A PDE-based model-free algorithm for Continuous-time Reinforcement Learning

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Aug 27, Benasque
X Partial differential equations, optimal design and numerics

The PDE problem we are interested in

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Question: Why not solving an inverse problem?

Step 1. Solve an inverse problem

$$\{s_0^j, s_{\Delta t}^j, \cdots, s_{m\Delta t}^j\}_{j=1}^J \longrightarrow \hat{b}(s_t), \hat{\sigma}(s_t)$$

Step 2. Solve the PDE with estimated dynamics

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- **Cumulative** error (Step 1 + Step 2)
- Computationally **expensive** to solve the inverse problem

$$- \sum_{i,j} L\left(p_{\hat{b},\hat{\sigma}}(s_{i\Delta t}^j, \Delta t), s_{(i+1)\Delta t}^j\right)$$

  - Especially when Δt is large or number of data are large

Mismatch between continuous-time dynamics and discrete-time data

Step 1. Solve an inverse problem

$$\{s_0^j, s_{\Delta t}^j, \cdots, s_{m\Delta t}^j\}_{j=1}^J \longrightarrow \|(\hat{b}, \hat{\sigma}) - (b, \sigma)\| \geq \min_{(\hat{b},\hat{\sigma})\in\mathcal{F}} \|(\hat{b}, \hat{\sigma}) - (b, \sigma)\|$$

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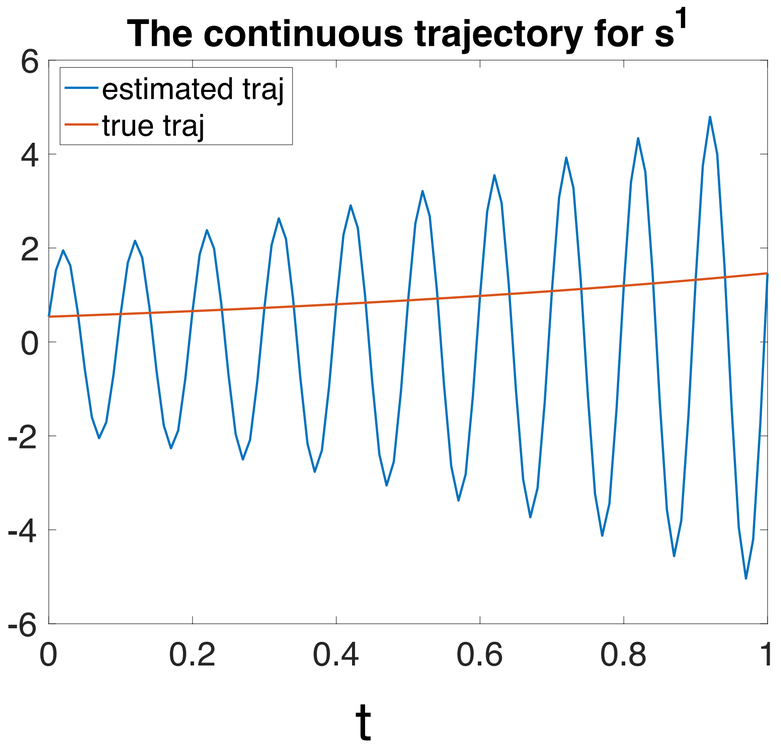
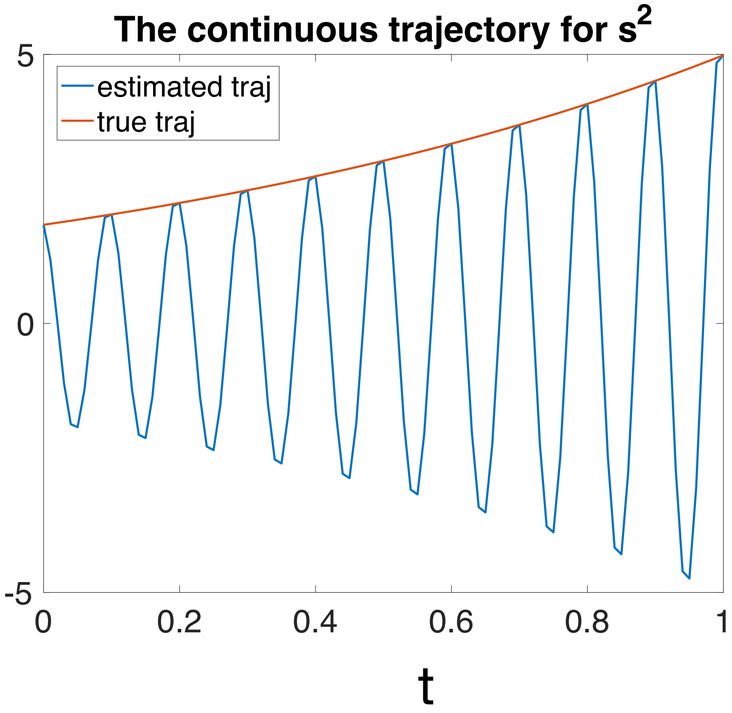
$$\hat{A} = \begin{bmatrix} 1, & \dfrac{2\pi}{\Delta t} \\ -\dfrac{2\pi}{\Delta t}, & 1 \end{bmatrix}$$

