Data-Driven Optimal Control:

An Inverse Optimization Model and Algorithm

Long, Youyuan

Supervisor: Peyman Mohajerin Esfahani

Daily Supervisors: Tolga Ok

Pedro Zattoni Scroccaro

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Contents

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Introduction of Inverse Optimization (IO)

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Inverse Optimization

Given a *state (input)*, the expert determines its optimal *action (output)* by optimizing an unknown cost

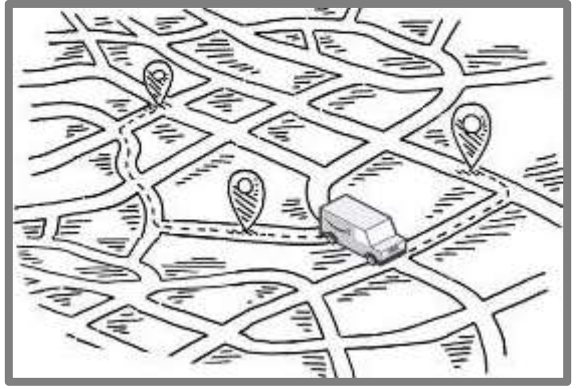
Expert

$$\hat{s} \longrightarrow \boxed{\arg\min_{u \in \mathbb{U}(\hat{s})} F(\hat{s}, u)} \longrightarrow \hat{u}$$

Market behavior

Saez-Gallego et al. ’16

Driver preference



Scroccaro et al. ’23

Control policy

Akhtar et al. ’21

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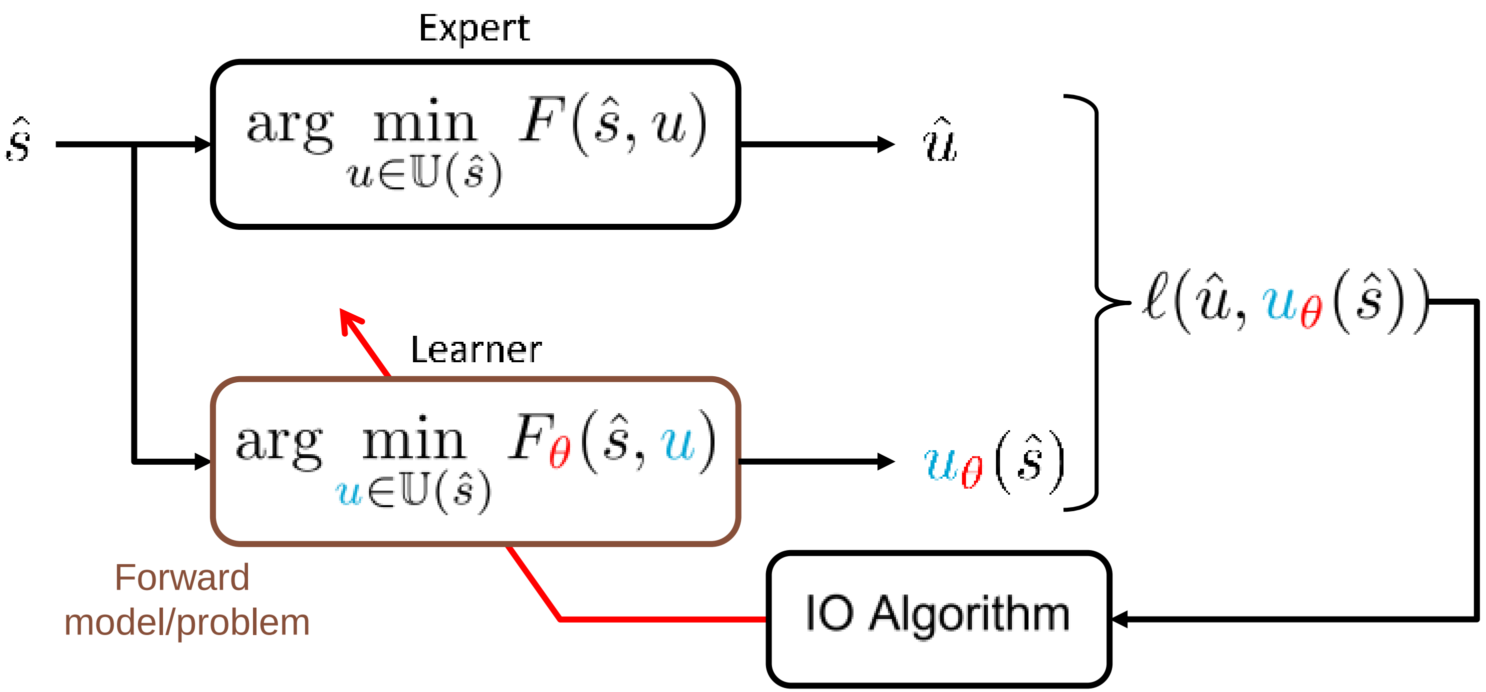
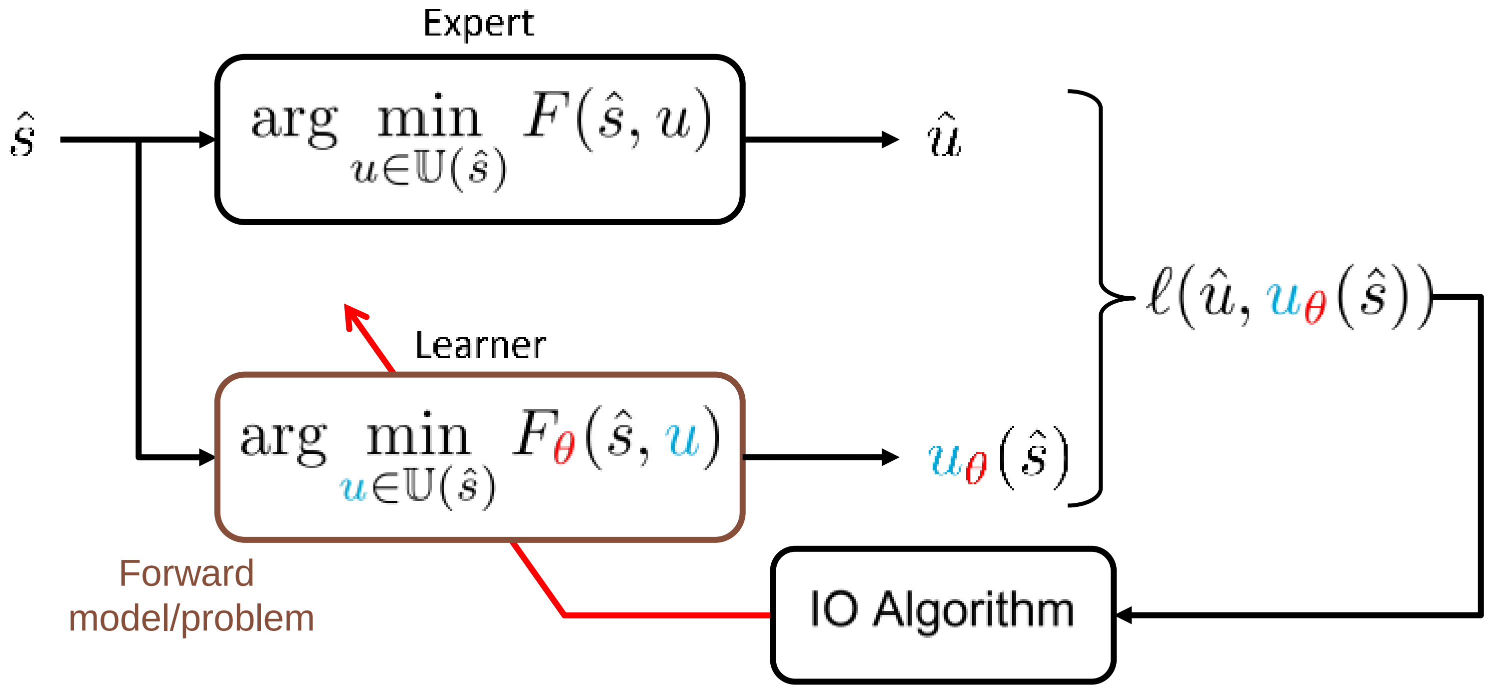
Supervised Learning Point of View

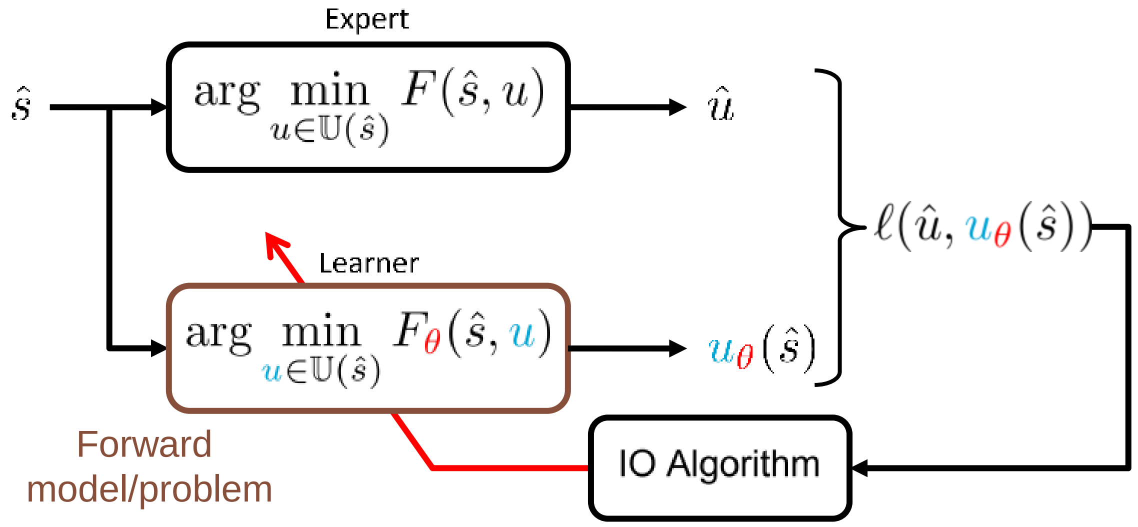


Supervised Learning Point of View



Inverse Optimization Summary

- Hypothesis space: $\{F_\theta \mid \theta \in \Theta\}$



- Loss function: $\ell(\hat{u}, u_\theta(\hat{s}))$

- Training: $\min_{\theta \in \Theta} \kappa \mathcal{R}(\theta) + \frac{1}{N} \sum_{i=1}^{N} \ell(\hat{u}_i, u_\theta(\hat{s}_i))$ $\qquad \hat{\mathcal{D}} = \{(\hat{s}_i, \hat{u}_i)\}_{i=1}^{N}$

