]$$

Theorem applies: Convergence to optimal policy (with model bias) in large data regime

SAA in learning (across context) instead of SAA in policy (conditional to context)

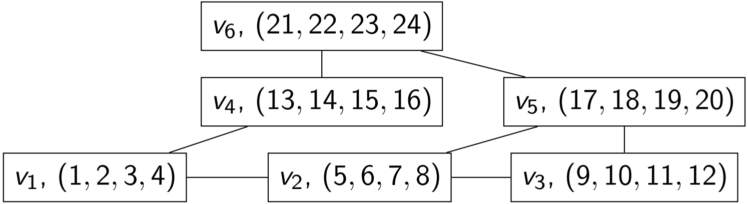
- No model needed on (X, ξ)
- CSO equivalent of a discriminative approach (by opposition to generative)

Assumption on problem

Assumption on instances and f^0 Partition

- There is a finite partition $\mathcal{G}$ of $\mathcal{X}$ into $(\mathcal{X}_G)_{G\in\mathcal{G}}$ such that $\mathcal{Y}(\boldsymbol{x})$ are constant and finite for all $\boldsymbol{x} \in \mathcal{X}_G$;
- The absolute value of the target function $|f^0|$ is uniformly bounded on $\mathcal{X}_G$ for each $G \in \mathcal{G}$ and, hence, its oscillation is finite, $\operatorname{osc}(f^0) < \infty$, with

$$\operatorname{osc}(f^0) := \sup f^0 - \inf f^0 .$$



Instance : Labelled graph

Feasible solutions : depend only on graph

Assumptions on statistical model and perturbation

Assumption on statistical model Lipschitz

For all $\boldsymbol{x} \in \mathcal{X}$, the function $\boldsymbol{w} \in \mathcal{W} \mapsto \psi_{\boldsymbol{w}}(\boldsymbol{x}) \in \mathbb{R}^{d(\boldsymbol{x})}$ is $L_{\mathcal{W}}$-Lipschitz continuous with a constant $L_{\mathcal{W}}$ which does not depend on $\boldsymbol{x}$.

Assumption on perturbation Gaussian

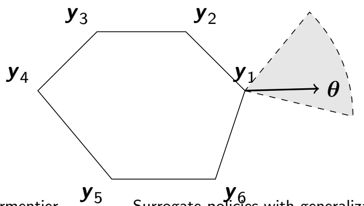
$$\forall \boldsymbol{x} \in \mathcal{X}_G\,, \quad \sqrt{d(G)}Z(\boldsymbol{x}) \sim \mathcal{N}(0, \mathrm{Id}_{d(G)})\,.$$

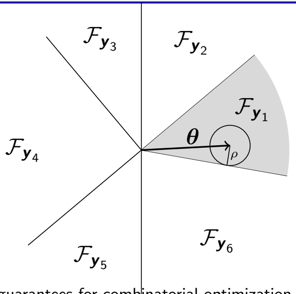
Under these assumptions, there exists an optimal $\boldsymbol{w}^\star \in \mathcal{W}$ and $\min_{\boldsymbol{w}\in\mathcal{W}} \mathcal{R}_{n,0}(h_{\boldsymbol{w}})$ has a minimizer.

Proposition Uniform Weak Moment Property

Under the previous assumptions, for all $\tau \in (0,1)$, it exists a positive constant $C_{0,\tau} > 0$ such that

$$\forall \boldsymbol{w} \in \mathcal{W}\,,\ \mathbb{E}_{X,Z}\left[\left(\frac{\rho(\psi_{\boldsymbol{w}}(X) + 0Z(X))}{\sqrt{d(X)}}\right)^{-\tau}\right] \leq C_{0,\tau}\,.$$





Key property to bound perturbation bias

$$|\mathcal{R}_0(h_{\boldsymbol{w}}) - \mathcal{R}_\lambda(h_{\boldsymbol{w}})|$$

Empirical process

To control the random variable

$$\Delta_n = \sup_{\boldsymbol{w} \in \mathcal{W}} \left| \mathcal{R}_{n,\lambda}(\boldsymbol{w}) - \mathcal{R}_\lambda(\boldsymbol{w}) \right| .$$

We use

- Bernstein inequality
- Dudley's entropy the partition assumption on

Partition assumption on oscillation function

$$\operatorname{osc}(f^0) := \sup f^0 - \inf f^0 .$$

And Lipschitz and Gauss assumption

to obtain: For all $\delta \in (0,1)$, it holds that

$$\Delta_n = \sup_{\boldsymbol{w} \in \mathcal{W}} \left| \mathcal{R}_{n,\lambda}(\boldsymbol{w}) - \mathcal{R}_\lambda(\boldsymbol{w}) \right| \leq \frac{\operatorname{osc}(f^0)}{\lambda \sqrt{n}} \left((\ln 2)^{\frac{-3}{4}} L_{\mathcal{W}} \mathcal{I}_{\mathcal{W}} \sqrt{d(\mathcal{X})} + 4 \sqrt{\ln \frac{8}{\delta}} \right),$$

with probability higher than $1 - \delta$.

Kernel Sum-of-Squares

Kernel Sum-of-Squares[3] (K-SoS) algorithm to solve

$$\min_{\boldsymbol{w}} \mathcal{R}_{n,\lambda}(\boldsymbol{w})$$

Exploit the smoothness to prove polynomial convergence

Practical performance

- comparable to a simple black box heuristic
- works when dimension of $\boldsymbol{w}$ is not too large (≤ 50)

Working with more specific problems enable deep learning compatible algorithms

[3] Alessandro Rudi, Ulysse Marteau-Ferey, and Francis Bach. "Finding global minima via kernel approximations". In: *Mathematical Programming* (2024), pp. 1–82.

Soon on arxiv

Generalization Bounds of Surrogate Policies
for Combinatorial Optimization Problems

Pierre Cyril Aubin-Frankowski[1], Yohann De Castro[2,3], Axel Parmentier[4], and Alessandro Rudi[5]

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[3] *Institut Universitaire de France (IUF)*
[4] *CERMICS, École des Ponts, France.*
[5] *SIERRA, INRIA Paris, France.*

July 24, 2024

Abstract

A recent stream of structured learning approaches has improved the practical state of the art for a range of combinatorial optimization problems with complex objectives encountered in operations research. Such approaches train policies that chain a statistical model with a surrogate combinatorial optimization oracle to map any instance of the problem to a feasible solution. The key idea is to exploit the statistical

Conclusion

Policies embedding a CO layer in a NN

- improved practical state of the art on several data driven problems
- when trained using decision aware learning

This study : theoretical guarantees on the policy obtained

- Results apply to contextual stochastic optimization

Smoothing them by perturbation trained using decision aware learning

- makes optimization easier (polynomial convergence guarantee)
- improves generalization (empirical process control)

Perspective: deep learning compatible risk minimization algorithms

References I

[1] Cheikh Ahmed et al. *DistrictNet: Decision aware learning for geographical districting*. Feb. 2024.

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