Mismatch between continuous-time dynamics and discrete-time data

Estimated trajectory is driven by $\hat{A}$; true trajectory is driven by A, $\Delta t = 0.1$





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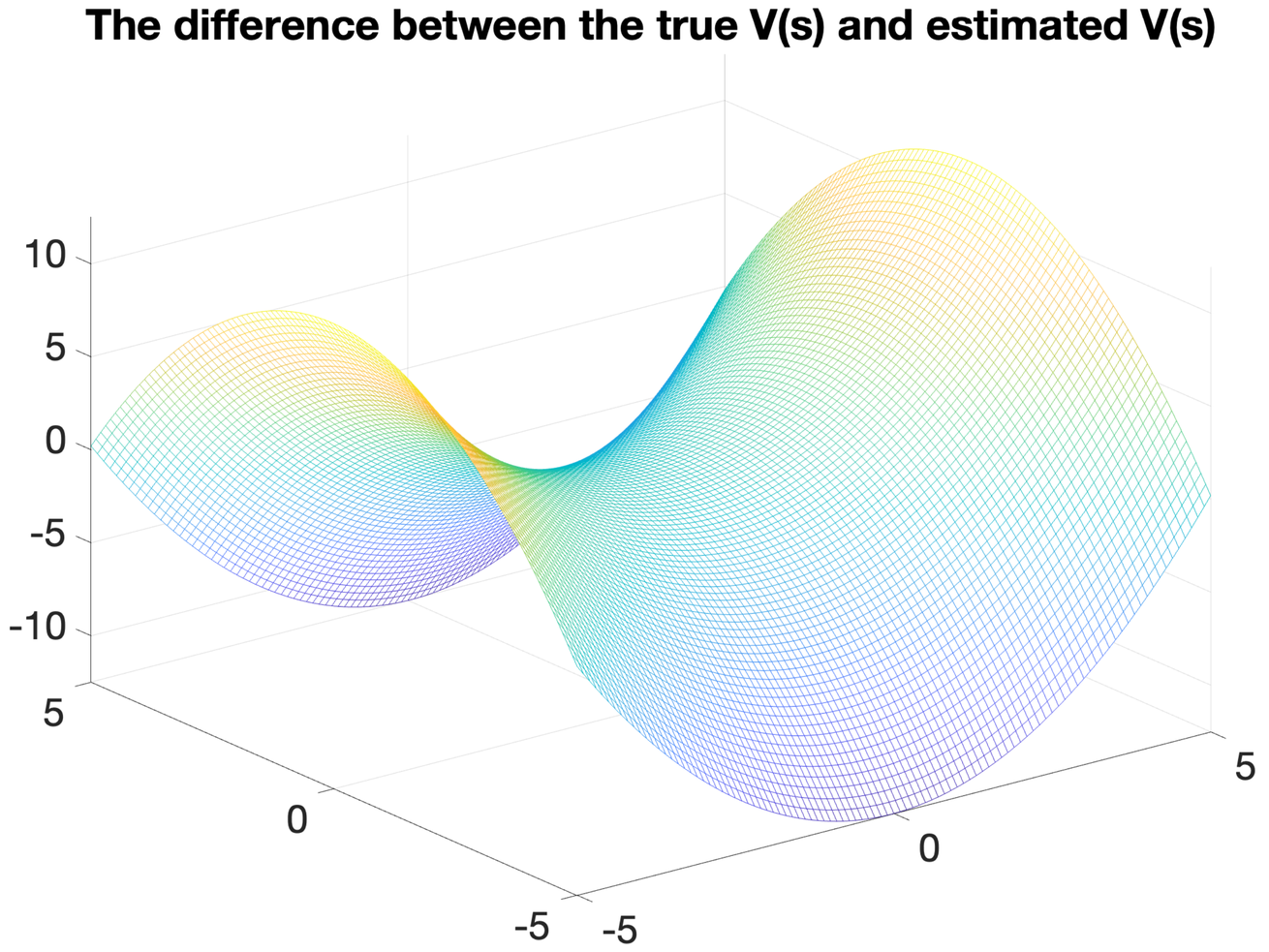

