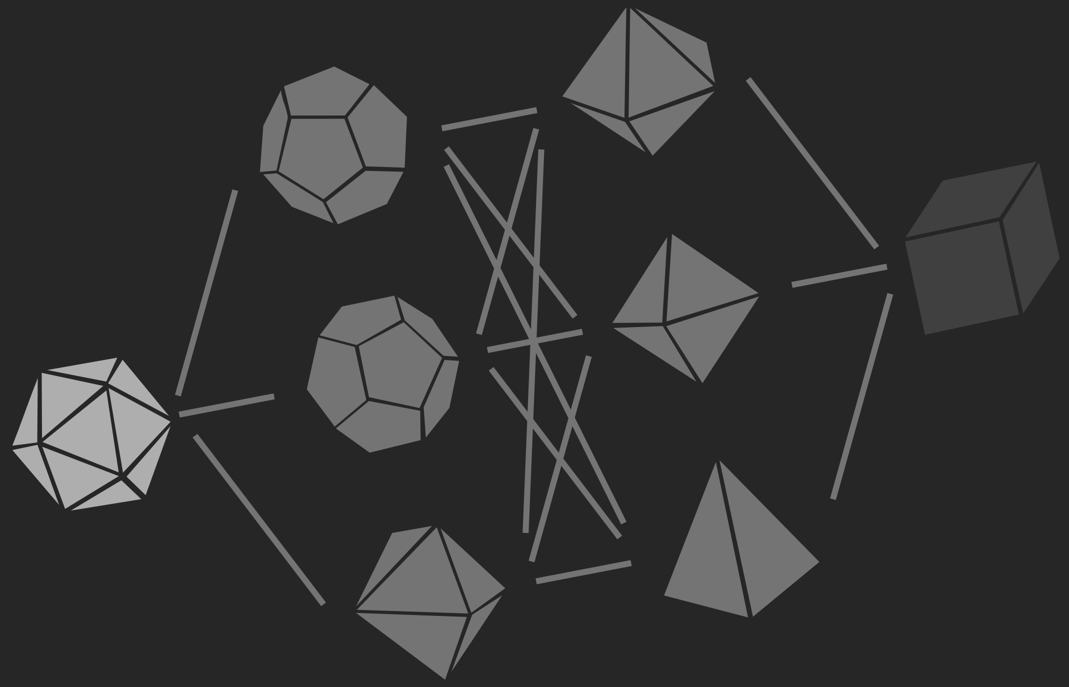
CPAIOR 2024 | Session 12: Decision-focused Learning

▸CaVE

A Cone-Aligned Approach for Fast Predict-then-Optimize



Mechanical & Industrial Engineering
UNIVERSITY OF TORONTO

Presented by Bo Tang

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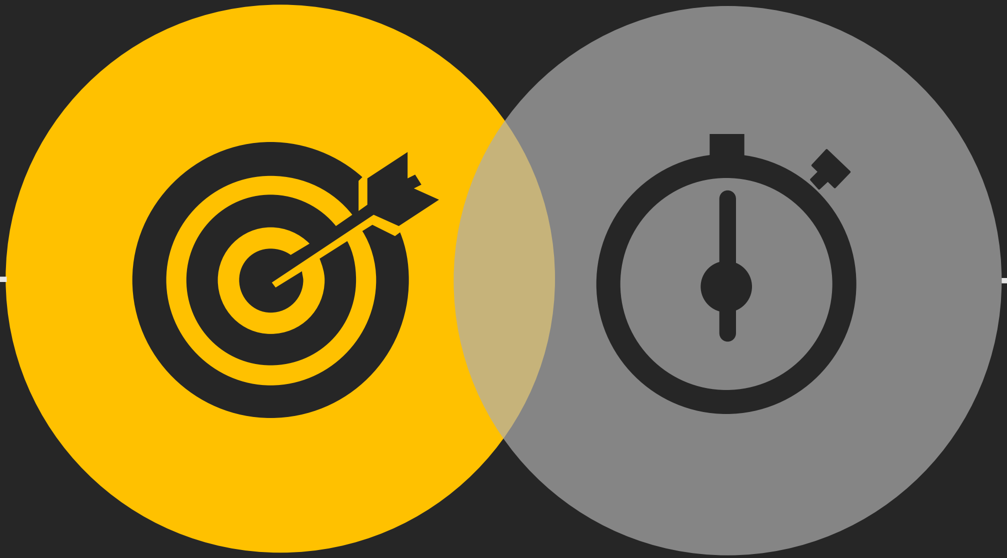
Introduction

CaVE (Cone-aligned Vector Estimation) is an efficient and accurate **Decision-focused Learning** approach for **Binary Linear Programs** (BLPs).



End-to-End:

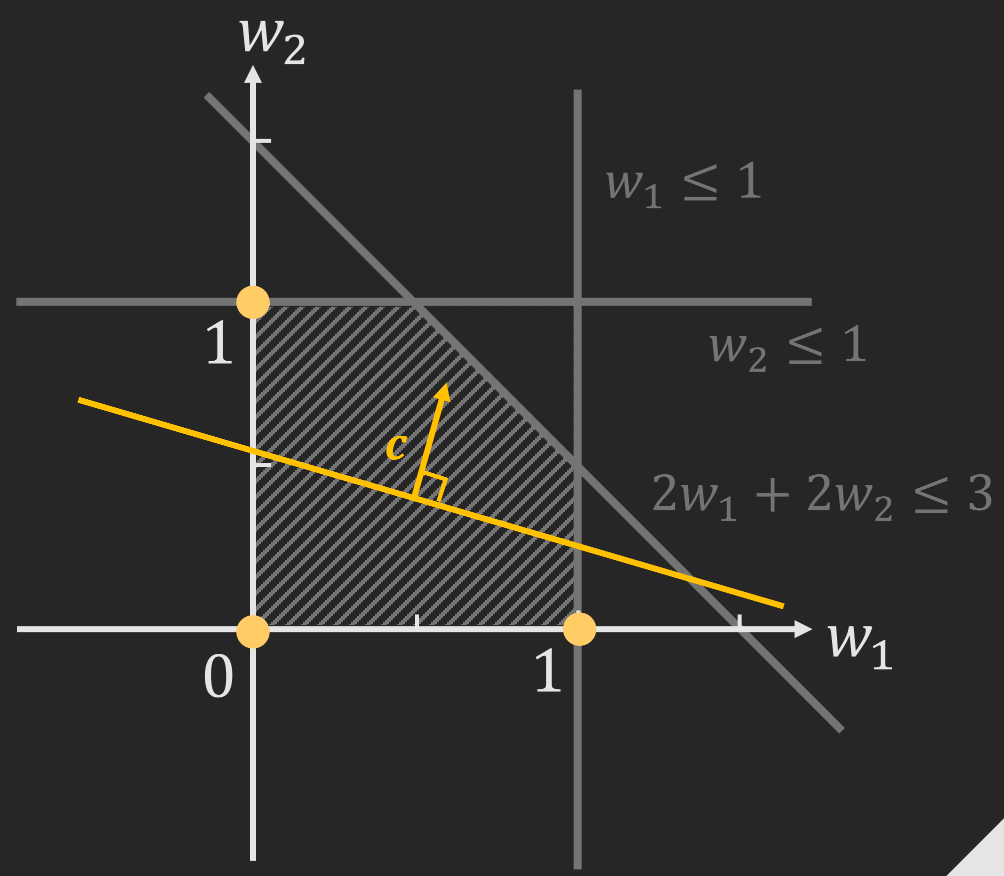
The loss function of CaVE focuses on decision quality.

Efficiency:

The algorithm of CaVE utilizes non-negative least squares (NNLSs) instead of solving BLPs.

Notation

$$\min_{\underbrace{\boldsymbol{w}}_{\text{Decision Variables}}} \{ \overbrace{\boldsymbol{c}^\top \boldsymbol{w}}^{\text{Linear Objective Function}} : \underbrace{\boldsymbol{w} \in S}_{\text{Feasible Region}}, \overbrace{\boldsymbol{w} \in \{0,1\}}^{\text{Binary Domain}} \}$$



Predict, then Optimize

$$\min_{\boldsymbol{w}} \{ \boldsymbol{c}_1^\top \boldsymbol{w} : \boldsymbol{w} \in \boldsymbol{S} \}$$

$$\min_{\boldsymbol{w}} \{ \boldsymbol{c}_2^\top \boldsymbol{w} : \boldsymbol{w} \in \boldsymbol{S} \}$$

$$\min_{\boldsymbol{w}} \{ \boldsymbol{c}_3^\top \boldsymbol{w} : \boldsymbol{w} \in \boldsymbol{S} \}$$

$$\ddots$$

Predict, then Optimize

Unknown Coefficients

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_1^\top \boldsymbol{w} : \boldsymbol{w} \in S\}$$

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_2^\top \boldsymbol{w} : \boldsymbol{w} \in S\}$$

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_3^\top \boldsymbol{w} : \boldsymbol{w} \in S\}$$

$$\ddots$$

Identical Constraints

Predict, then Optimize

Unknown Coefficients

$$\min_{\boldsymbol{w}} \{ \boldsymbol{c}_1^\top \boldsymbol{w} : \boldsymbol{w} \in S \}$$

$$\min_{\boldsymbol{w}} \{ \boldsymbol{c}_2^\top \boldsymbol{w} : \boldsymbol{w} \in S \}$$

$$\min_{\boldsymbol{w}} \{ \boldsymbol{c}_3^\top \boldsymbol{w} : \boldsymbol{w} \in S \}$$

$\ddots$

Identical Constraints

Observed Feature Vector

$\boldsymbol{x}_1$

$\boldsymbol{x}_2$

$\boldsymbol{x}_3$

$\vdots$

Predict, then Optimize

Unknown Coefficients

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_1^\top \boldsymbol{w} : \boldsymbol{w} \in S\}$$

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_2^\top \boldsymbol{w} : \boldsymbol{w} \in S\}$$

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_3^\top \boldsymbol{w} : \boldsymbol{w} \in S\}$$

$$\ddots$$

Identical Constraints

$\hat{\boldsymbol{c}} = g(\boldsymbol{x}; \boldsymbol{\theta})$

Prediction

Observed Feature Vector

$\boldsymbol{x}_1$

$\boldsymbol{x}_2$

$\boldsymbol{x}_3$

$\vdots$

Predict, then Optimize

Unknown Coefficients

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_1^{\top}\boldsymbol{w}: \boldsymbol{w} \in S\}$$

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_2^{\top}\boldsymbol{w}: \boldsymbol{w} \in S\}$$

$$\min_{\boldsymbol{w}}\{\boldsymbol{c}_3^{\top}\boldsymbol{w}: \boldsymbol{w} \in S\}$$

$\ddots$

Identical Constraints

Predicted Coefficients

Model Parameters

$$\hat{\boldsymbol{c}} = g(\boldsymbol{x}; \boldsymbol{\theta})$$

Prediction

Observed Feature Vector

$\boldsymbol{x}_1$

$\boldsymbol{x}_2$

$\boldsymbol{x}_3$

$\vdots$

Examples

- Vehicle Routing
- Energy Scheduling
- Portfolio Optimization

Examples

- ❖ Vehicle Routing
- ❖ Energy Scheduling
- ❖ Portfolio Optimization

Unknown Costs: Travel Time, Electricity Prices, Asset Returns

Examples

❖Vehicle Routing

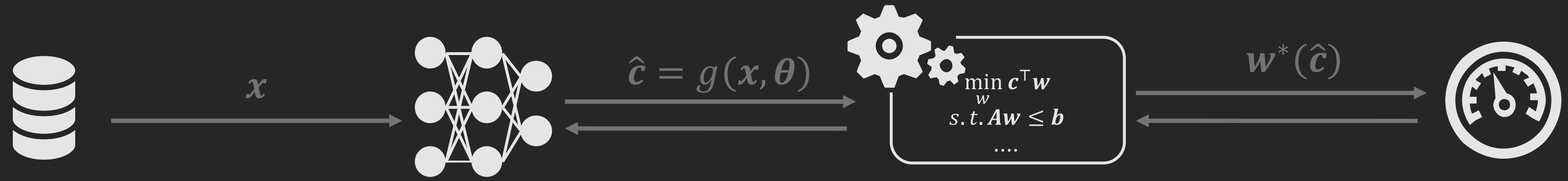
❖Energy Scheduling

❖Portfolio Optimization

Unknown Costs: Travel Time, Electricity Prices, Asset Returns

Observed Features: Distance, Time, Weather, Financial Factors...