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Quadratic Hypothesis Space

Augmented state/feature

Quadratic cost: $F_\theta(\hat{s}, u) = u^T \theta_{uu} u + 2\phi(\hat{s})^T \theta_{su} u, \;\; \theta := (\theta_{uu}, \theta_{su})$

Linear constraints: $\mathbb{U}(\hat{s}) = \{u \in \mathbb{R}^n \mid M(\hat{s})u \leq W(\hat{s})\}$

$$\min_{u \in \mathbb{U}(\hat{s})} F_\theta(\hat{s}, u)$$

To ensure the **convexity** of the Forward Problem w.r.t u, extra constraints should be imposed on θ:

$$\theta \in \{(\theta_{uu}, \theta_{su}) \mid \theta_{uu} \succeq I\}$$

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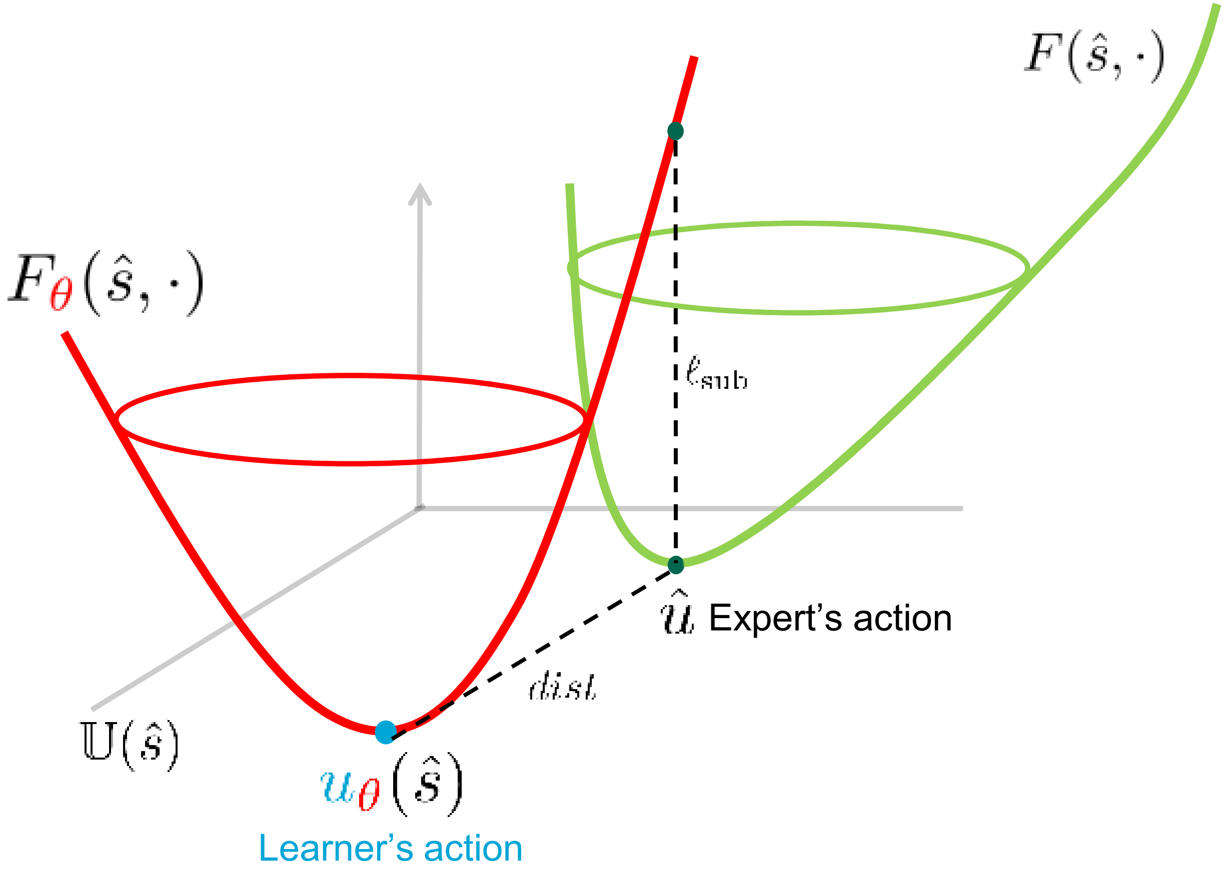
Suboptimality Loss Function [1]

$$\ell_{\text{sub}}(\hat{s},\hat{u}) := F_\theta(\hat{s},\hat{u}) - F_\theta(\hat{s}, u_\theta(\hat{s}))$$

$$u_\theta(\hat{s}) = \arg\min_{u\in\mathbb{U}(\hat{s})} F_\theta(\hat{s}, u)$$



[1] Mohajerin Esfahani P, Shafieezadeh-Abadeh S, Hanasusanto G A, et al. Data-driven inverse optimization with imperfect information[J]. Mathematical Programming, 2018, 167: 191-234.

Suboptimality Loss Function[1]

$$\ell_{\text{sub}}(\hat{s}, \hat{u}) := F_\theta(\hat{s}, \hat{u}) - F_\theta(\hat{s}, u_\theta(\hat{s}))$$

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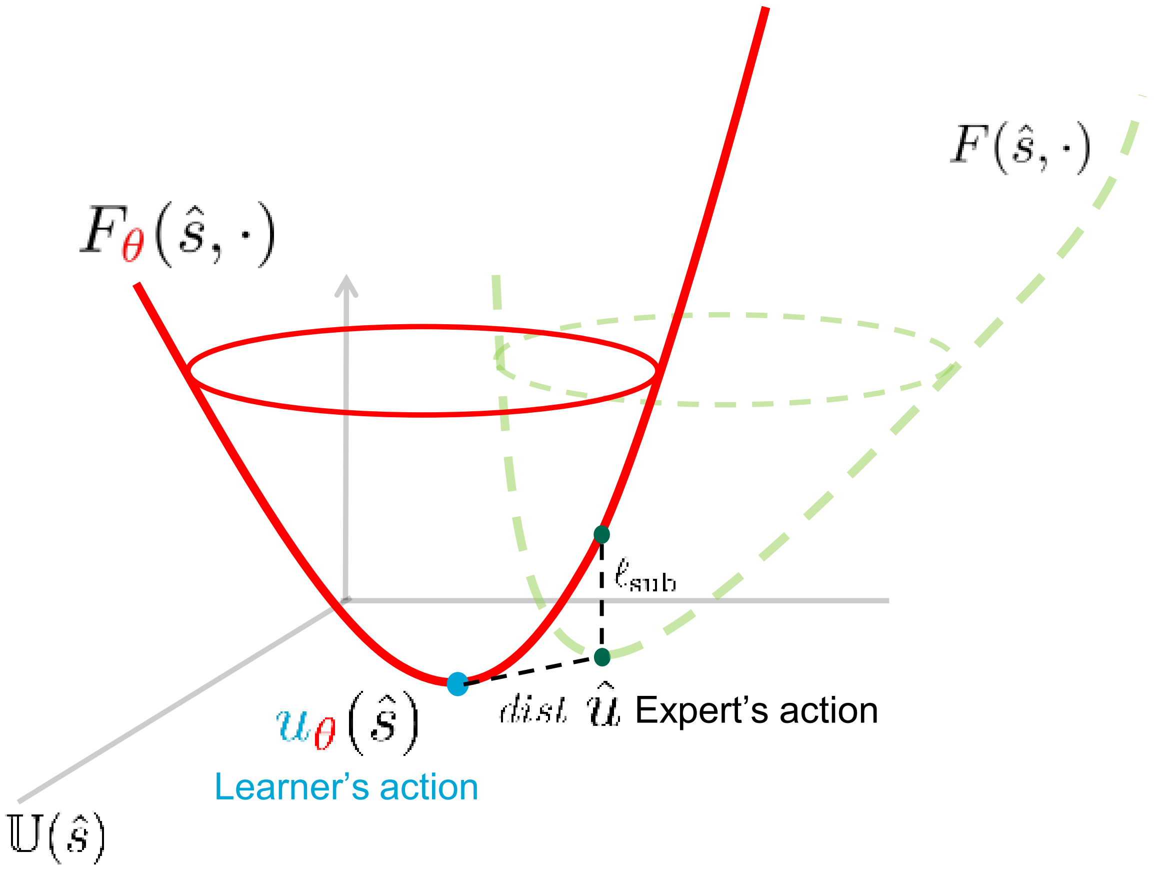

[1] Mohajerin Esfahani P, Shafieezadeh-Abadeh S, Hanasusanto G A, et al. Data-driven inverse optimization with imperfect information[J]. Mathematical Programming, 2018, 167: 191-234.