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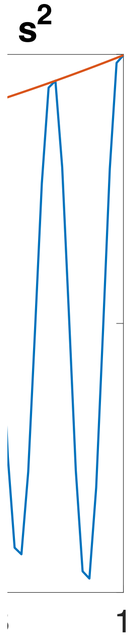

Model-based PDE formulation

Cons

- **Hard** to find a suitable functional space $\mathscr{F}$ for the dynamics
- **Cumulative** error (Step 1 + Step 1)
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- Keep the **PDE form** to estimate $V(s)$
  - Model error small, then $\hat{V}(s)$ is close to $V(s)$
  - Well-developed PDE analysis tool
  - Keep the continuous-time structure

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Can we skip the inverse problem and directly estimate $V(s)$?

Schedule

Problem Setting

Bellman equation ——Why it is not good

A PDE-based Bellman equation —— Why it is better

Algorithm

Continuous-time RL

Discrete-time RL (Markov Decision Process)

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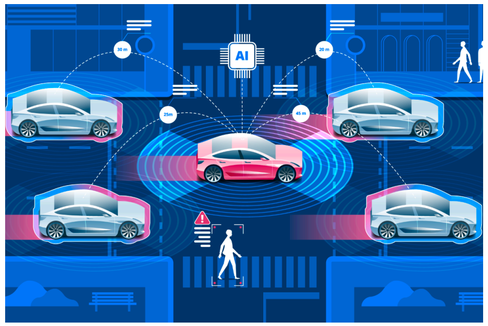

Autonomous vehicle

Robotics

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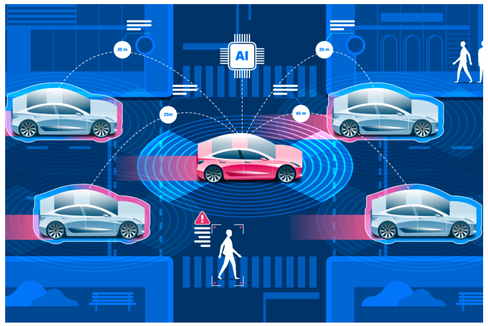

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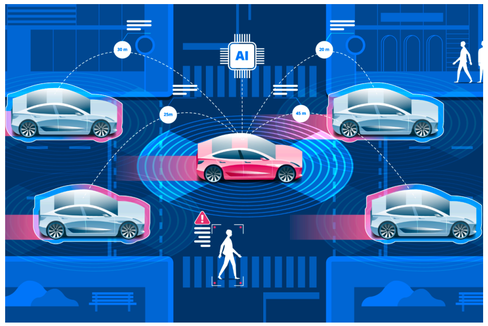

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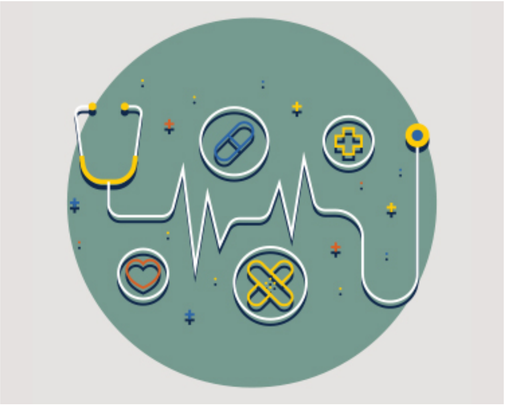

Dynamic Treatment

Question: Why bother studying continuous-time RL?

Discrete-time data  why not treat it as a discrete-time RL?