Decision-focused Learning



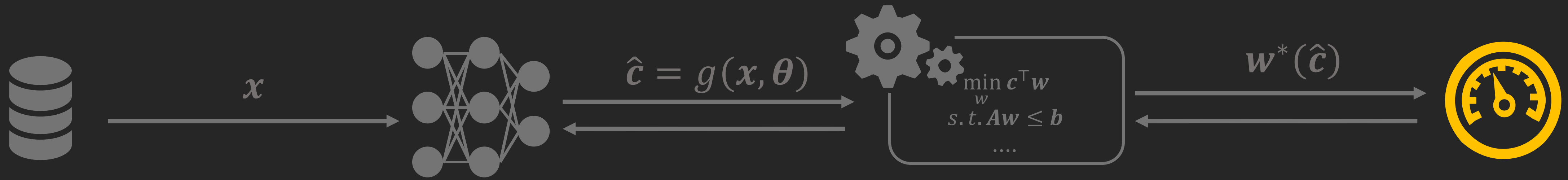
Dataset $\mathcal{D}$ with data points $(\boldsymbol{x}, \boldsymbol{c})$

Prediction model $g(\boldsymbol{x}, \boldsymbol{\theta})$ with parameters $\boldsymbol{\theta}$

Optimization solver $\boldsymbol{w}^*(\hat{\boldsymbol{c}}) = \operatorname{argmin}_{\boldsymbol{w} \in S} \hat{\boldsymbol{c}}^\top \boldsymbol{w}$

Loss function $\mathcal{L}(\cdot)$ to measure decision error

Decision-focused Learning



Dataset $\mathcal{D}$ with data points (x, c)

Prediction model $g(x, \theta)$ with parameters θ

Optimization solver $w^*(\hat{c}) = \operatorname{argmin}_{w \in S} \hat{c}^\top w$

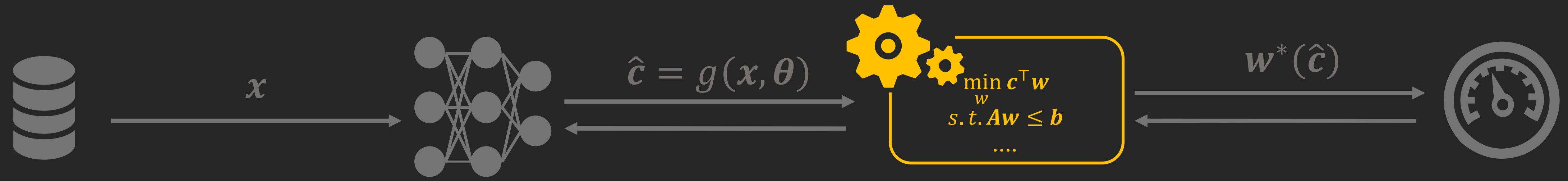
Loss function $\mathcal{L}(\cdot)$ to measure decision error

e.g.

$$\mathcal{L}_{\text{Regret}}(\hat{c}, c) = c^\top w^*(\hat{c}) - c^\top w^*(c)$$

$$\mathcal{L}_{\text{Square}}(\hat{c}, c) = \frac{1}{2} \| w^*(c) - w^*(\hat{c}) \|_2^2$$

Decision-focused Learning



Dataset $\mathcal{D}$ with data points (x, c)

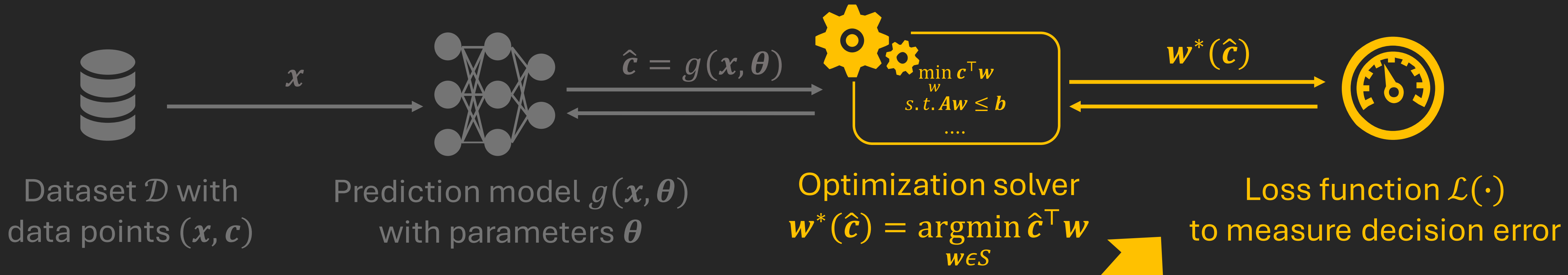
Prediction model $g(x, \theta)$ with parameters θ

Optimization solver $w^*(\hat{c}) = \operatorname{argmin}_{w \in S} \hat{c}^{\top} w$

Loss function $\mathcal{L}(\cdot)$ to measure decision error

Computational Bottleneck:
All state-of-the-art methods require repeated solving during the iteration.

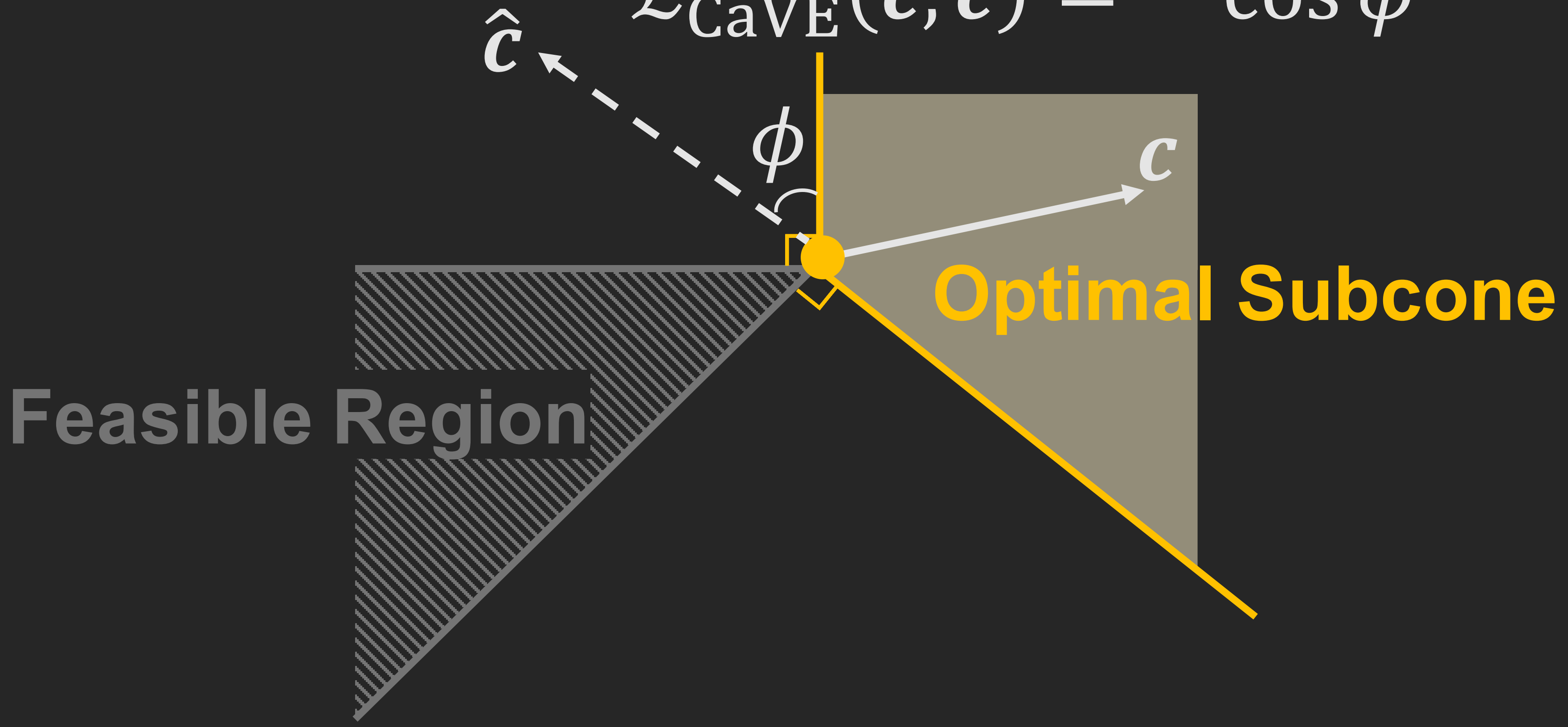
Decision-focused Learning



Cone-aligned Vector Estimation:
Replace the original optimization problem with projection (quadratic programming).