Regularized training

$$\min_{\theta} k\|\theta_{uu}\|_F^2 + k\|\theta_{su}\|_F^2 + \frac{1}{N}\sum_{i=1}^{N}\left\{F_\theta(\hat{s}_i, \hat{u}_i) - \min_{u\in\mathbb{U}(\hat{s}_i)} F_\theta(\hat{s}_i, u)\right\}$$
$$\text{s.t. } \theta_{uu} \succeq I$$

Convex w.r.t θ !

$$\hat{\mathcal{D}} = \{(\hat{s}_i, \hat{u}_i)\}_{i=1}^N$$

Quadratic cost: $F_\theta(\hat{s}, u) = u^T\theta_{uu}u + 2\phi(\hat{s})^T\theta_{su}u, \ \theta_{uu} \succeq I$

Suboptimality loss: $\ell_{\text{sub}}(\hat{s}, \hat{u}) := F_\theta(\hat{s}, \hat{u}) - F_\theta(\hat{s}, u_\theta(\hat{s}))$

$$u_\theta(\hat{s}) = \arg\min_{u\in\mathbb{U}(\hat{s})} F_\theta(\hat{s}, u)$$

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Theorem 1 (LMI reformulation[1])

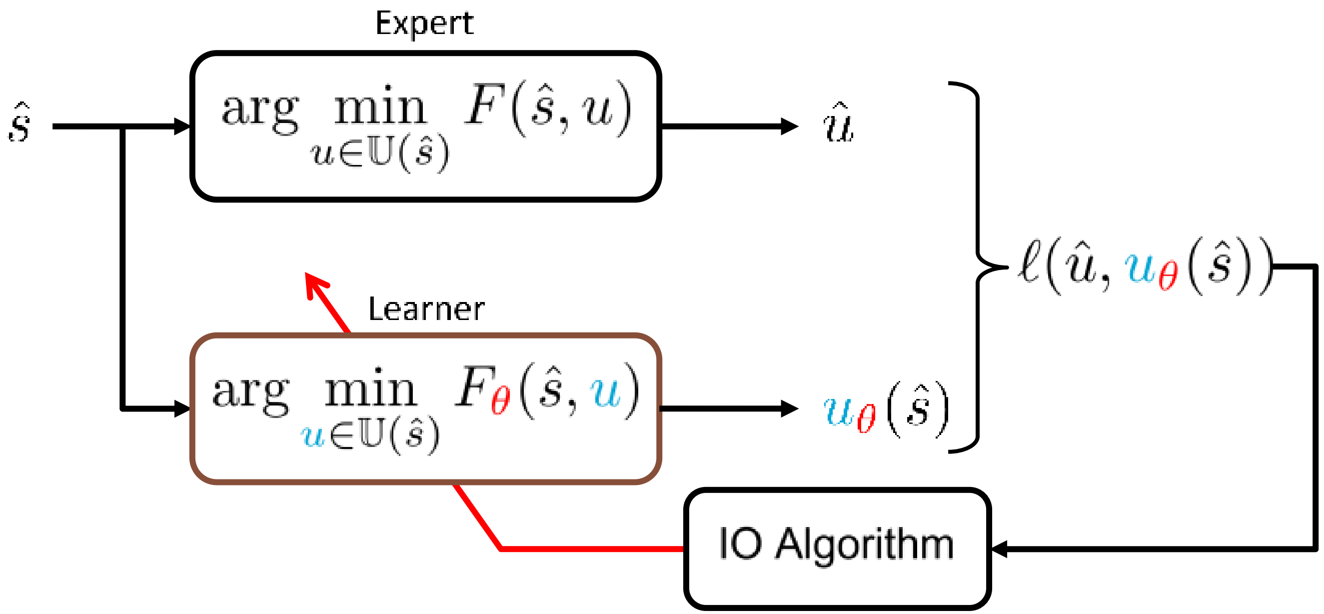
$$\min_{\theta} k\|\theta_{uu}\|_F^2 + k\|\theta_{su}\|_F^2 + \frac{1}{N}\sum_{i=1}^{N}\left\{F_\theta(\hat{s}_i,\hat{u}_i) - \min_{u\in\mathbb{U}(\hat{s}_i)} F_\theta(\hat{s}_i,u)\right\}$$
$$\text{s.t.}\quad \theta_{uu} \succeq I$$

$$\theta := (\theta_{uu}, \theta_{su})$$

Equivalent !

$$\begin{aligned}
\min_{\theta_{uu},\theta_{su},\lambda_i,\gamma_i}\quad & k\|\theta_{uu}\|_F^2 + k\|\theta_{su}\|_F^2 \\
& +\frac{1}{N}\sum_{i=1}^{N}\left(\hat{u}_i^T\theta_{uu}\hat{u}_i + 2\phi(\hat{s}_i)^T\theta_{su}\hat{u}_i + \frac{1}{4}\gamma_i + W(\hat{s}_i)^\top\lambda_i\right) \\
\text{s.t.}\quad & \theta_{uu}\succeq I,\ \lambda_i\in\mathbb{R}_+^d,\ \gamma_i\in\mathbb{R},\quad \forall i\leq N \\
& \begin{bmatrix} \theta_{uu} & M(\hat{s}_i)^\top\lambda_i + 2\theta_{su}^T\phi(\hat{s}_i) \\ * & \gamma_i \end{bmatrix}\succeq 0,\quad \forall i\leq N
\end{aligned}$$

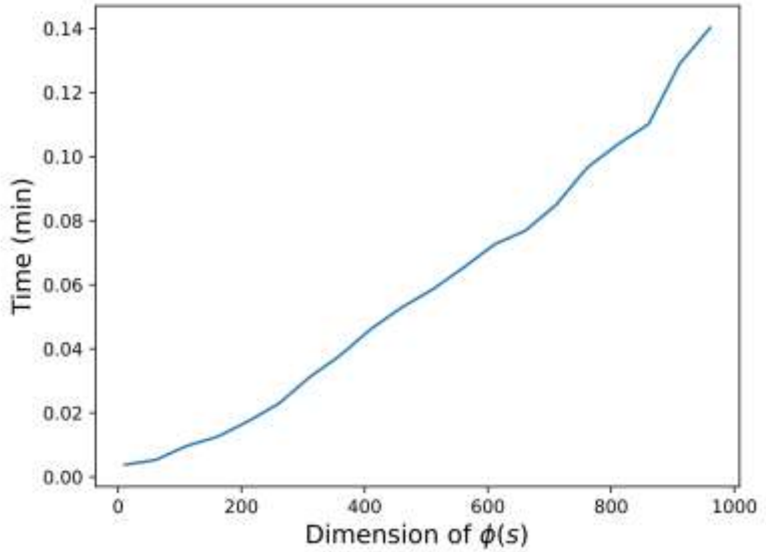
[1] Akhtar S A, Kolarijani A S, Esfahani P M. Learning for control: An inverse optimization approach[J]. IEEE Control Systems Letters, 2021, 6: 187-192.



Expert
$\hat{s}$
$\arg\min_{u \in \mathbb{U}(\hat{s})} F(\hat{s}, u)$
$\hat{u}$
$\ell(\hat{u}, u_\theta(\hat{s}))$
Learner
$\arg\min_{u \in \mathbb{U}(\hat{s})} F_\theta(\hat{s}, u)$
$u_\theta(\hat{s})$
IO Algorithm

Contributions

- Heavy computational burden by high-dimensional augmented feature



- Challenges of feature engineering

KIOM

- Scalability issues caused by large datasets

Data size	Memory (RAM)
5K	16GB
10K	64GB
15K	128GB
20K	256GB

Table: The relationship between the dataset size and the required memory on the Halfcheetah-expert task.

SSO

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Kernel Inverse Optimization Machine

(KIOM)

---- Solution for heavy computational burden by high-dimensional augmented feature and challenges of feature engineering

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Theorem 2 (Kernel reformulation)

$$\begin{aligned}
\min_{\theta_{uu},\theta_{su},\lambda_i,\gamma_i} \quad & k\|\theta_{uu}\|_F^2 + k\|\theta_{su}\|_F^2 + \frac{1}{N}\sum_{i=1}^{N}\left(\hat{u}_i^T\theta_{uu}\hat{u}_i + 2\phi(\hat{s}_i)^T\theta_{su}\hat{u}_i + \frac{1}{4}\gamma_i + W\left(\hat{s}_i\right)^\top\lambda_i\right) \\
\text{s.t.} \quad & \theta_{uu} \succeq I,\ \lambda_i \in \mathbb{R}_+^d,\ \gamma_i \in \mathbb{R}, \quad \forall i \leq N \\
& \begin{bmatrix} \theta_{uu} & M\left(\hat{s}_i\right)^\top\lambda_i + 2\theta_{su}^T\phi(\hat{s}_i) \\ * & \gamma_i \end{bmatrix} \succeq 0, \quad \forall i \leq N
\end{aligned}$$

[LMI reformulation]