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Reinforcement Learning

Policy Evaluation

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Reinforcement Learning

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Update the policy using gradient ascent

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Update the policy using gradient ascent → $\pi_{k+1} = \pi_k + \eta \nabla_{\pi} V^{\pi_k}$

Reinforcement Learning

This talk

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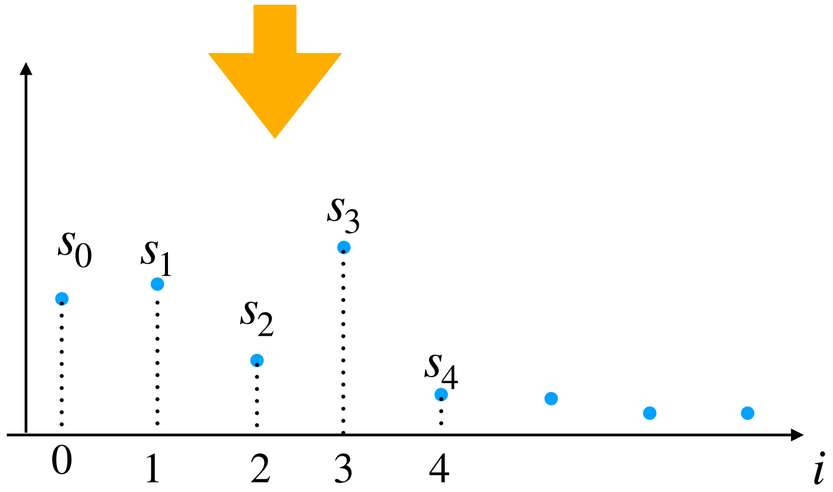

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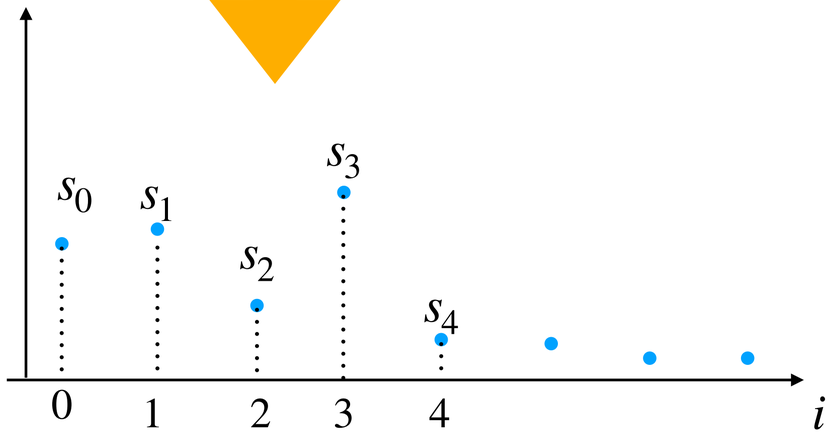

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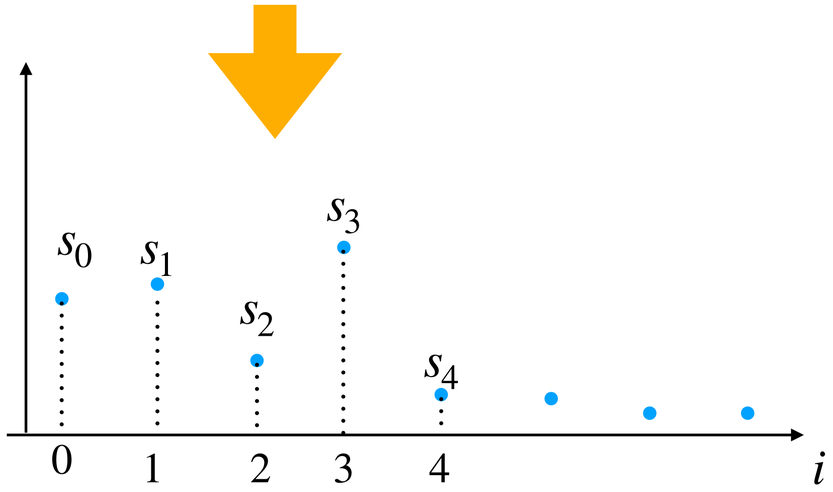