Similarity Loss Function

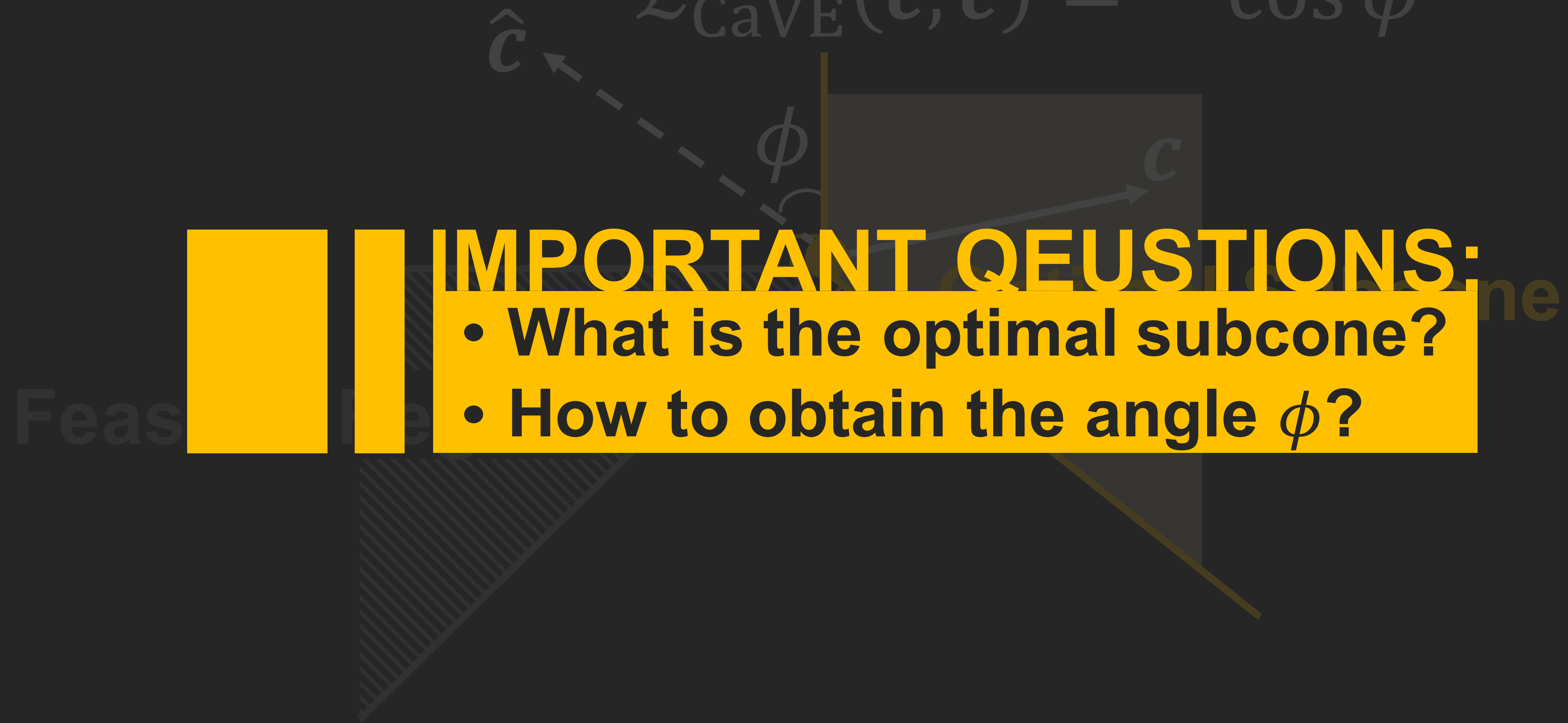
$$\mathcal{L}_{\text{CaVE}}(\hat{\boldsymbol{c}}, \boldsymbol{c}) = -\cos\phi$$



When the predicted cost vector lies inside the **optimal subcone**, the optimal solution to the linear relaxation is the optimal of original BLP problem.

Similarity Loss Function

$$\mathcal{L}_{\text{CaVE}}(\hat{\boldsymbol{c}}, \boldsymbol{c}) = -\cos\phi$$

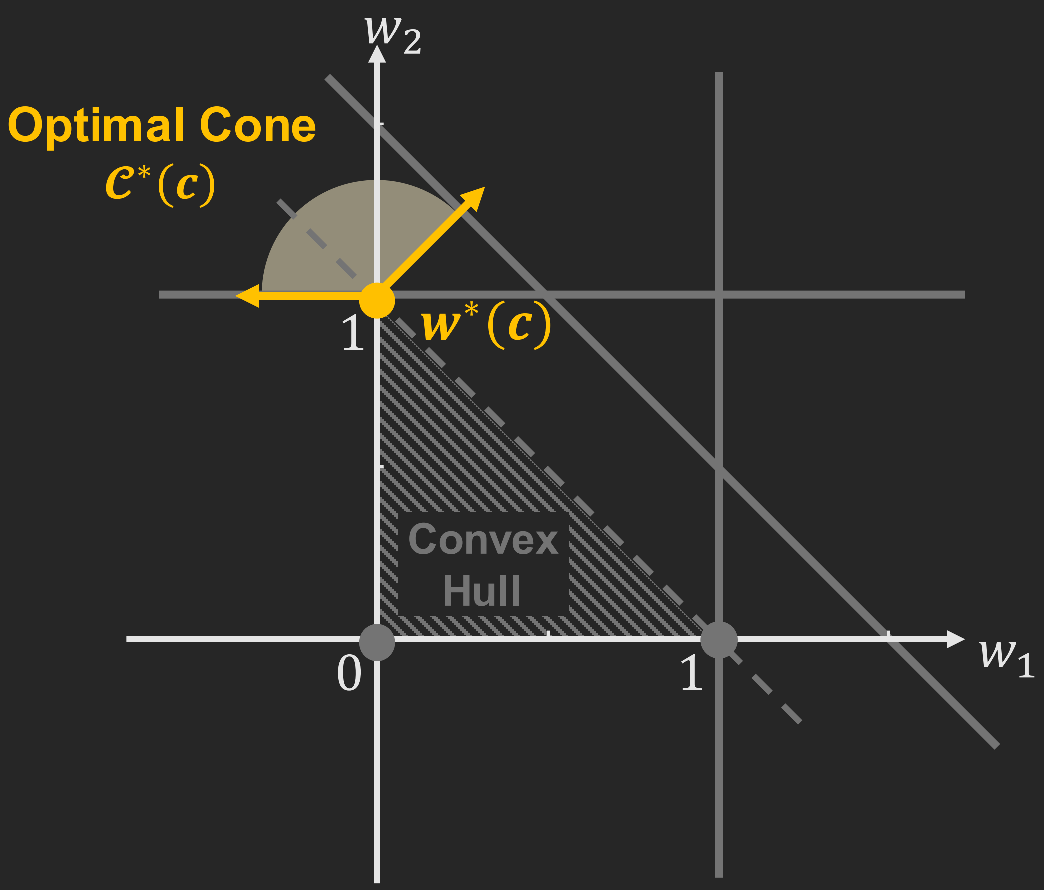


IMPORTANT QEUSTIONS:

- **What is the optimal subcone?**
- **How to obtain the angle ϕ?**

When the predicted cost vector lies inside the **optimal subcone**, the optimal solution to the linear relaxation is the optimal of original BLP problem.

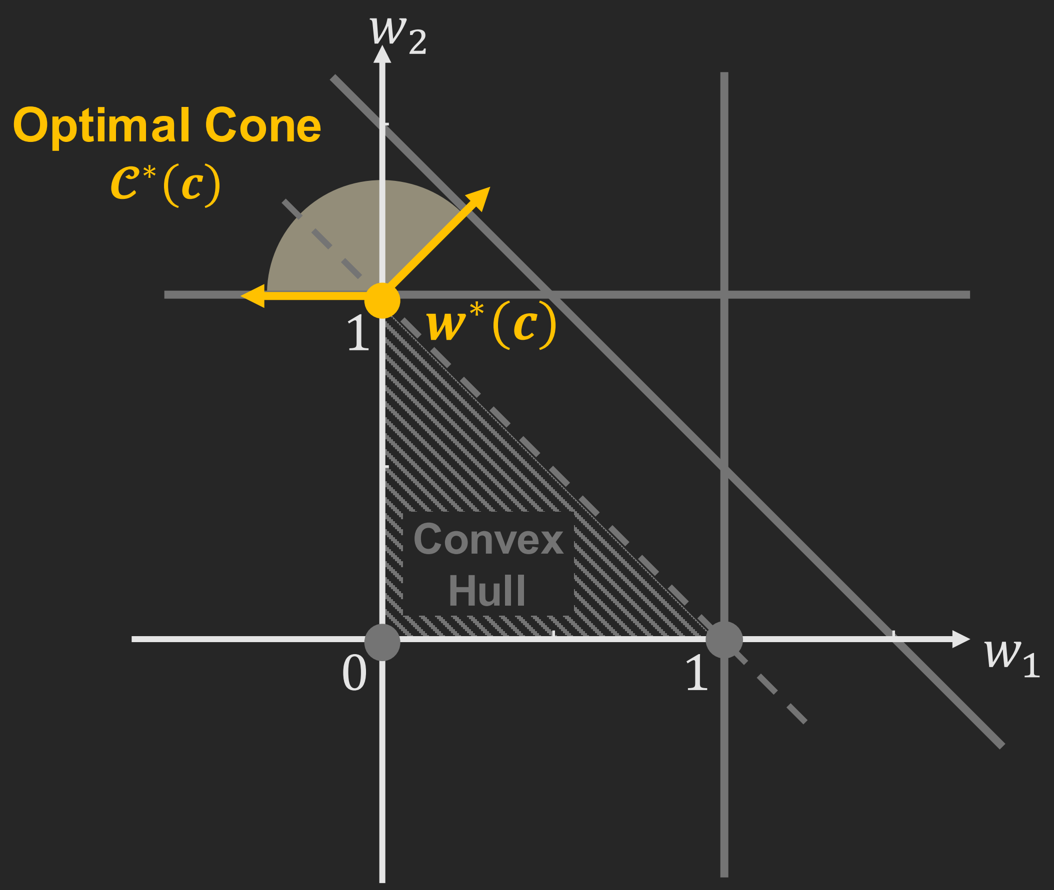
Optimal Subcone



Binary Linear Program

1. For ILP, the normal cone to the convex hull at the optimal solution $\boldsymbol{w}^*(\boldsymbol{c})$ is defined as optimal cone $\mathcal{C}^*(\boldsymbol{c})$.

Optimal Subcone



Binary Linear Program

1. For ILP, the normal cone to the convex hull at the optimal solution $\boldsymbol{w}^*(\boldsymbol{c})$ is defined as optimal cone $\mathcal{C}^*(\boldsymbol{c})$.