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Theorem 2 (Kernel reformulation)

$$\begin{aligned}\min_{\theta_{uu},\theta_{su},\lambda_i,\gamma_i} \quad & k\|\theta_{uu}\|_F^2 + k\|\theta_{su}\|_F^2 + \frac{1}{N}\sum_{i=1}^{N}\left(\hat{u}_i^T\theta_{uu}\hat{u}_i + 2\phi(\hat{s}_i)^T\theta_{su}\hat{u}_i + \frac{1}{4}\gamma_i + W(\hat{s}_i)^\top\lambda_i\right)\\ \text{s.t.} \quad & \theta_{uu} \succeq I_n,\ \lambda_i \in \mathbb{R}_+^d,\ \gamma_i \in \mathbb{R}, \quad \forall i \le N\\ & \begin{bmatrix}\theta_{uu} & M(\hat{s}_i)^\top\lambda_i + 2\theta_{su}^T\phi(\hat{s}_i)\\ * & \gamma_i\end{bmatrix} \succeq 0, \quad \forall i \le N\end{aligned}$$

Primal

Dual

$$\begin{aligned}\min_{P,\Lambda_i,\Gamma_i} \quad & \frac{1}{4k}\left\|\left(\sum_{i=1}^{N}\frac{\hat{u}_i\hat{u}_i^T}{N} - \Lambda_i\right) - P\right\|_F^2 - \mathrm{Tr}(P)\\ & + \frac{1}{k}\sum_{i=1}^{N}\sum_{j=1}^{N}\kappa(\hat{s}_i,\hat{s}_j)\left(\frac{\hat{u}_i}{N} - 2\Gamma_i\right)^T\left(\frac{\hat{u}_j}{N} - 2\Gamma_j\right)\\ \text{s.t.} \quad & P \succeq 0,\ \frac{W(\hat{s}_i)}{N} - 2M(\hat{s}_i)\Gamma_i \ge 0, \quad \forall i \le N\\ & \begin{bmatrix}\Lambda_i & \Gamma_i\\ * & \frac{1}{4N}\end{bmatrix} \succeq 0, \quad \forall i \le N\end{aligned}$$

$$\kappa(\hat{s}_i,\hat{s}_j) = \phi(\hat{s}_i)^T\phi(\hat{s}_j)$$

Recover θ

KIOM

$$\theta_{uu} = -\frac{\left(\sum_{i=1}^{N}\frac{\hat{u}_i\hat{u}_i^T}{N} - \Lambda_i\right) - P}{2k}$$

$$\theta_{su} = -\frac{\sum_{i=1}^{N}\phi(\hat{s}_i)\left(\frac{\hat{u}_i^T}{N} - 2\Gamma_i{}^T\right)}{k}$$

Theorem 2 (Kernel reformulation)

KIOM

$$\theta_{uu} = -\frac{\left(\sum_{i=1}^{N} \frac{\hat{u}_i \hat{u}_i^T}{N} - \Lambda_i\right) - P}{2k}$$

$$\theta_{su} = -\frac{\sum_{i=1}^{N} \phi(\hat{s}_i) \left(\frac{\hat{u}_i^T}{N} - 2{\Gamma_i}^T\right)}{k}$$

$$\begin{aligned} \min_{P,\Lambda_i,\Gamma_i} \quad & \frac{1}{4k}\left\| \left(\sum_{i=1}^{N} \frac{\hat{u}_i \hat{u}_i^T}{N} - \Lambda_i\right) - P \right\|_F^2 - \mathrm{Tr}(P) \\ & + \frac{1}{k}\sum_{i=1}^{N}\sum_{j=1}^{N} \kappa(\hat{s}_i, \hat{s}_j)\left(\frac{\hat{u}_i}{N} - 2\Gamma_i\right)^T \left(\frac{\hat{u}_j}{N} - 2\Gamma_j\right) \\ \text{s.t.} \quad & P \succeq 0, \quad \frac{W(\hat{s}_i)}{N} - 2M(\hat{s}_i)\Gamma_i \geq 0, \quad \forall i \leq N \\ & \begin{bmatrix} \Lambda_i & \Gamma_i \\ * & \frac{1}{4N} \end{bmatrix} \succeq 0, \quad \forall i \leq N \end{aligned}$$

$$\kappa(\hat{s}_i, \hat{s}_j) = \phi(\hat{s}_i)^T \phi(\hat{s}_j)$$

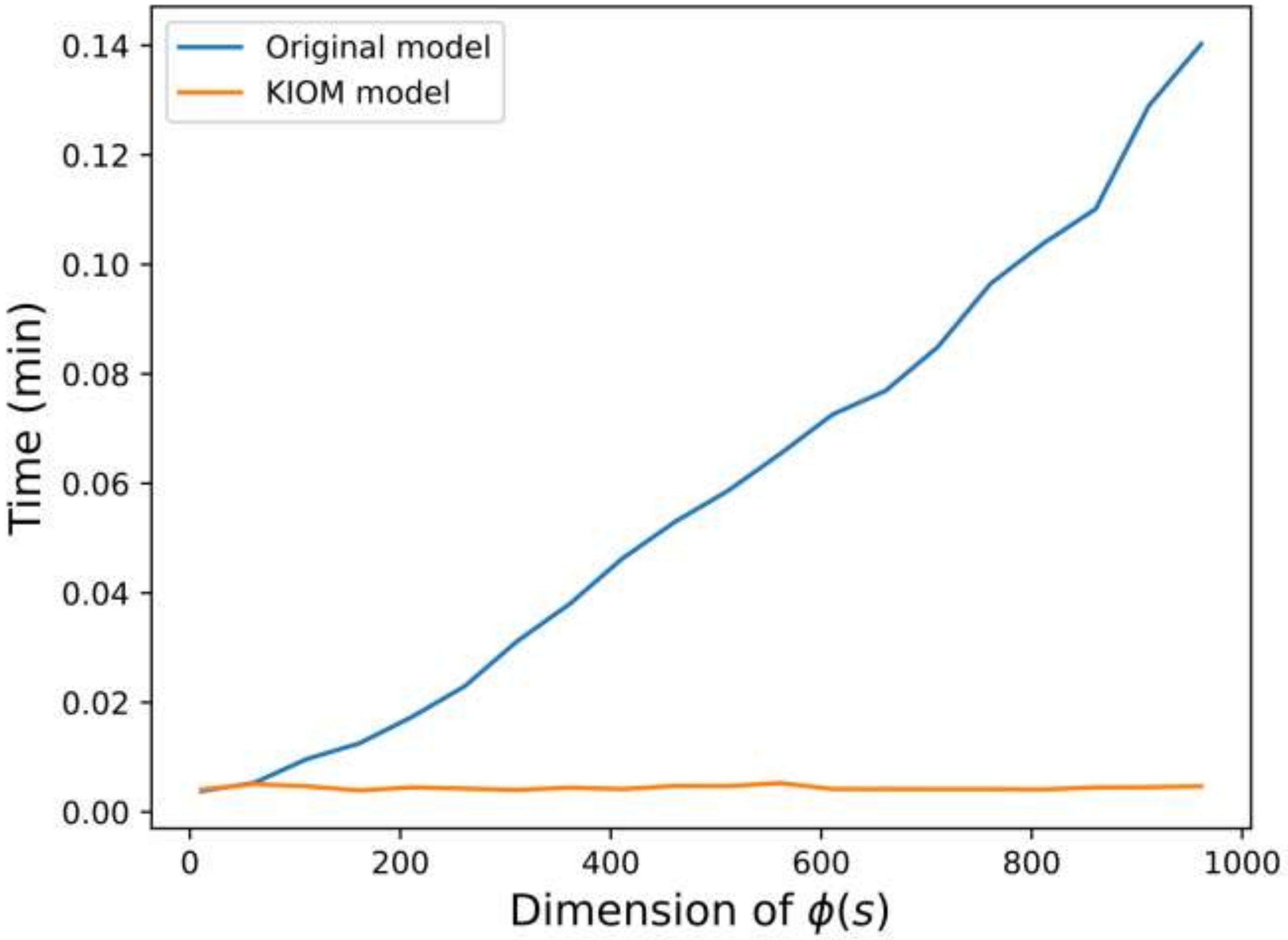
Recover θ

Forward problem:

$$\min_{u \in \mathbb{U}(s)} u^T \theta_{uu} u + \underbrace{2\phi(s)^T \theta_{su}}_{-\frac{1}{k}\sum_{i=1}^{N} \kappa(s, \hat{s}_i)\left(\frac{\hat{u}_i^T}{N} - 2{\Gamma_i}^T\right)} u$$

Does the KIOM model address the first two deficiencies mentioned before?