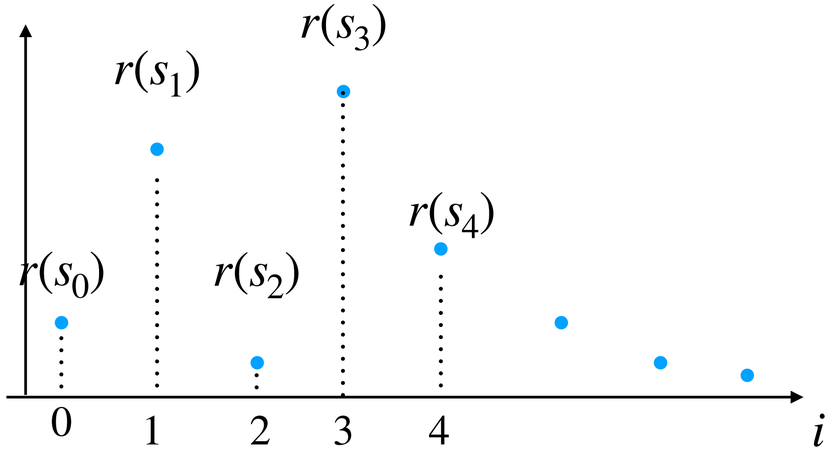

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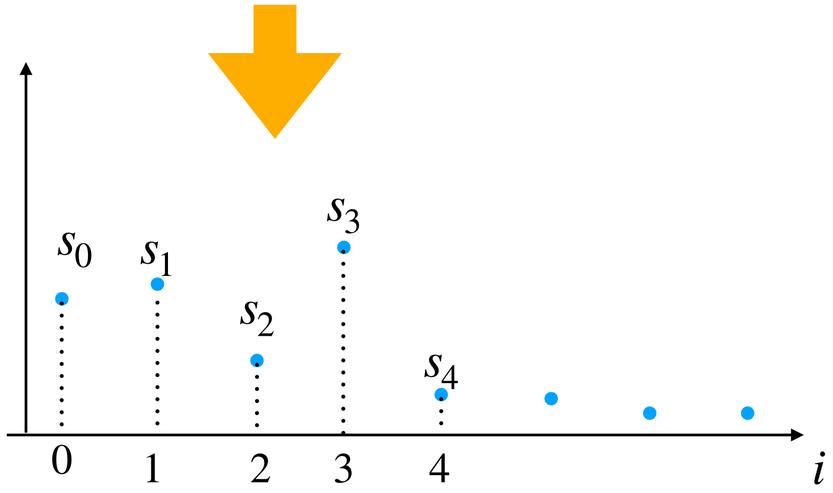
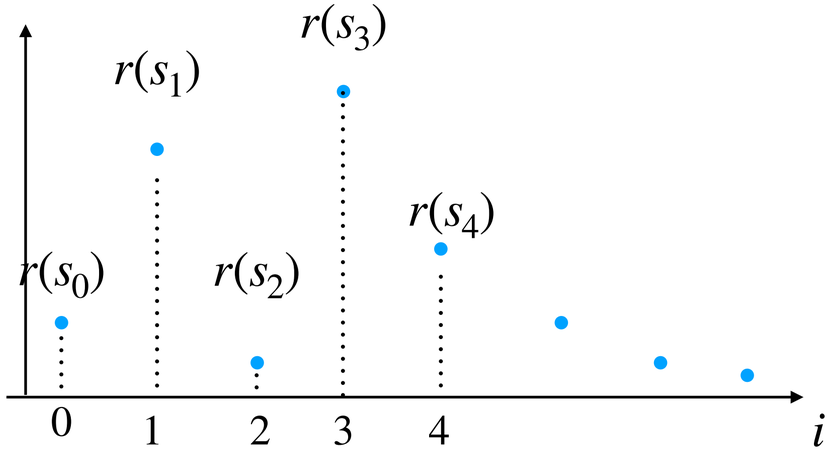
$$s_0\,,\ a_0 \sim \pi(a \mid s_0) \longrightarrow \quad s_1,\quad a_1 \sim \pi(a \mid s_1) \longrightarrow \ \ldots\ldots \quad V^{\pi}(s) = \mathbb{E}\left[\sum_{i=0}^{\infty} \gamma^i r(s_i) \mid s_0 = s\right]$$