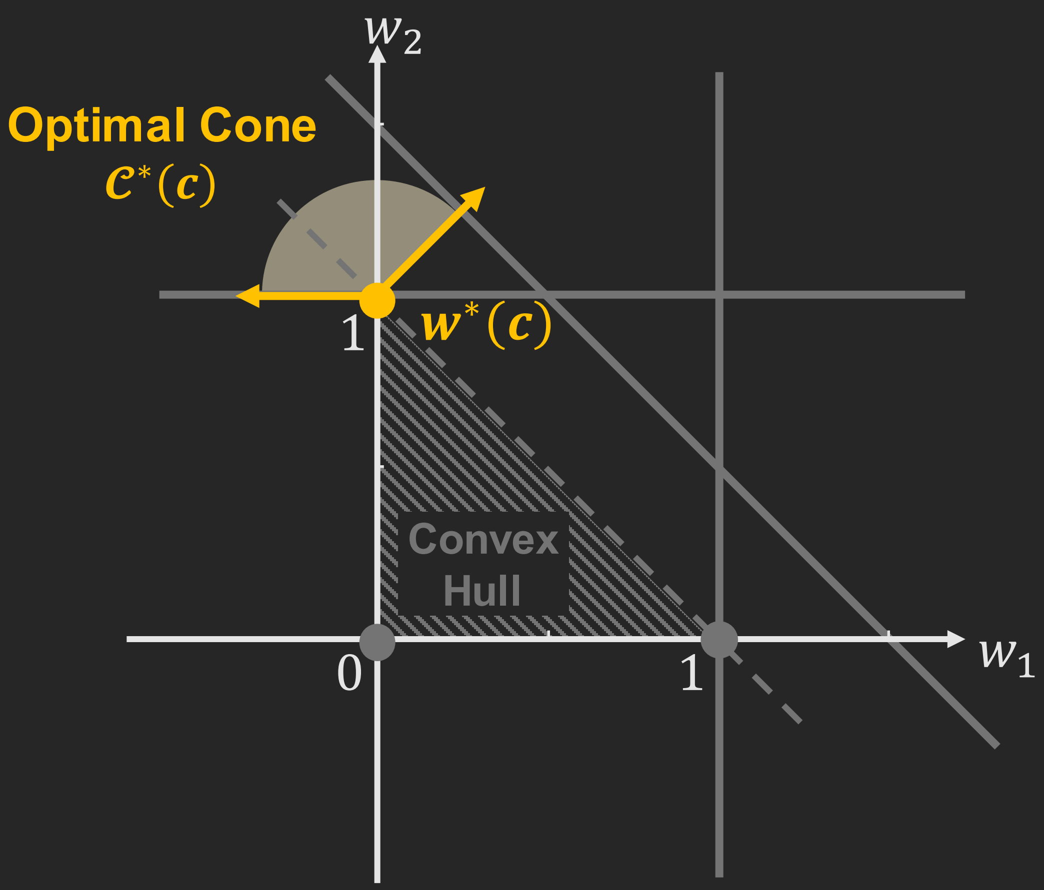
2. $\forall \boldsymbol{c}' \in \mathcal{C}^*(\boldsymbol{c}), \boldsymbol{w}^*(\boldsymbol{c}') = \boldsymbol{w}^*(\boldsymbol{c})$. Cost vectors yield the same optimal solution if and only if they are in the same optimal cone.

Optimal Subcone

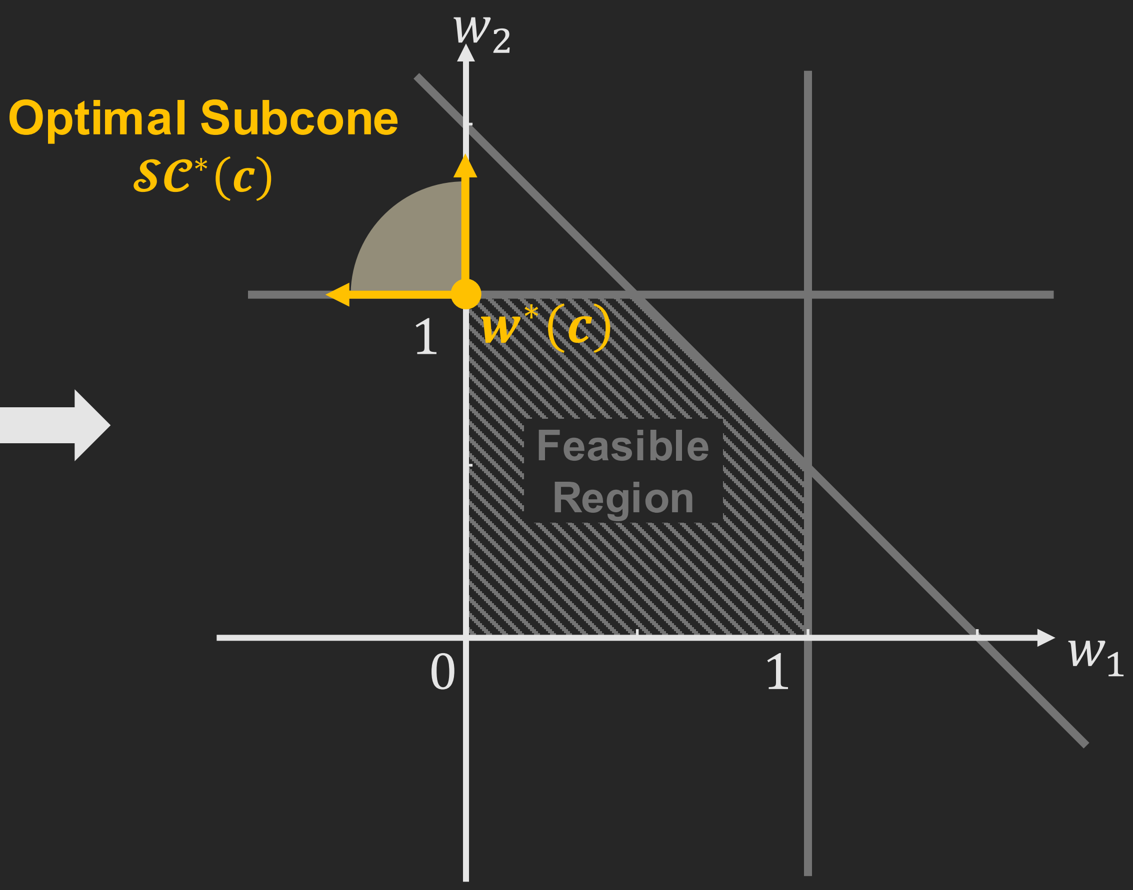
Binary Linear Program

1. For ILP, the normal cone to the convex hull at the optimal solution $\boldsymbol{w}^*(\boldsymbol{c})$ is defined as optimal cone $\boldsymbol{\mathcal{C}}^*(\boldsymbol{c})$.
2. $\forall \boldsymbol{c}' \in \boldsymbol{\mathcal{C}}^*(\boldsymbol{c}), \boldsymbol{w}^*(\boldsymbol{c}') = \boldsymbol{w}^*(\boldsymbol{c})$. Cost vectors yield the same optimal solution if and only if they are in the same optimal cone.
3. However, for ILP, obtaining the convex hull is NOT trivial. e.g., Cutting Plane method...

Optimal Subcone



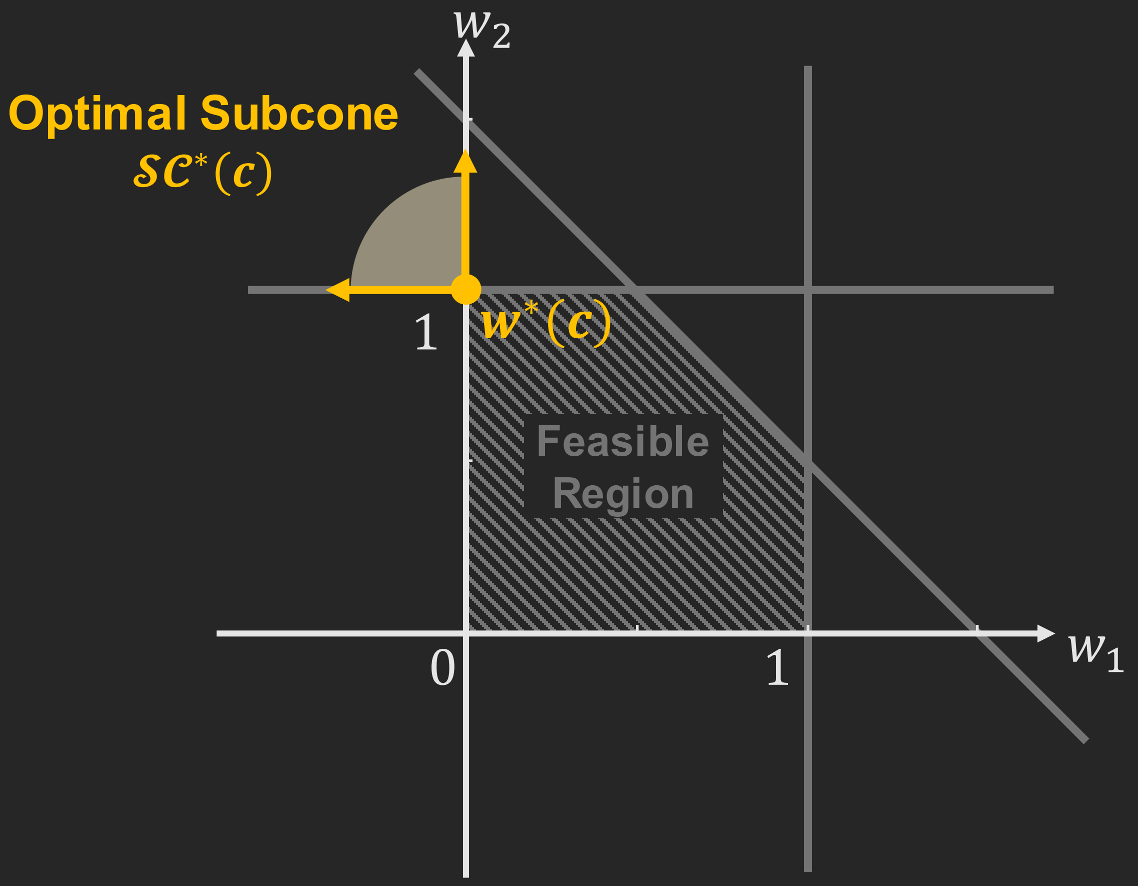
Binary Linear Program



Linear Relaxation

Optimal Subcone

1. For BLP, the normal cone to the feasible region of linear relaxation at the optimal solution $\boldsymbol{w}^*(\boldsymbol{c})$ is defined as optimal subcone $\mathcal{SC}^*(\boldsymbol{c})$.