- Heavy computational burden by high-dimensional augmented feature
- Challenges of feature engineering



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Variant: A Simpler Version with $\theta_{uu} = I$

KIOM

$$\theta_{uu} = -\frac{\left(\sum_{i=1}^{N} \frac{\hat{u}_i \hat{u}_i^T}{N} - \Lambda_i\right) - P}{2k}$$

$$\theta_{su} = -\frac{\sum_{i=1}^{N} \phi(\hat{s}_i)\left(\frac{\hat{u}_i^T}{N} - 2{\Gamma_i}^T\right)}{k}$$

$$\begin{aligned}
\min_{P,\Lambda_i,\Gamma_i} \quad & \frac{1}{4k}\left\|\left(\sum_{i=1}^{N} \frac{\hat{u}_i \hat{u}_i^T}{N} - \Lambda_i\right) - P\right\|_F^2 - \operatorname{Tr}(P) \\
& + \frac{1}{k}\sum_{i=1}^{N}\sum_{j=1}^{N} \kappa(\hat{s}_i, \hat{s}_j)\left(\frac{\hat{u}_i}{N} - 2\Gamma_i\right)^T\left(\frac{\hat{u}_j}{N} - 2\Gamma_j\right) \\
\text{s.t.} \quad & P \succeq 0, \quad \frac{W(\hat{s}_i)}{N} - 2M(\hat{s}_i)\Gamma_i \geq 0, \quad \forall i \leq N \\
& \begin{bmatrix} \Lambda_i & \Gamma_i \\ * & \frac{1}{4N} \end{bmatrix} \succeq 0, \quad \forall i \leq N
\end{aligned}$$

$\theta_{uu} = I$

Simple KIOM

$$\begin{aligned}
\min_{\Lambda_i,\Gamma_i} \quad & \frac{1}{k}\sum_{i=1}^{N}\sum_{j=1}^{N} \kappa(\hat{s}_i, \hat{s}_j)\left(\frac{\hat{u}_i}{N} - 2\Gamma_i\right)^T\left(\frac{\hat{u}_j}{N} - 2\Gamma_j\right) + \sum_{i=1}^{N} \operatorname{Tr}(\Lambda_i) \\
\text{s.t.} \quad & \frac{W(\hat{s}_i)}{N} - 2M(\hat{s}_i)\Gamma_i \geq 0, \quad \forall i \leq N \\
& \begin{bmatrix} \Lambda_i & \Gamma_i \\ * & \frac{1}{4N} \end{bmatrix} \succeq 0, \quad \forall i \leq N
\end{aligned}$$

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Scalability issues caused by large datasets

Data size	Memory (RAM)
5K	16GB
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Table: The relationship between the dataset size and the required memory on the Halfcheetah-expert task.

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Sequential Selection Optimization (SSO)

- ---- Solution for Scalability issues caused by large datasets

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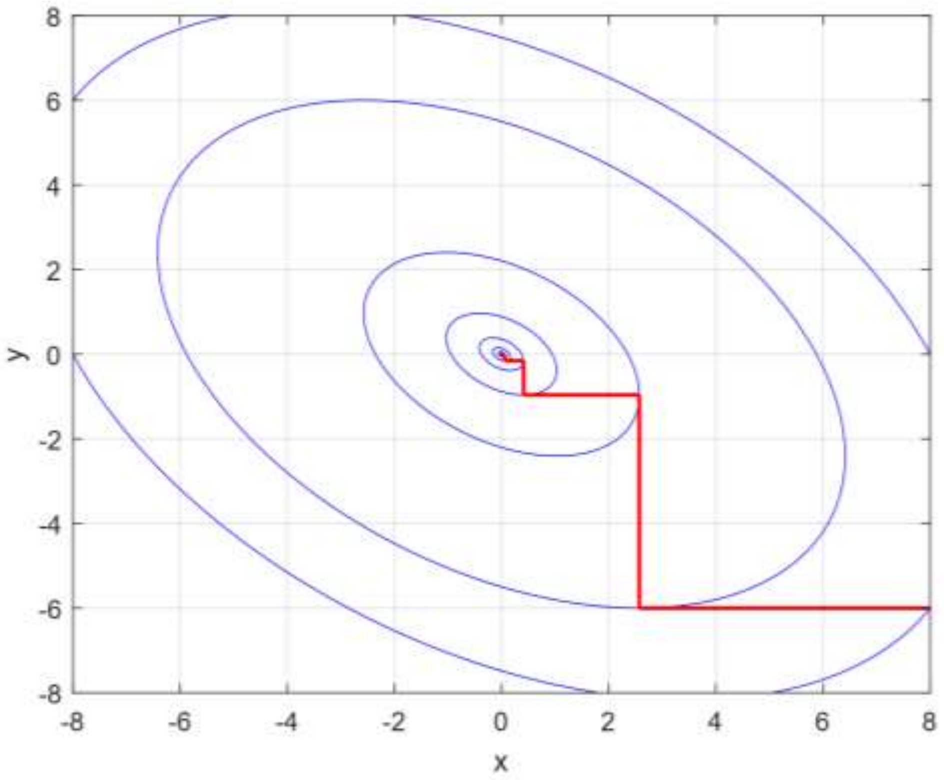
Coordinate Descent Method

- Coupled cost, decoupled constraints

$$\min_{x^1,\dots x^N} f(x^1,\dots,x^N)$$
$$\text{s.t. } x^i \in \mathcal{X}^i, \forall i \leq N$$



- Coordinate descent method

$$x^i_{k+1} = \arg\min_{\xi \in X_i} f\left(x^1_{k+1},\dots,x^{i-1}_{k+1},\xi,x^{i+1}_k,\dots,x^N_k\right)$$

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Why Does the Coordinate Descent (CD) Method Suit?

- Simple KIOM problem

$$
\begin{aligned}
\min_{\Lambda_i,\Gamma_i} \quad & \frac{1}{k}\sum_{i=1}^{N}\sum_{j=1}^{N}\kappa(\hat{s}_i,\hat{s}_j)\left(\frac{\hat{u}_i}{N}-2\Gamma_i\right)^T\left(\frac{\hat{u}_j}{N}-2\Gamma_j\right)+\sum_{i=1}^{N}\mathrm{Tr}(\Lambda_i) \\
\text{s.t.} \quad & \frac{W(\hat{s}_i)}{N}-2M(\hat{s}_i)\Gamma_i \geq 0, \quad \forall i \leq N \\
& \begin{bmatrix} \Lambda_i & \Gamma_i \\ * & \frac{1}{4N} \end{bmatrix} \succeq 0, \quad \forall i \leq N
\end{aligned}
$$

$$
\rightarrow \quad
\begin{aligned}
\min_{x^1,\ldots x^N} \; & f(x^1,\ldots,x^N) \\
\text{s.t.} \; & x^i \in \mathcal{X}^i, \forall i \leq N
\end{aligned}
$$

- Definition of coordinate

$$
\text{coordinate i} := \{\Lambda_i, \Gamma_i\}
$$

Each coordinate is decoupled in constraints !

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Two heuristics for SSO

- a. Heuristics for choosing which coordinates to optimize

Given the current values of $\{\Lambda_i, \Gamma_i\}_{i=1}^{N}$, we choose ***p*** coordinates that satisfy the condition

$$\frac{W(\hat{s}_i)}{N} - 2M(\hat{s}_i)\Gamma_i > 0$$

and have the largest KKT violators which is defined as

$$\text{KKT\_violator}(i) = \left| \mathrm{Tr}\left(\begin{bmatrix} \Lambda_i & \Gamma_i \\ * & \frac{1}{4N} \end{bmatrix} \begin{bmatrix} I_n & 2\theta_{su}^{\top}\phi(\hat{s}_i) \\ * & \|2\theta_{su}^{\top}\phi(\hat{s}_i)\|_2^2 \end{bmatrix} \right) \right|.$$

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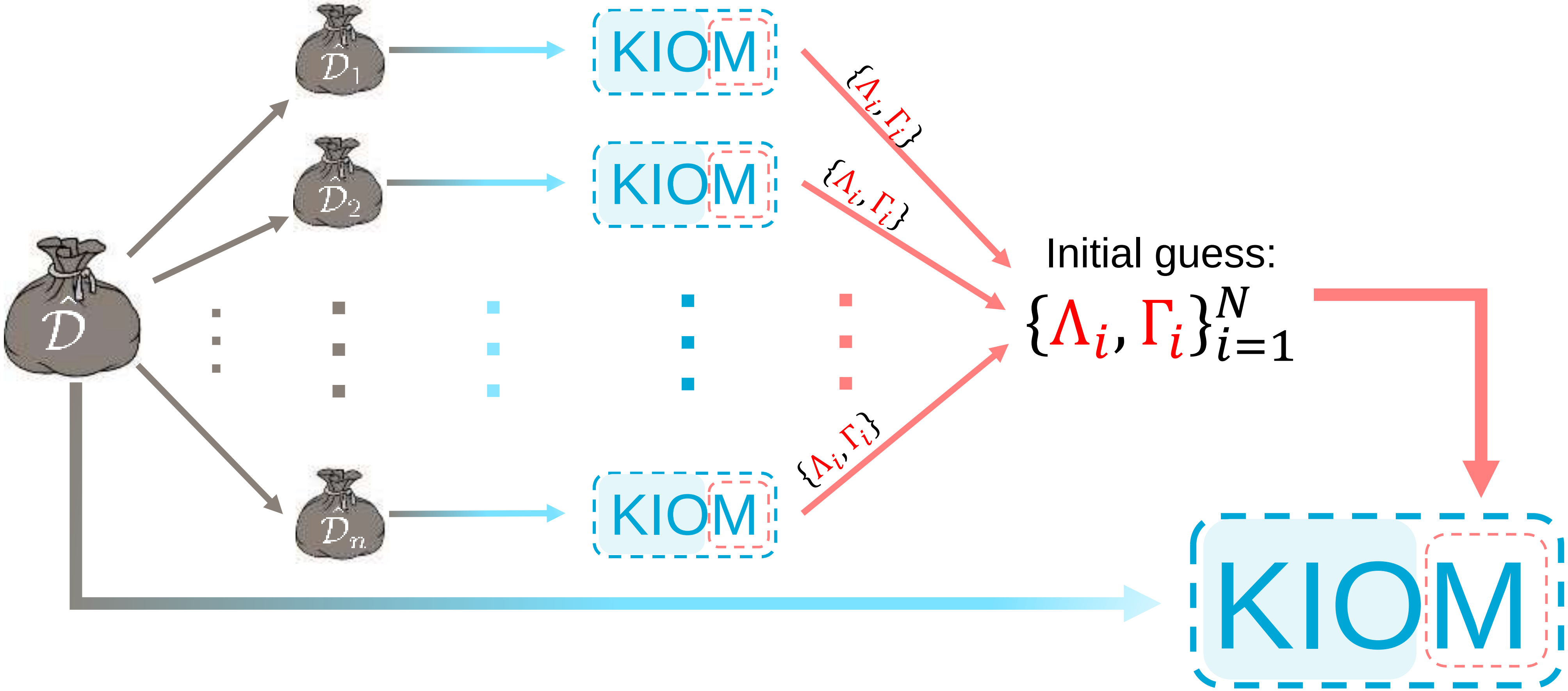
Two heuristics for SSO