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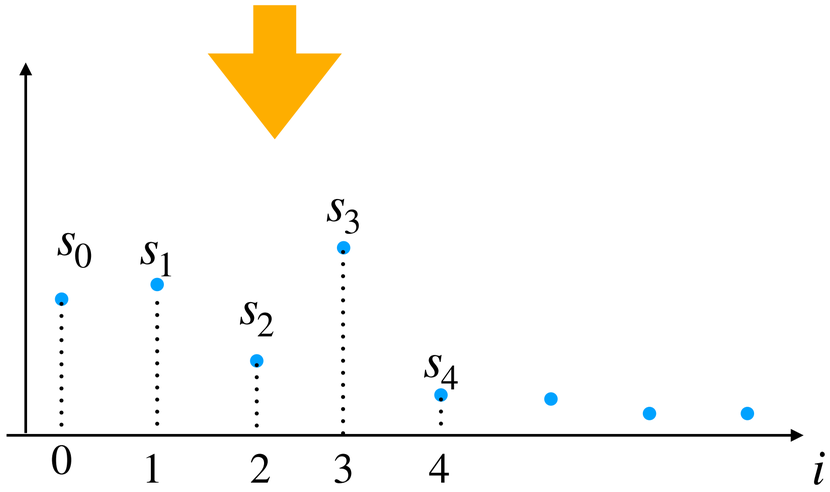

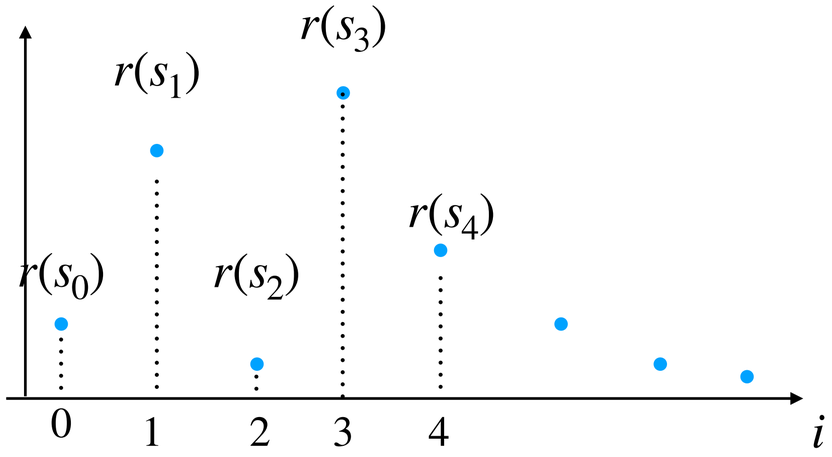

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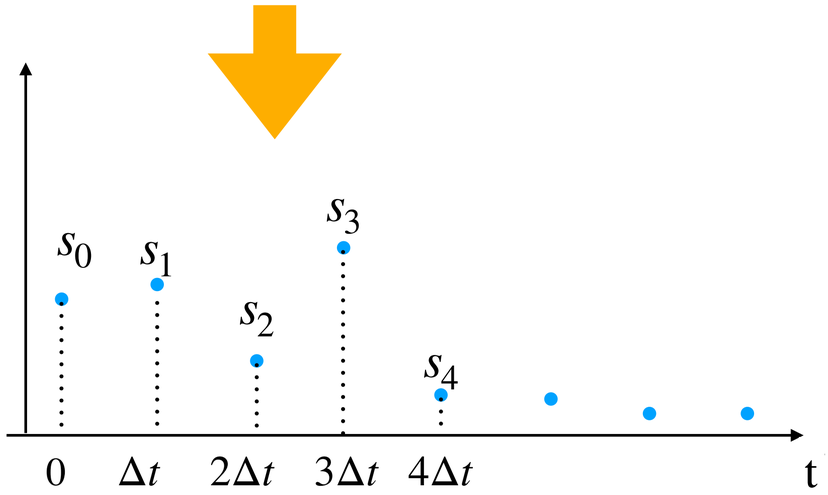