Linear Relaxation

Optimal Subcone

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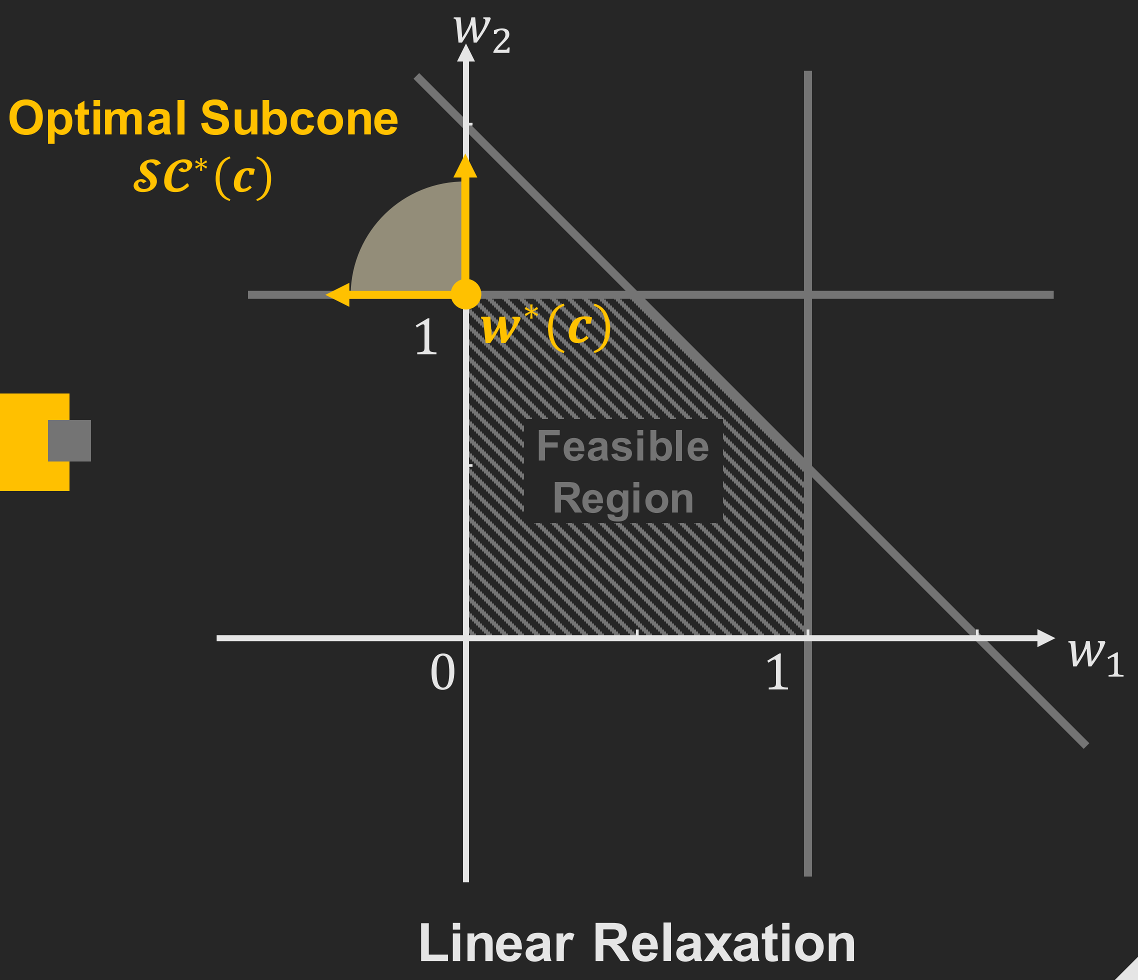
Note: This does not apply to general ILP!

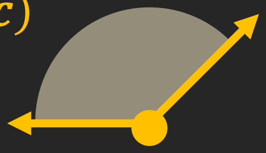


Optimal Subcone

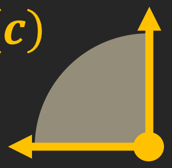
1. For BLP, the normal cone to the feasible region of linear relaxation at the optimal solution $\boldsymbol{w}^*(\boldsymbol{c})$ is defined as optimal subcone $\mathcal{SC}^*(\boldsymbol{c})$.

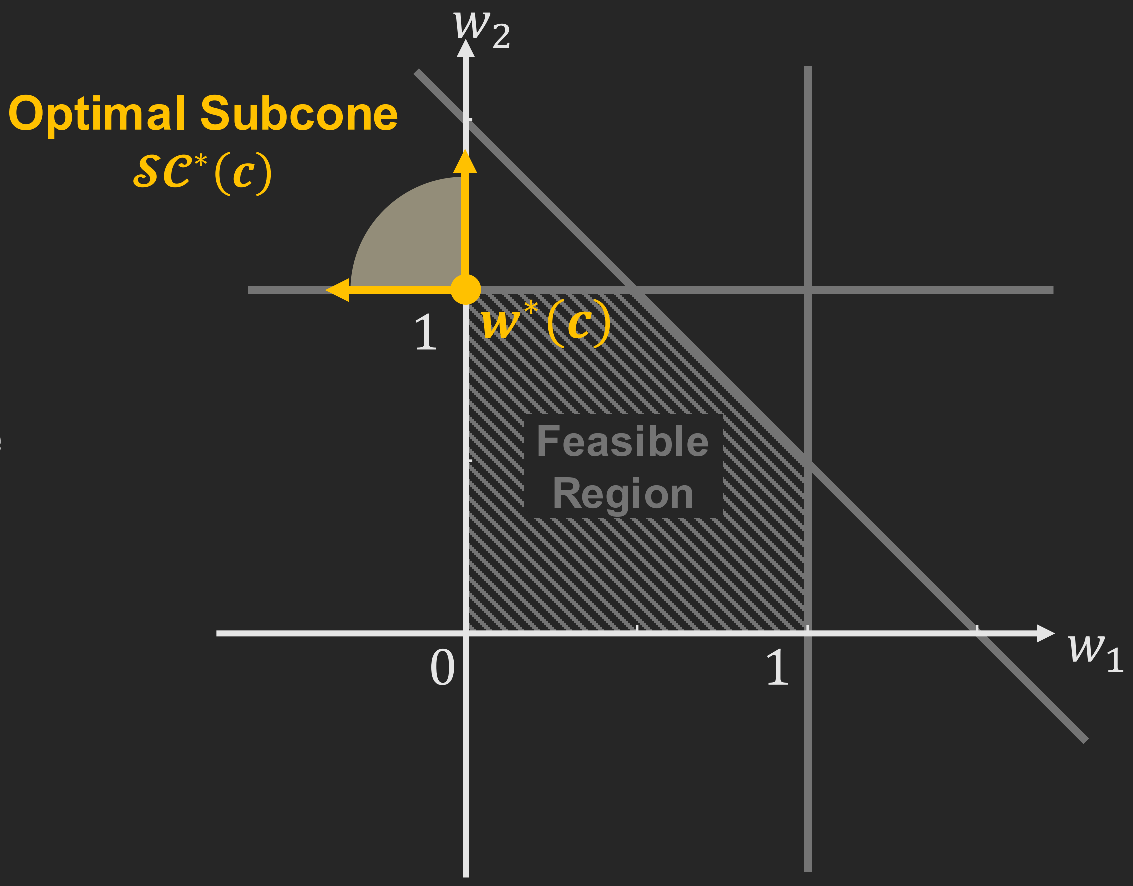
2. $\mathcal{SC}^*(\boldsymbol{c}) \subseteq \mathcal{C}^*(\boldsymbol{c})$. Thus, cost vectors yield the same optimal solution if they are in the same optimal subcone.

Optimal Cone
$\mathcal{C}^*(\boldsymbol{c})$



Optimal Subcone
$\mathcal{SC}^*(\boldsymbol{c})$





Linear Relaxation

Optimal Subcone

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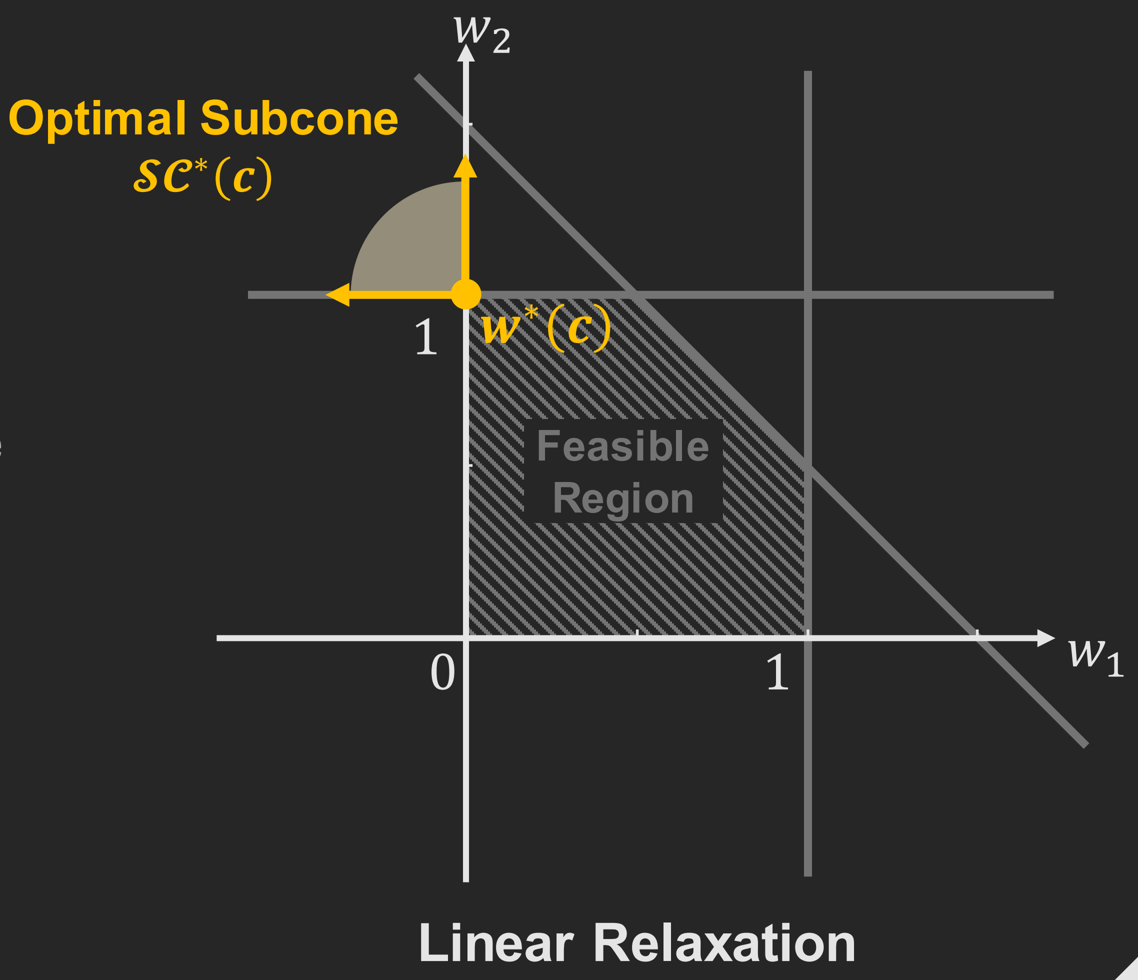
2. $\mathcal{SC}^*(\boldsymbol{c}) \subseteq \mathcal{C}^*(\boldsymbol{c})$. Thus, cost vectors yield the same optimal solution if they are in the same optimal subcone.
3. The optimal subcone is the conic combination of tight constraints, which is trivial.