- b. Warm-up trick for improved initial guess



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SSO Algorithm

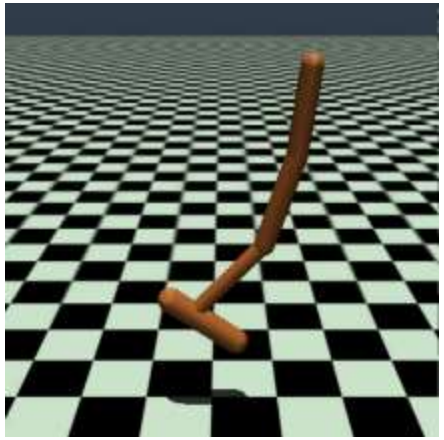
Algorithm 1 SSO

1: Initialize variable: $\{\Lambda_i, \Gamma_i\}_{i=1,\ldots,N} \leftarrow \text{WarmUp}(\{\hat{s}_i, \hat{u}_i\}_{i=1,\ldots N})$
2: **for** iteration = 1 to T **do**
3: $\quad \{\Lambda_{a_i}, \Gamma_{a_i}\}_{i=1,\ldots,p} \leftarrow \text{HeuristicSelection}(\{\hat{s}_i, \hat{u}_i\}_{i=1,\ldots N}, \{\Lambda_i, \Gamma_i\}_{i=1,\ldots,N})$
4: $\quad \text{Update}(\{\Lambda_{a_i}, \Gamma_{a_i}\}_{i=1,\ldots,p})$ (Update selected coordinates)
5: **end for**

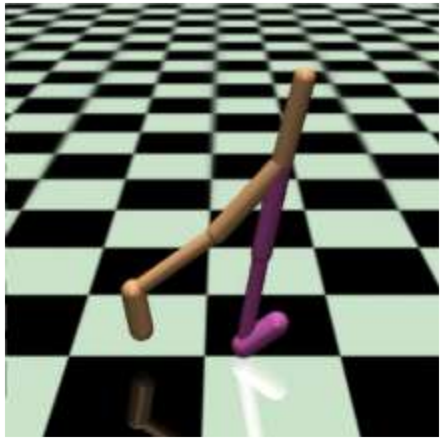
Numerical Experiments

Numerical Experiments

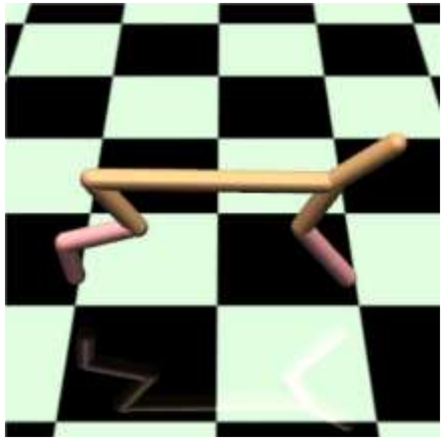
- Experimental environment



Hopper



Walker2d



HalfCheetah

Task	Action Dim	State Dim
Hopper	3	11
Walker2d	6	17
HalfCheetah	6	17

- Dataset

D4RL

- Expert dataset
- Medium dataset

- Solver

SCS
SPLITTING CONIC SOLVER

- Open-source
- Parallel processing

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Performance Evaluation of KIOM

Task	KIOM	IO	BC(TD3+BC)[1]	BC(CQL)[2]	Teacher agent
Hopper-expert	**109.9**(5k)	31.8	**111.5**	**109.0**	**108.5**
Hopper-medium	**50.2**(5k)	20.6	30.0	29.0	44.3
Walker2d-expert	108.5(10k)	0.9	56.0	**125.7**	107.1
Walker2d-medium	**74.6**(5k)	0.0	11.4	6.6	62.1
Halfcheetah-expert	84.4(10k)	-1.7	105.2	**107.0**	88.1
Halfcheetah-medium	**39.0**(5k)	-3.1	36.6	36.1	**40.7**

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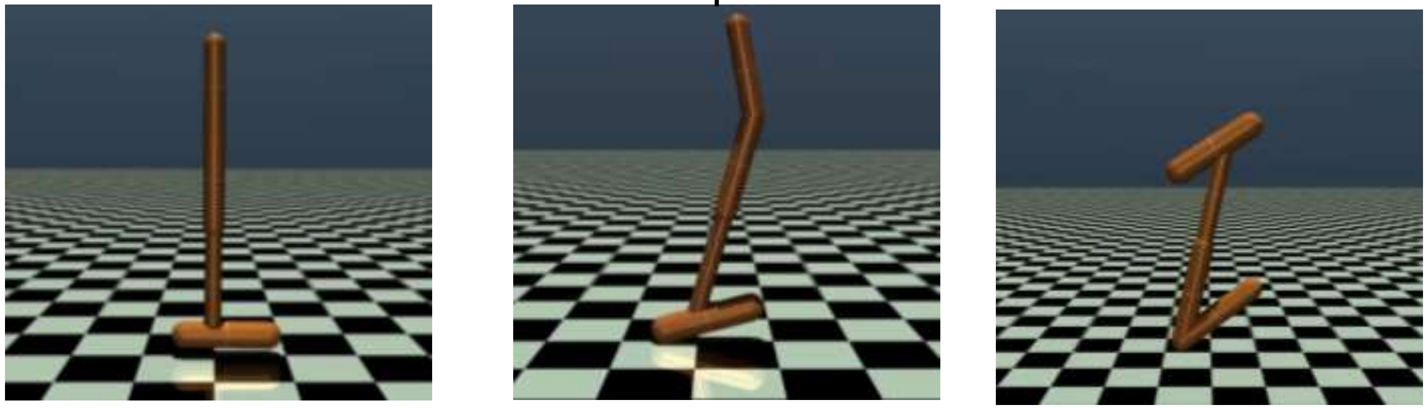
[1] Fujimoto S, Gu S S. A minimalist approach to offline reinforcement learning[J]. Advances in neural information processing systems, 2021, 34: 20132-20145.
[2] Kumar A, Zhou A, Tucker G, et al. Conservative q-learning for offline reinforcement learning[J]. Advances in Neural Information Processing Systems, 2020, 33: 1179-1191

Performance Evaluation of KIOM

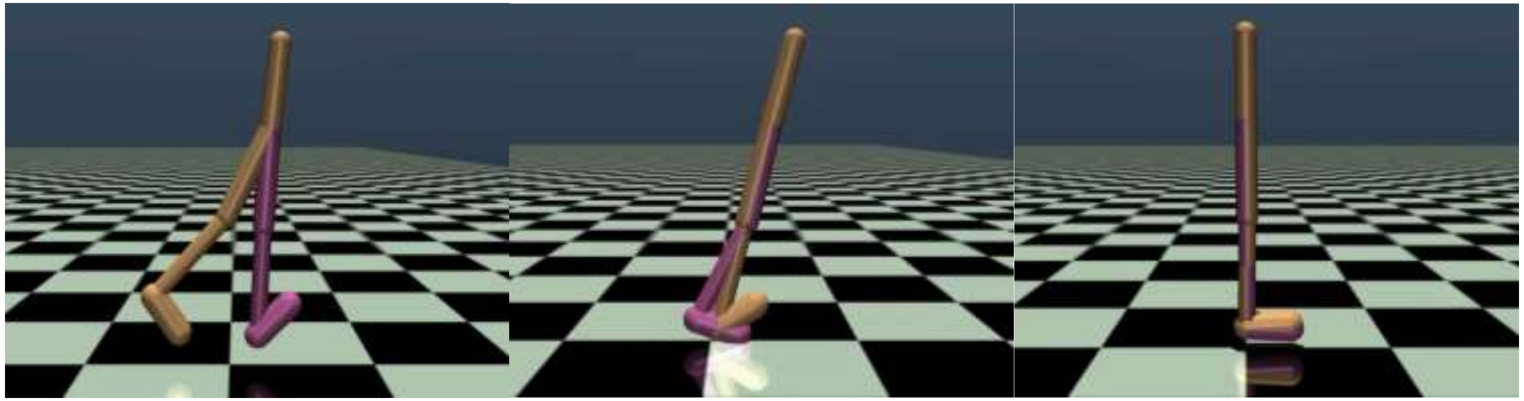
Task	KIOM	IO	BC(TD3+BC)[1]	BC(CQL)[2]	Teacher agent
Hopper-expert	**109.9**(5k)	31.8	**111.5**	**109.0**	**108.5**
Hopper-medium	**50.2**(5k)	20.6	30.0	29.0	44.3
Walker2d-expert	108.5(10k)	0.9	56.0	**125.7**	107.1
Walker2d-medium	**74.6**(5k)	0.0	11.4	6.6	62.1
Halfcheetah-expert	84.4(10k)	-1.7	105.2	**107.0**	88.1
Halfcheetah-medium	**39.0**(5k)	-3.1	36.6	36.1	**40.7**