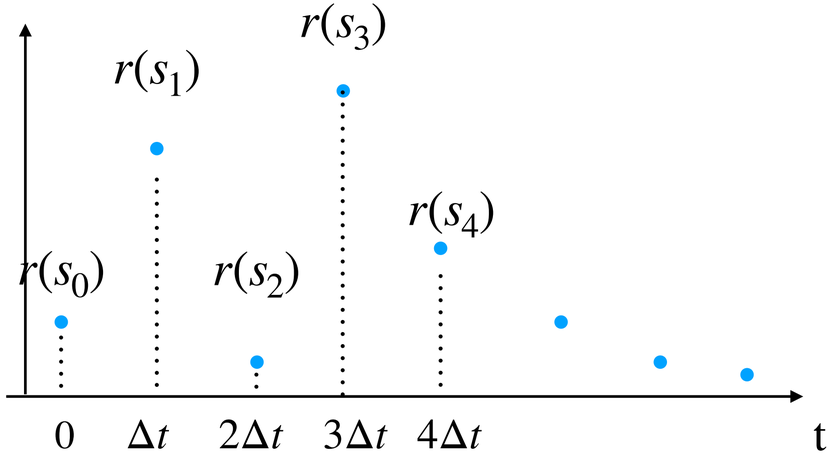

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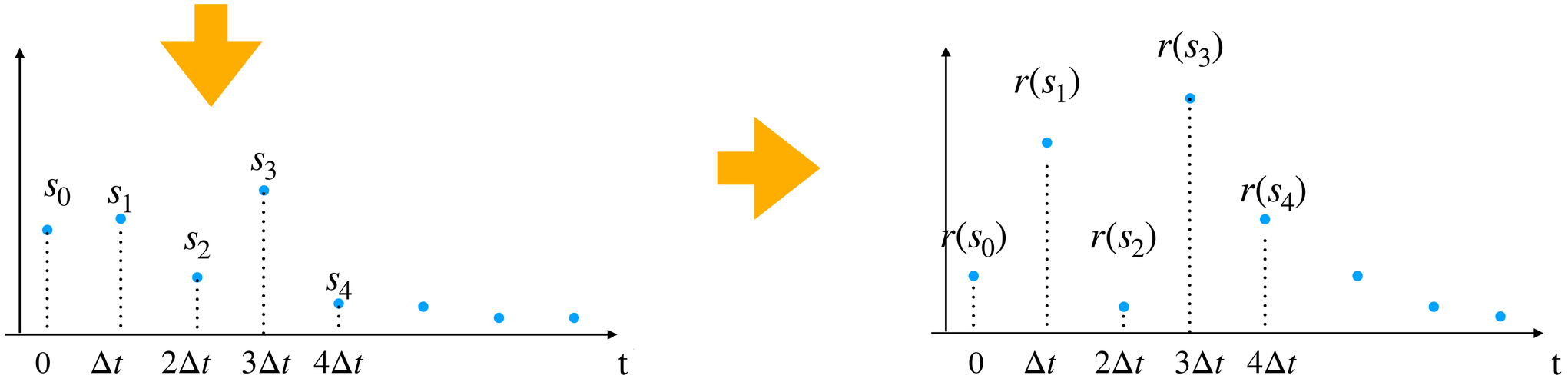

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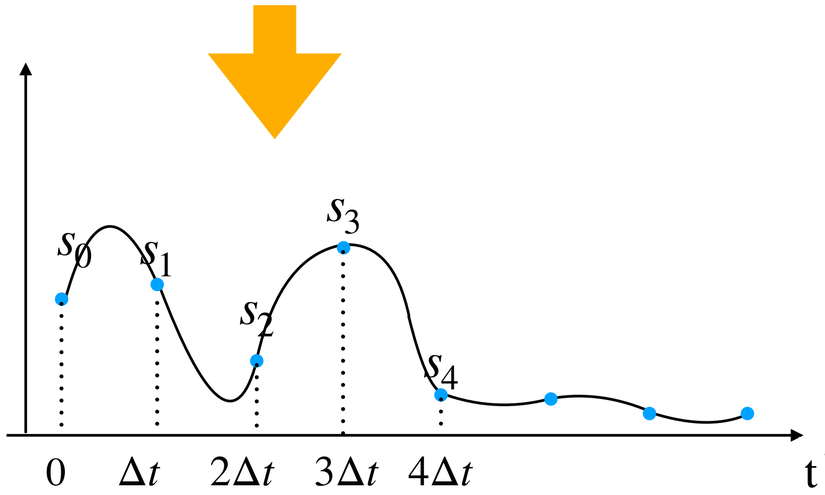