Optimal Subcone

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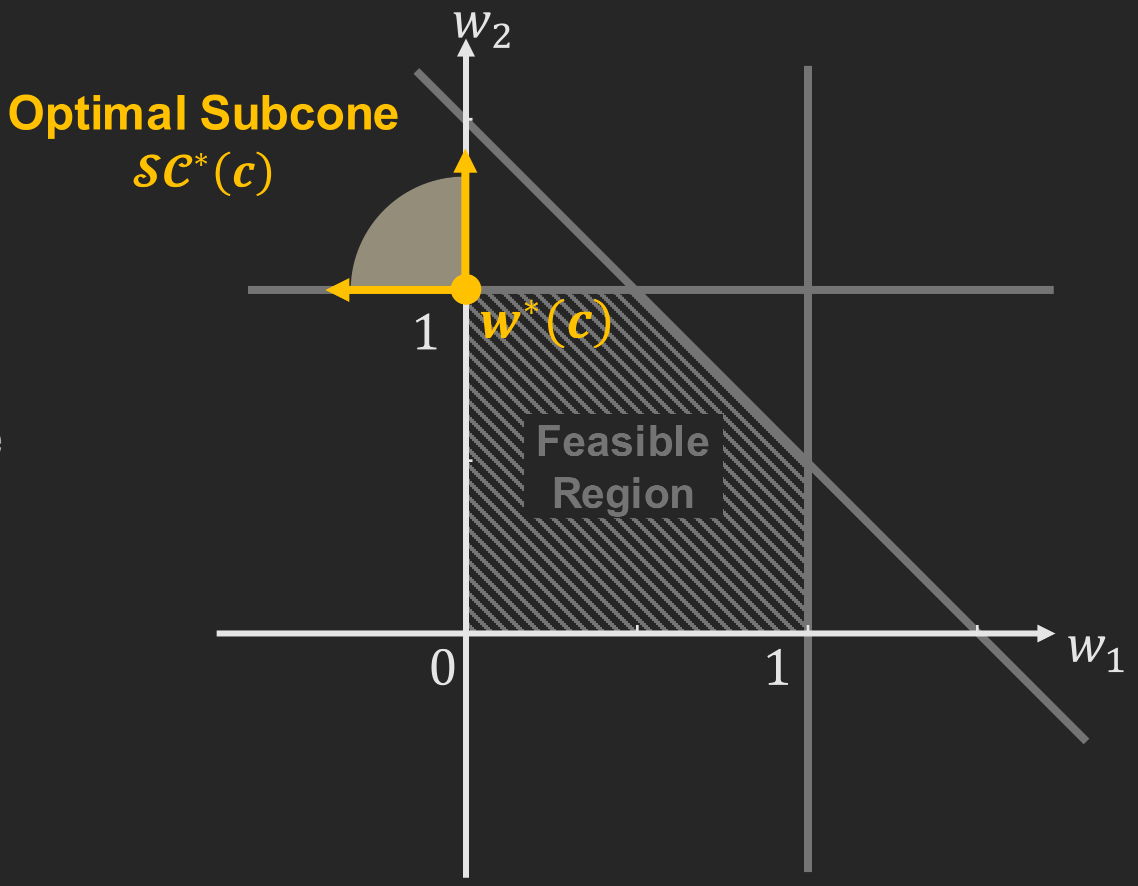
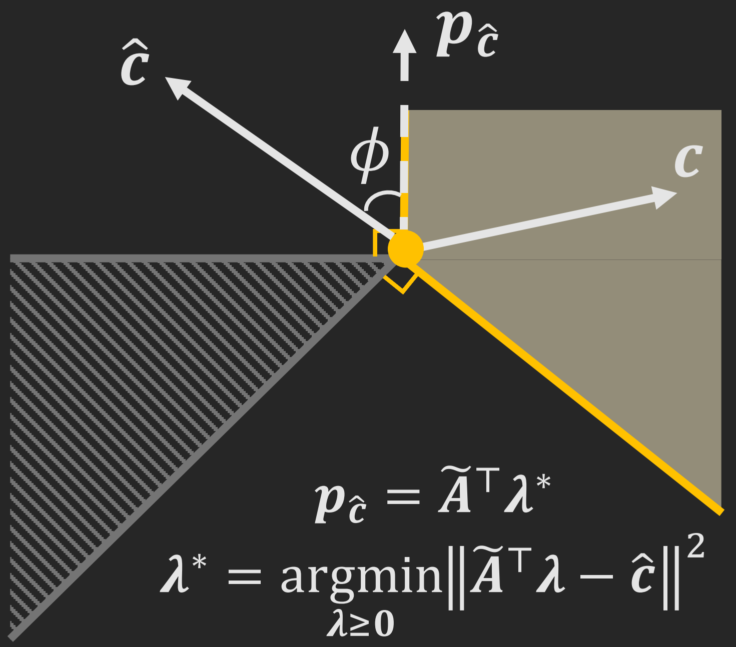
$\tilde{A}(\boldsymbol{c})$: $\tilde{A}(\boldsymbol{c})^\top \boldsymbol{w}^*(\boldsymbol{c}) = \boldsymbol{b}$



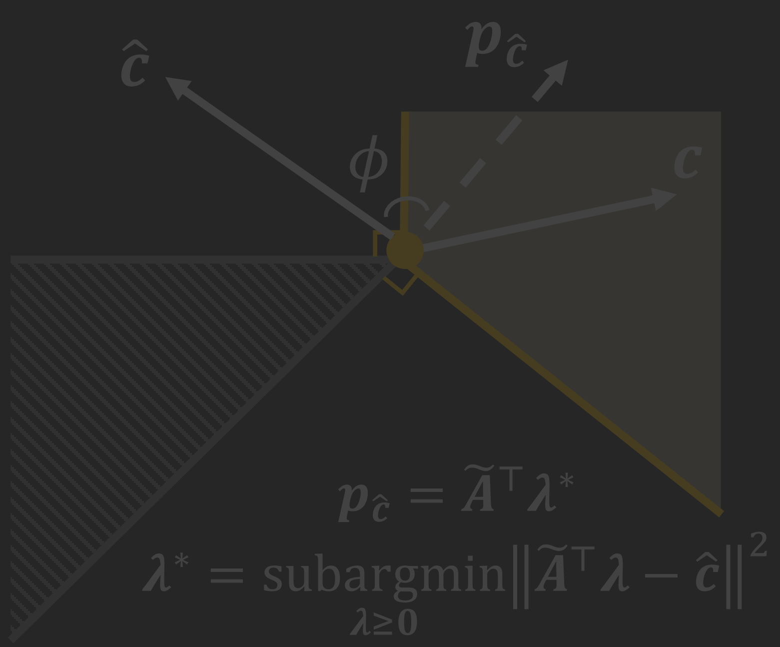
Linear Relaxation

Projection



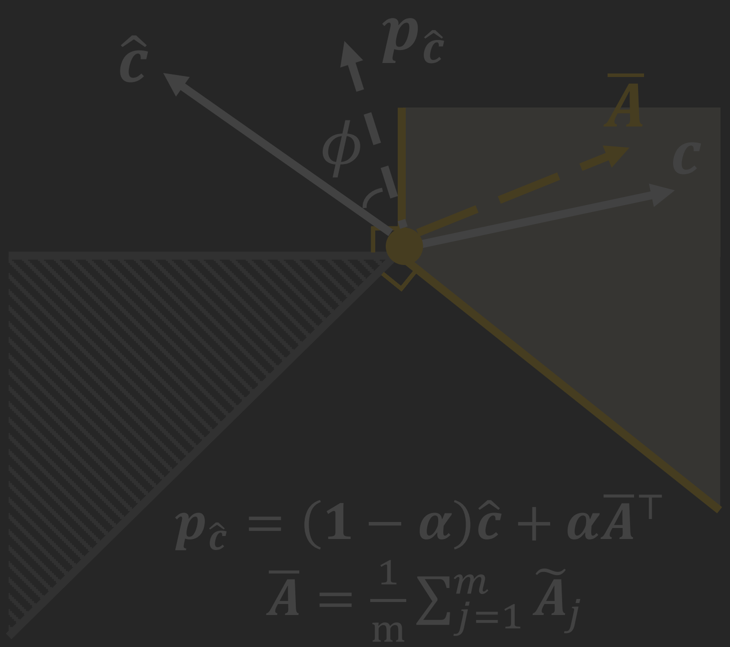
$$p_{\hat{c}} = \widetilde{A}^{\top}\lambda^{*}$$
$$\lambda^{*} = \underset{\lambda \geq 0}{\operatorname{argmin}} \left\| \widetilde{A}^{\top}\lambda - \hat{c} \right\|^{2}$$

Exact Projection



$$p_{\hat{c}} = \widetilde{A}^{\top}\lambda^{*}$$
$$\lambda^{*} = \underset{\lambda \geq 0}{\operatorname{subargmin}} \left\| \widetilde{A}^{\top}\lambda - \hat{c} \right\|^{2}$$

Inner Projection

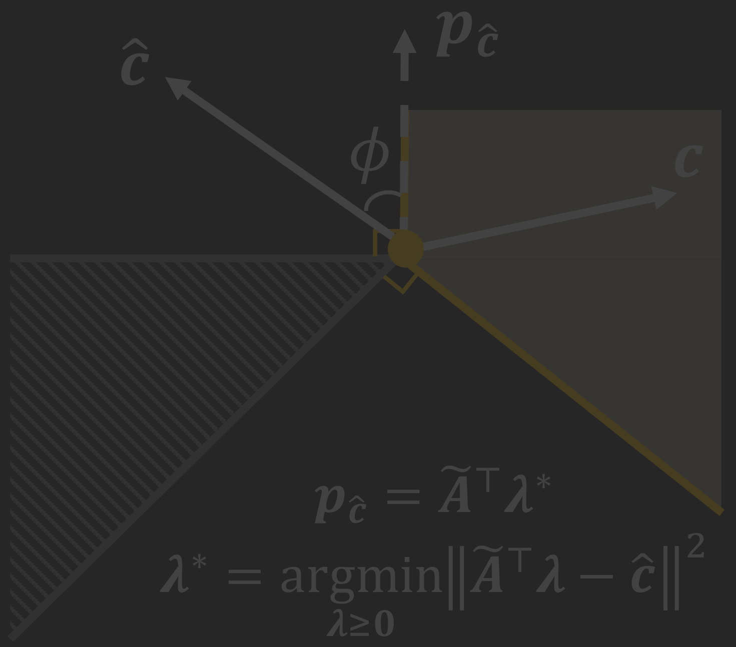


$$p_{\hat{c}} = (1-\alpha)\hat{c} + \alpha \overline{A}^{\top}$$
$$\overline{A} = \frac{1}{m}\sum_{j=1}^{m} \widetilde{A}_{j}$$

Heuristic Projection

CaVE Exact performs exact projection, wherein the optimal solution of the NNLS is on the surface of the cone.
This approach results in the vanishing gradients as the predicted cost vector close the surface.