KIOM Expert IO

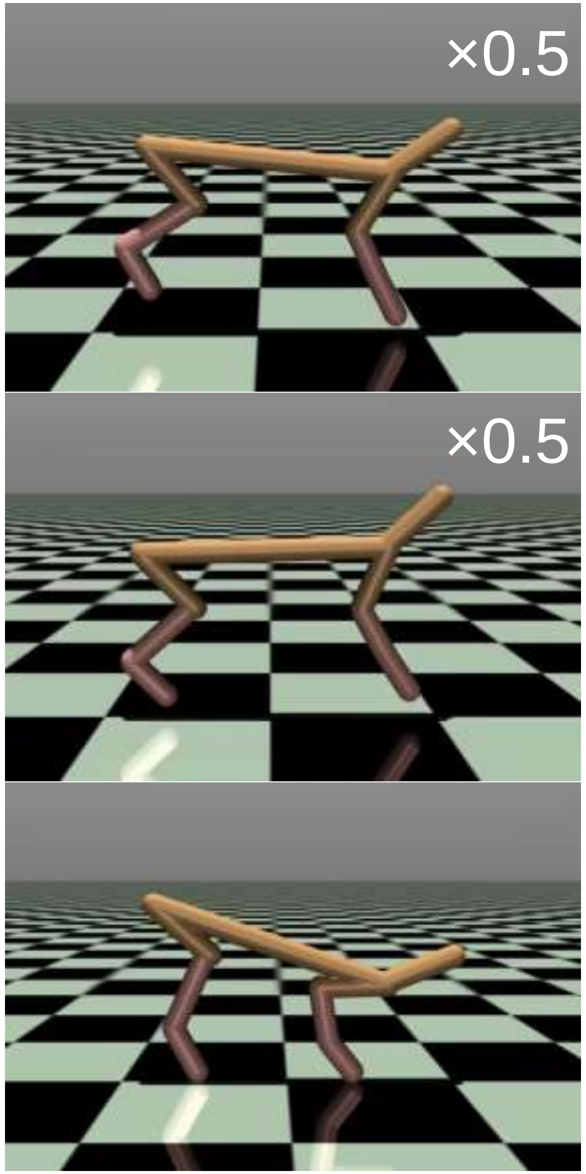
Hopper



Walker



Halfcheetah



KIOM

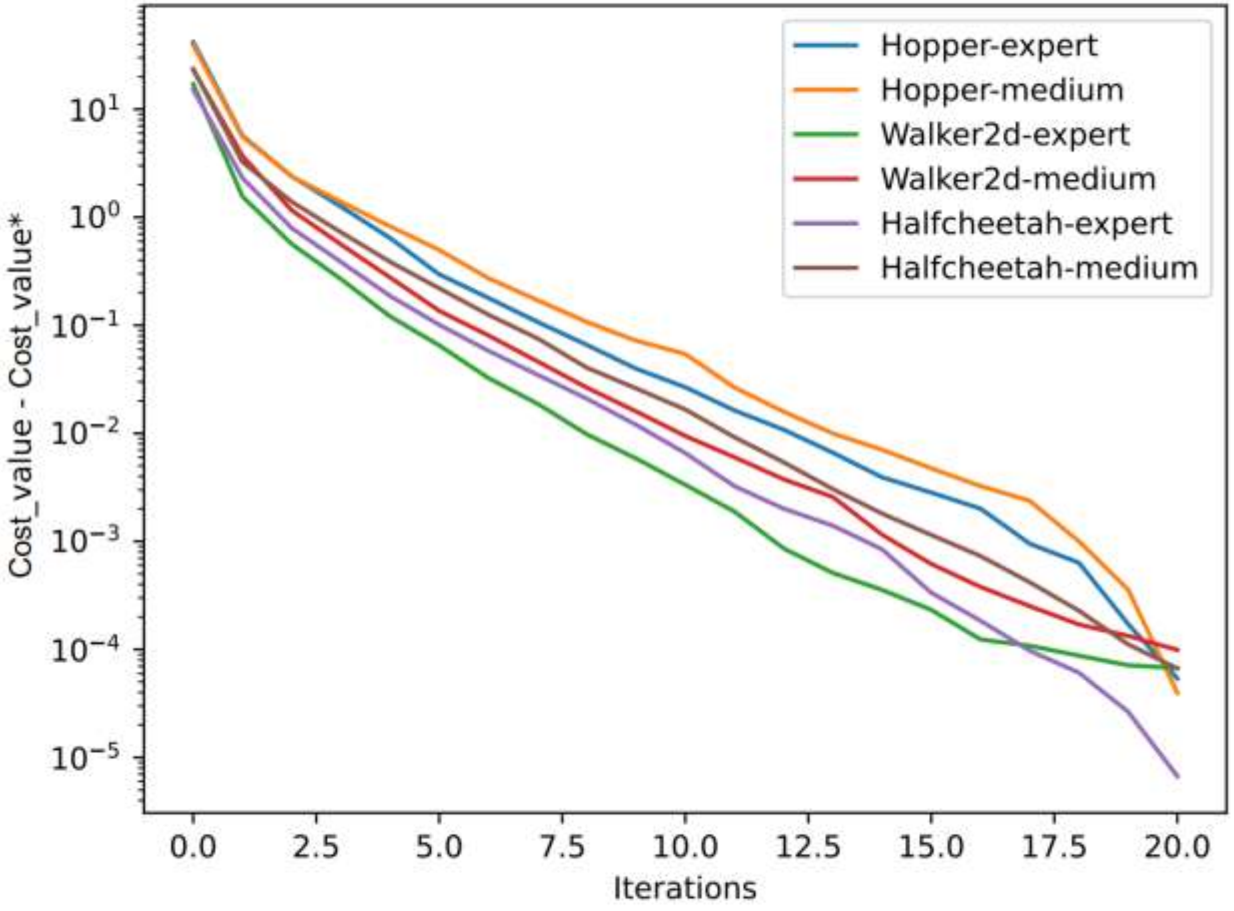
Expert

IO

Performance Evaluation of SSO

Task	SCS		SSO	
	Cost Value	Score	Cost Value	Score
Hopper-expert	185.219	109.9	185.220	110.2
Hopper-medium	218.761	50.2	218.761	51.8
Walker2d-expert	140.121	108.5	140.121	109.2
Walker2d-medium	151.117	74.6	151.117	74.9
Halfcheetah-expert	165.041	84.4	165.041	83.8
Halfcheetah-medium	188.184	39.0	188.184	39.7

Performance Evaluation of SSO



Task	SCS		SSO	
	Cost Value	**Score**	**Cost Value**	**Score**
Hopper-expert	185.219	109.9	185.220	110.2
Hopper-medium	218.761	50.2	218.761	51.8
Walker2d-expert	140.121	108.5	140.121	109.2
Walker2d-medium	151.117	74.6	151.117	74.9
Halfcheetah-expert	165.041	84.4	165.041	83.8
Halfcheetah-medium	188.184	39.0	188.184	39.7