Projection



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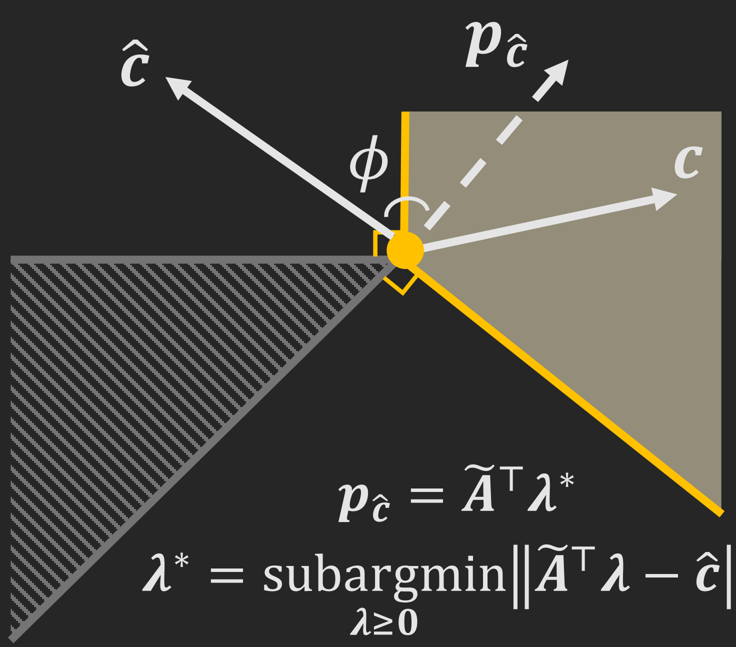
Exact Projection



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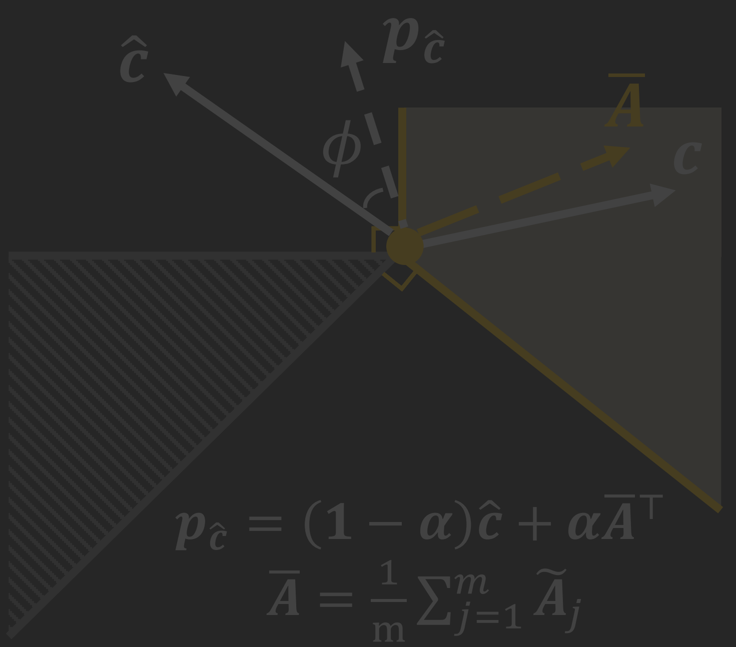
Inner Projection

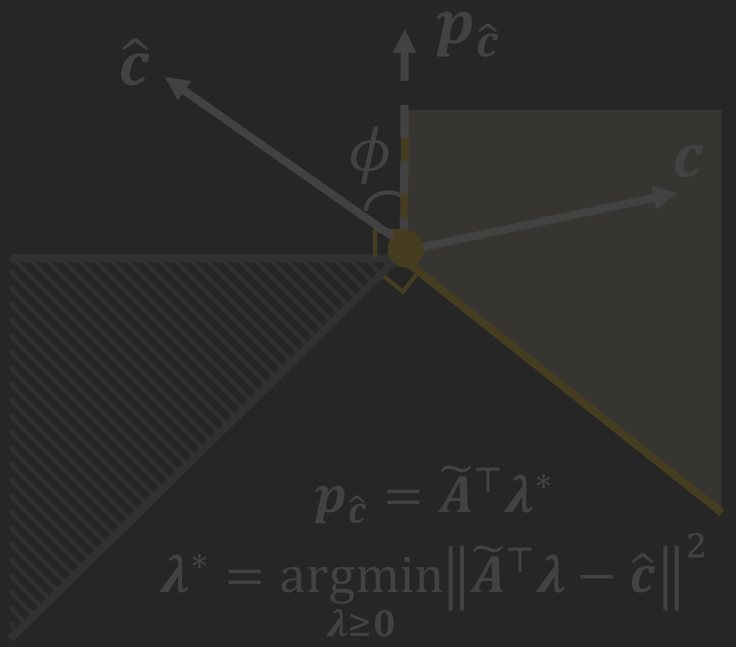


$$p_{\hat{c}} = (1-\alpha)\hat{c} + \alpha \bar{A}^{\top}$$
$$\bar{A} = \frac{1}{m}\sum_{j=1}^{m} \widetilde{A}_j$$

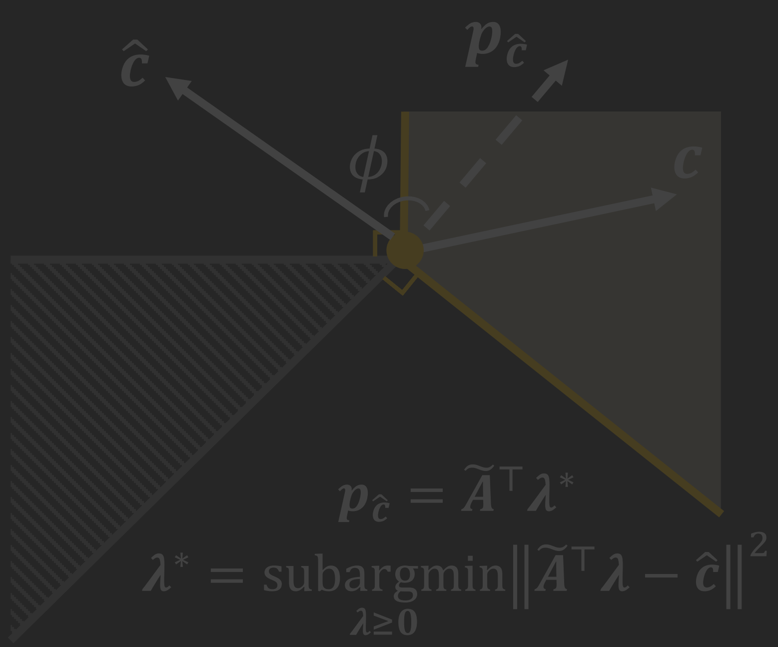
Heuristic Projection

The goal is to obtain a projection of the predicted cost vector that lies inside the subcone. (suboptimal solution)
Since the solver (Clarabel) uses the primal-dual interior point, the feasibility is guaranteed at each iteration. We can simply set the maximum iterations.

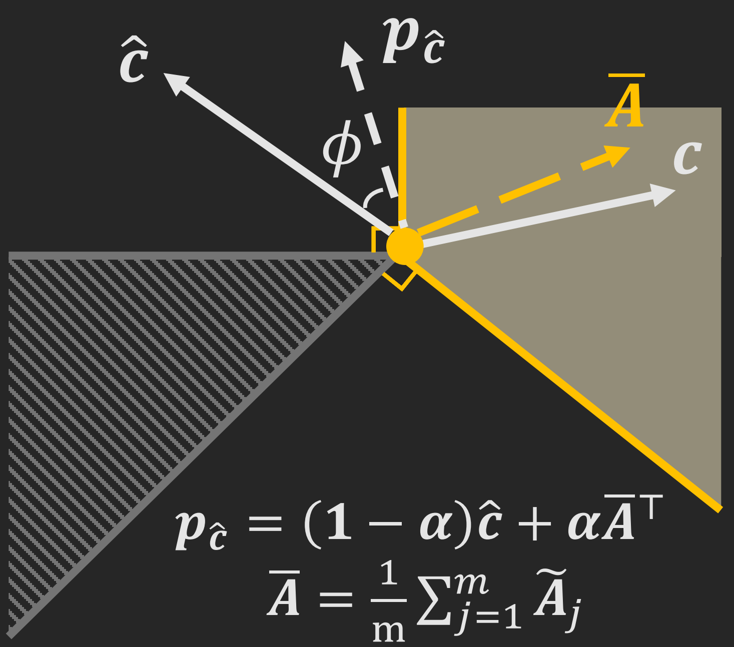
Projection



Exact Projection



Inner Projection

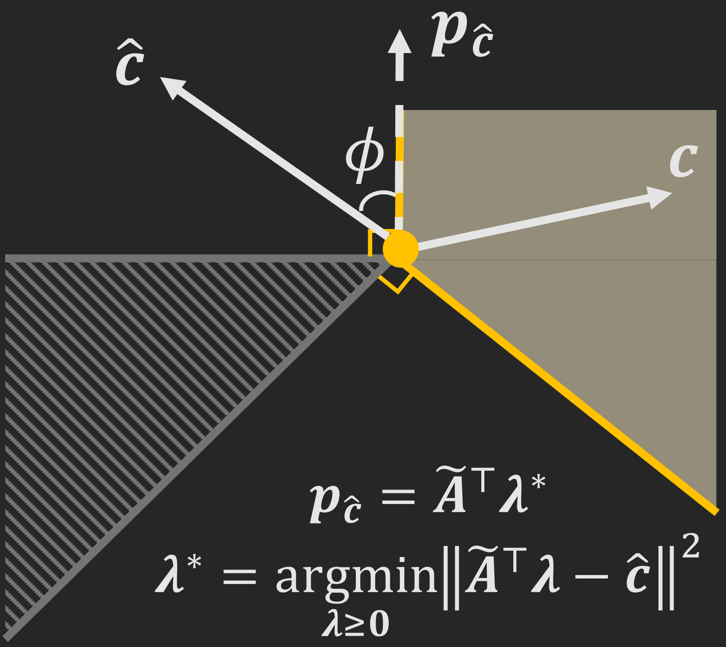


Heuristic Projection

A heuristic projection that does not require solving NNLS and relies on simple operations.

This approach does NOT guarantee feasibility, yet it ensures that the cost vector is pushed towards the cone.