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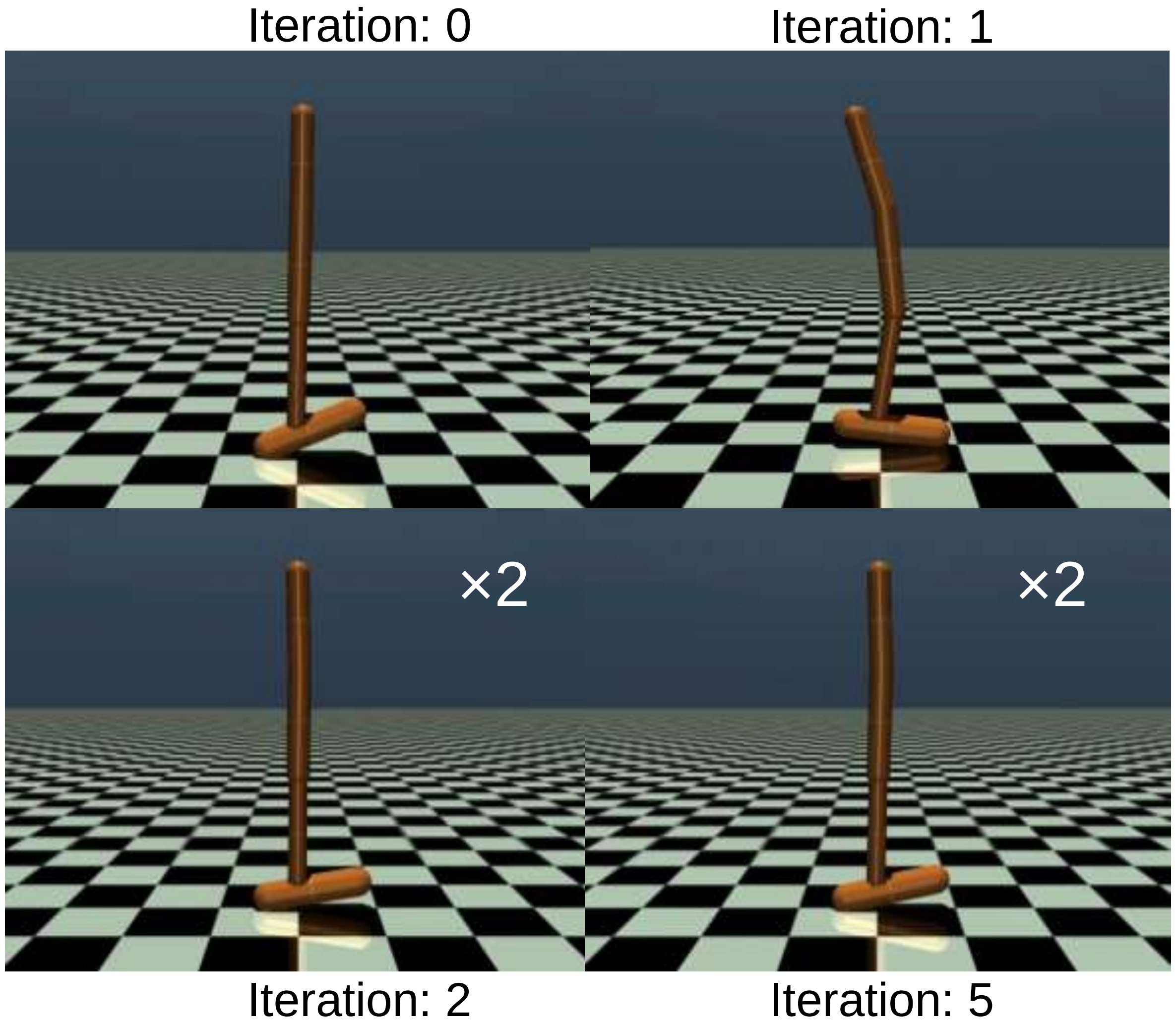
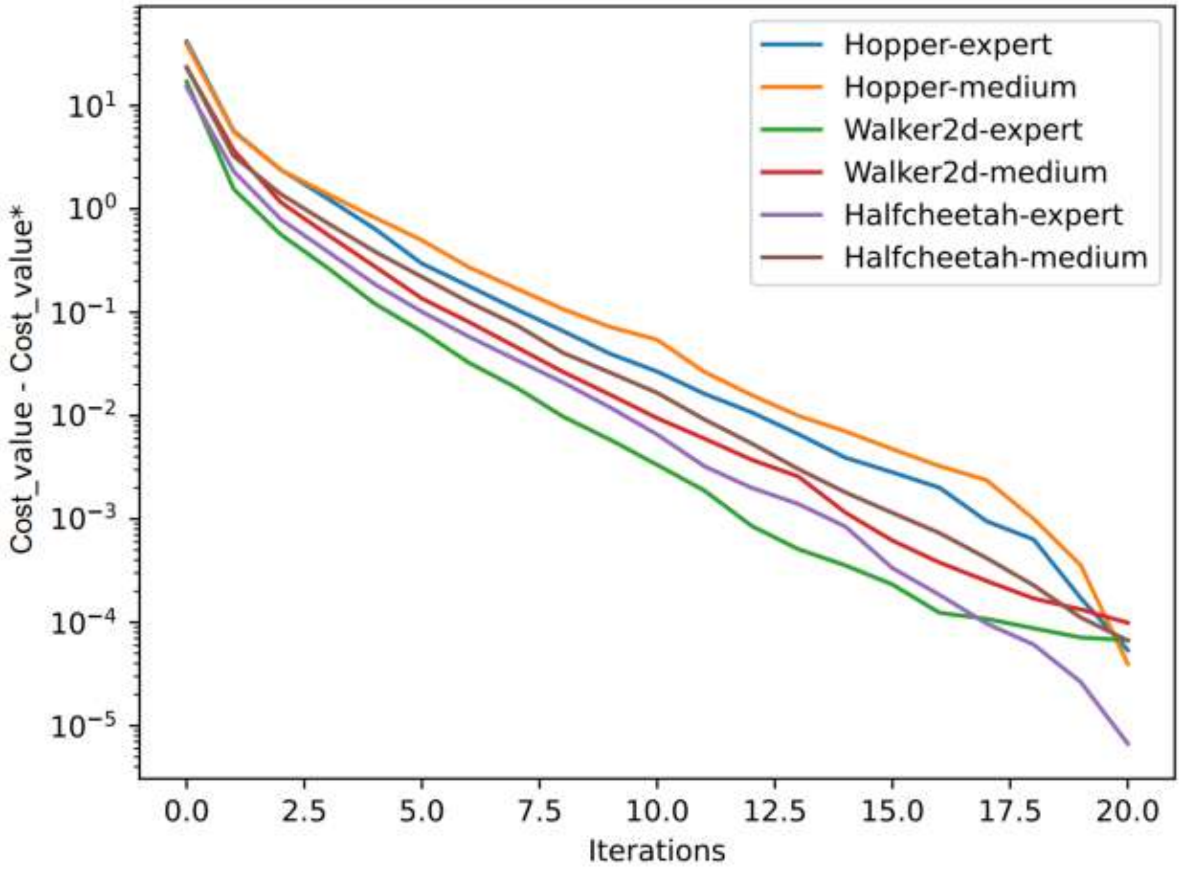
Performance Evaluation of SSO

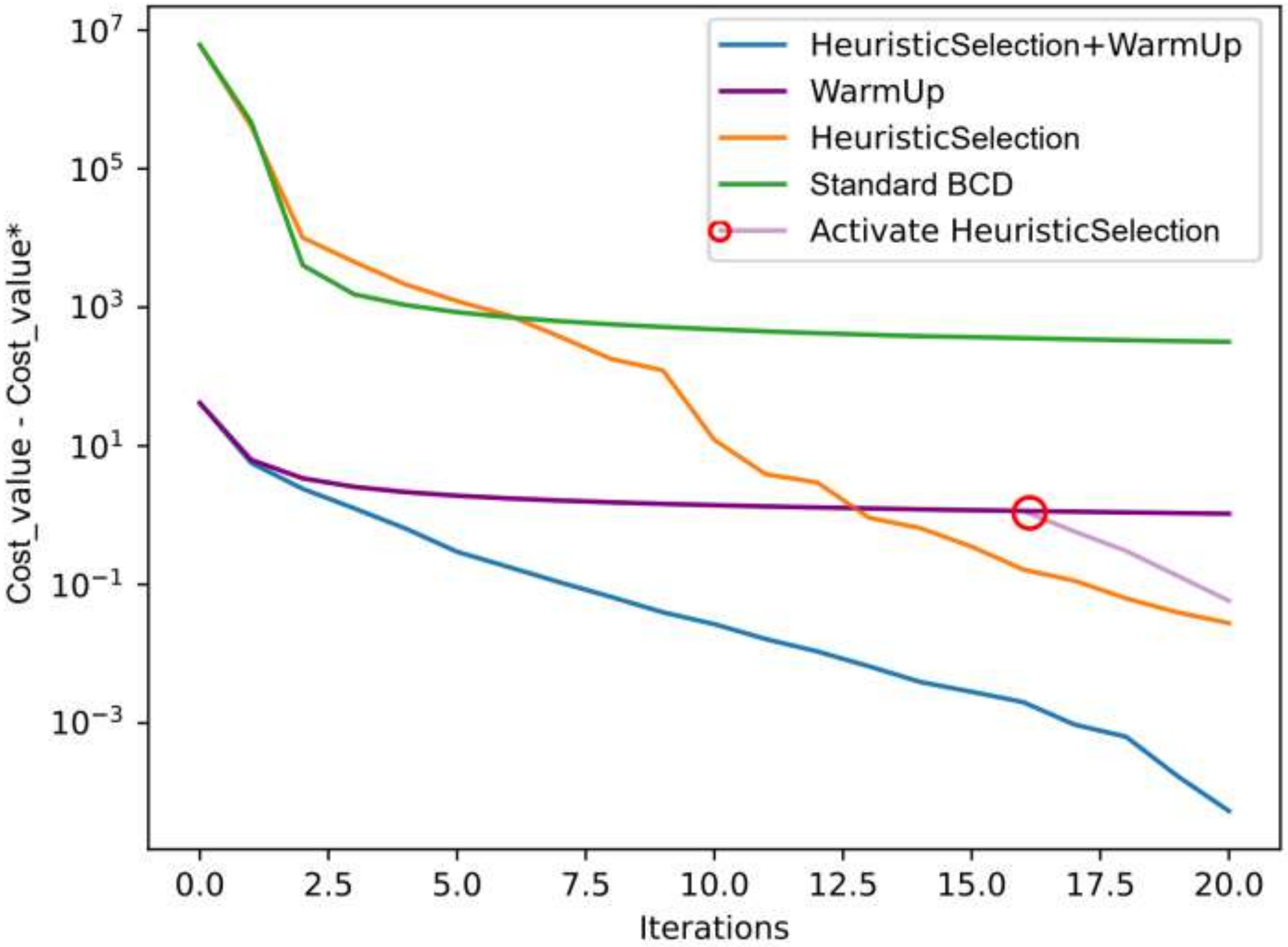
- a. Performance evaluation



Task	SCS		SSO	
	Cost Value	Score	Cost Value	Score
Hopper-expert	185.219	109.9	185.220	110.2
Hopper-medium	218.761	50.2	218.761	51.8
Walker2d-expert	140.121	108.5	140.121	109.2
Walker2d-medium	151.117	74.6	151.117	74.9
Halfcheetah-expert	165.041	84.4	165.041	83.8
Halfcheetah-medium	188.184	39.0	188.184	39.7



Ablation studies of SSO



Conclusion and Future Study

Conclusion and Future Study

- Conclusion

Introduction of Inverse Optimization

Primal

IO Model

Quadratic hypothesis space
Suboptimality loss

Dual

KIOM

Kernel Method

$\theta_{uu} = I$

Simple KIOM

SSO (CD based)

HeuristicSelection
WarmUp

- Future study

Establish the convergence analysis for the SSO

Thank you for your attention

Long, Youyuan

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