Projection



$$p_{\hat{c}} = \tilde{A}^{\top}\lambda^{*}$$
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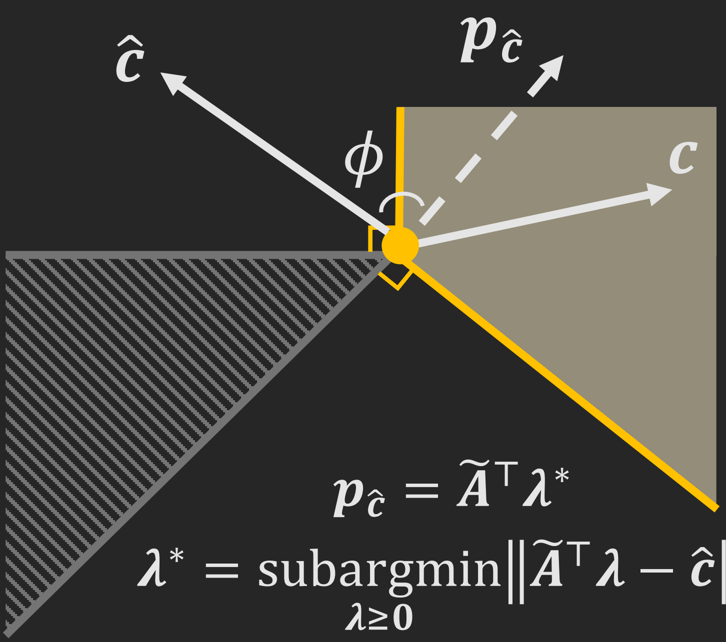
Exact Projection

↓

CaVE Exact



$$p_{\hat{c}} = \tilde{A}^{\top}\lambda^{*}$$
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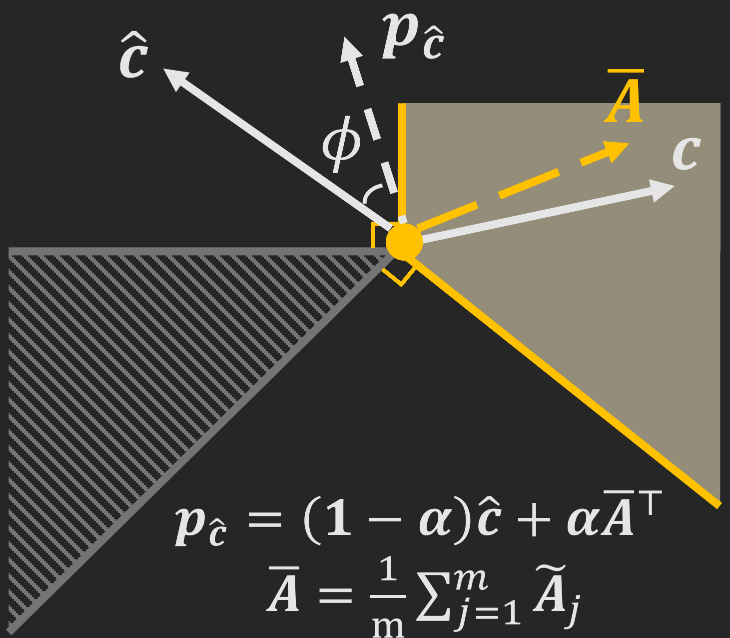
Inner Projection

↓

CaVE+



$$p_{\hat{c}} = (1-\alpha)\hat{c} + \alpha\bar{A}^{\top}$$
$$\bar{A} = \frac{1}{m}\sum_{j=1}^{m}\tilde{A}_j$$

Heuristic Projection

↓

CaVE Hybrid

Algorithm

Algorithm Cone-aligned Vector Estimation (`CaVE`)

Require: Pairs of feature vectors and binding constraints $\{(\boldsymbol{x}^i, \widetilde{\boldsymbol{A}}^i)\}_{i=1}^n$ for n training instances; learning rate $\alpha > 0$

Initialize model parameters $\boldsymbol{\theta}$
for each training epoch **do**
    for each batch of training samples $(\boldsymbol{x}, \widetilde{\boldsymbol{A}})$ **do**
        Predict cost coefficient $\hat{\boldsymbol{c}} \leftarrow g(\boldsymbol{x}, \boldsymbol{\theta})$
        Compute projection $\boldsymbol{p}_{\hat{\boldsymbol{c}}}$ with quadratic program
        Compute cosine similarity loss $\mathcal{L}_{\text{CaVE}}(\hat{\boldsymbol{c}}, \widetilde{\boldsymbol{A}})$
        Compute the gradient $\nabla_\theta \mathcal{L}_{\text{CaVE}}(\hat{\boldsymbol{c}}, \widetilde{\boldsymbol{A}})$ with backpropagation
        Update ML model parameters $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \alpha \nabla_\theta \mathcal{L}_{\text{CaVE}}(\hat{\boldsymbol{c}}, \widetilde{\boldsymbol{A}})$
    end for
end for
return $g(\cdot, \boldsymbol{\theta})$

Algorithm

Algorithm Cone-aligned Vector Estimation (`CaVE`)

Require: Pairs of feature vectors and binding constraints $\{(\boldsymbol{x}^i, \widetilde{\boldsymbol{A}}^i)\}_{i=1}^n$ for n training instances; learning rate $\alpha > 0$

```
Initialize model parameters θ
for each training epoch do
    for each batch of training samples (x, Ã) do
        Predict cost coefficient ĉ ← g(x, θ)
        Compute projection p_ĉ with quadratic program
        Compute cosine similarity loss L_CaVE(ĉ, Ã)
        Compute the gradient ∇_θ L_CaVE(ĉ, Ã) with backpropagation
        Update ML model parameters θ ← θ − α∇_θ L_CaVE(ĉ, Ã)
    end for
end for
return g(·, θ)
```

Faster than solving BLP!

Experiments - SP5

Shortest Path on 5 × 5 Grid

Average Test Normalized Regret (%) with Standard Deviation

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	8.82 ± 1.15	10.73 ± 1.54	8.39 ± 0.95	8.35 ± 0.88	7.79 ± 1.00	**7.68** ± 0.99	11.34 ± 1.11
Deg 6	12.58 ± 2.14	11.30 ± 1.30	8.89 ± 0.90	8.84 ± 1.00	**7.72** ± 1.11	7.86 ± 0.96	13.78 ± 1.58

Average Training Time (Sec) with Standard Deviation

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	1.52 ± 0.14	4.64 ± 0.09	4.89 ± 0.12	**2.57** ± 0.19	17.64 ± 0.12	18.52 ± 0.31	4.50 ± 0.48
Deg 6	1.38 ± 0.13	3.52 ± 0.11	3.72 ± 0.14	**2.39** ± 0.19	18.68 ± 0.40	17.78 ± 0.13	4.38 ± 0.42

Experiments – TSP20

Traveling Salesperson with 20 Nodes

Average Test Normalized Regret (%) with Standard Deviation

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	12.12 ± 0.89	7.35 ± 0.40	6.20 ± 0.24	7.69 ± 0.33	**5.95** ± 0.16	6.56 ± 0.21	12.21 ± 0.88
Deg 6	21.32 ± 1.81	8.01 ± 0.45	**6.97** ± 0.37	9.52 ± 0.64	7.48 ± 0.36	7.41 ± 0.37	14.31 ± 0.40

Average Training Time (Sec) with Standard Deviation

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	1.52 ± 0.10	113.56 ± 3.16	107.15 ± 3.80	27.06 ± 2.17	175.23 ± 4.95	220.21 ± 24.20	**25.92** ± 4.23
Deg 6	1.53 ± 0.19	158.66 ± 9.65	102.19 ± 10.38	30.17 ± 2.62	185.13 ± 7.44	185.02 ± 5.09	**25.48** ± 3.66

Experiments – TSP50

Traveling Salesperson with 50 Nodes

Average Test Normalized Regret (%) with Standard Deviation

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	28.16 ± 1.08	15.19 ± 0.65	7.69 ± 0.22	9.59 ± 0.44	**7.57** ± 0.20	8.03 ± 0.23	14.31 ± 0.40
Deg 6	52.61 ± 2.36	23.25 ± 2.41	**8.57** ± 0.38	11.28 ± 0.80	10.26 ± 0.46	9.00 ± 0.52	17.12 ± 0.48

Average Training Time (Sec) with Standard Deviation

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	1.55 ± 0.18	611.47 ± 23.52	518.07 ± 51.89	196.96 ± 35.92	1220.68 ± 85.39	1328.99 ± 28.87	**151.80** ± 24.21
Deg 6	1.16 ± 0.13	502.71 ± 16.03	573.87 ± 20.19	253.93 ± 27.67	1191.29 ± 42.63	1456.21 ± 34.18	**155.95** ± 24.46

Experiments – CVRP20

Capacity Vehicle Routing with 20 Nodes

Average Test Normalized Regret (%) with Standard Deviation

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	10.10 ± 0.64	9.26 ± 1.56	6.44 ± 0.24	7.92 ± 0.52	**5.94** ± 0.25	6.32 ± 0.28	15.77 ± 0.96
Deg 6	19.50 ± 1.22	11.64 ± 0.25	**7.94** ± 0.54	11.44 ± 1.14	8.75 ± 0.28	8.09 ± 0.57	18.96 ± 1.01

Average Training Time (Sec) with Standard Deviation

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	1.65 ± 0.48	213.56 ± 42.36	153.56 ± 11.08	**44.52** ± 6.27	7020.11 ± 1043.05	3773.31 ± 288.84	583.56 ± 170.67
Deg 6	1.54 ± 0.25	208.95 ± 12.90	127.94 ± 13.84	**51.83** ± 8.78	2204.83 ± 99.86	6197.84 ± 288.63	470.20 ± 84.46

Experiments – CVRP30

Due to the scale of the problem, we did not repeat our experimental evaluation with random seeds.

Capacity Vehicle Routing with 30 Nodes

Test Normalized Regret (%)

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	19.72	12.54	**9.13**	9.99	N/A		18.28

Training Time (Sec)

Methods	2-Stage	CaVE-E	CaVE+	CaVE-H	SPO+	PFYL	NCE
Deg 4	9.27	331.73	287.77	**132.62**	≥100h		884.95

Experiments – Relaxation

Traveling Salesperson with 50 Nodes

Average Test Normalized Regret (%)

Methods	CaVE+	SPO+ Rel	PFYL Rel
Deg 4	**7.69** ± 0.22	10.17 ± 0.23	11.11 ± 0.33
Deg 6	**8.57** ± 0.38	13.14 ± 0.46	13.38 ± 0.58

Average Training Time (Sec)

Methods	CaVE+	SPO+ Rel	PFYL Rel
Deg 4	518.07 ± 51.89	**386.06** ± 9.69	536.67 ± 4.94
Deg 6	573.87 ± 20.19	636.99 ± 3.04	**510.37** ± 3.46

Capacity Vehicle Routing with 20 Nodes

Average Test Normalized Regret (%)

Methods	CaVE+	SPO+ Rel	PFYL Rel
Deg 4	**6.44** ± 0.24	8.03 ± 0.38	17.07 ± 0.63
Deg 6	**7.94** ± 0.54	15.73 ± 0.39	19.19 ± 1.66

Average Training Time (Sec)

Methods	CaVE+	SPO+ Rel	PFYL Rel
Deg 4	153.56 ± 11.08	78.95 ± 0.73	**78.80** ± 1.19
Deg 6	127.94 ± 13.84	**78.74** ± 3.82	81.80 ± 0.86

Thank You

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