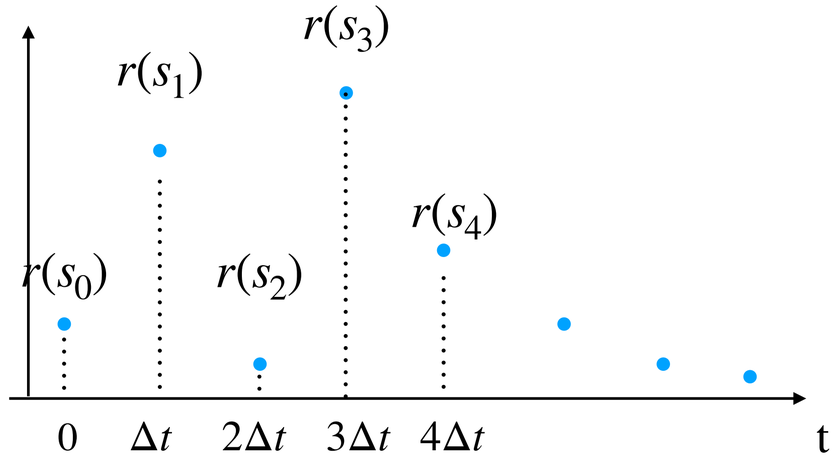

The underlying dynamics: $ds_t = b^{\pi}(s_t)\,dt + \sigma^{\pi}(s_t)\,dB_t$

Policy Evaluation

Given a policy $a \sim \pi(a \mid s)$ → $V^{\pi}(s)$: Measures how good the policy π is

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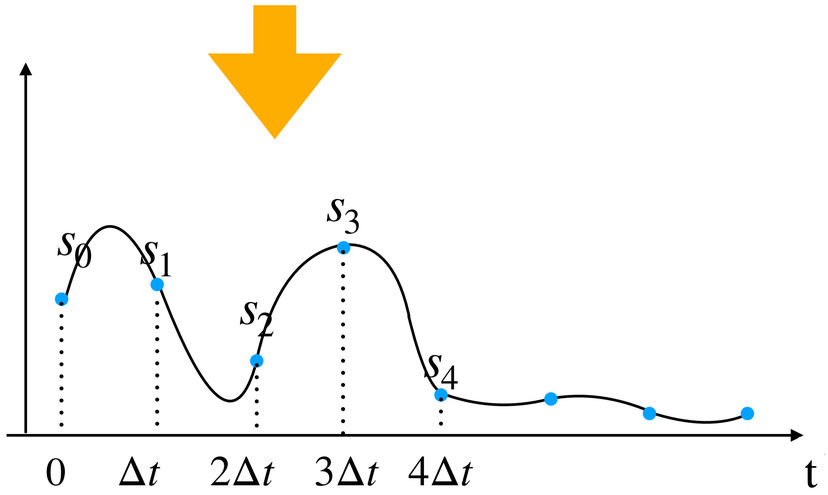

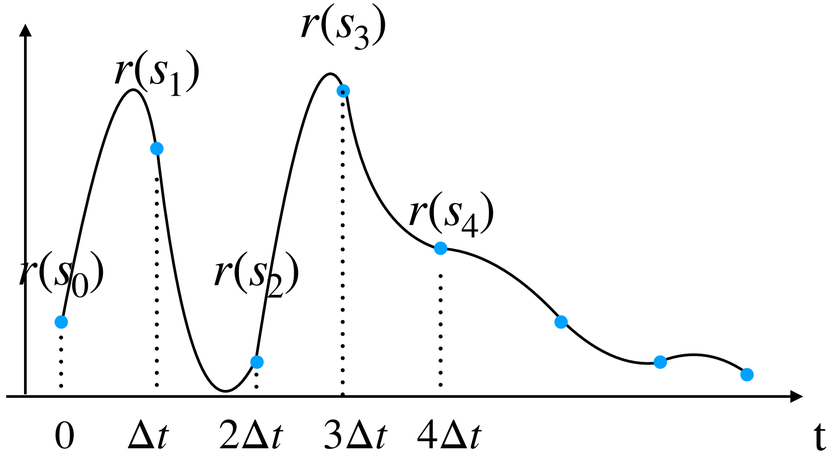

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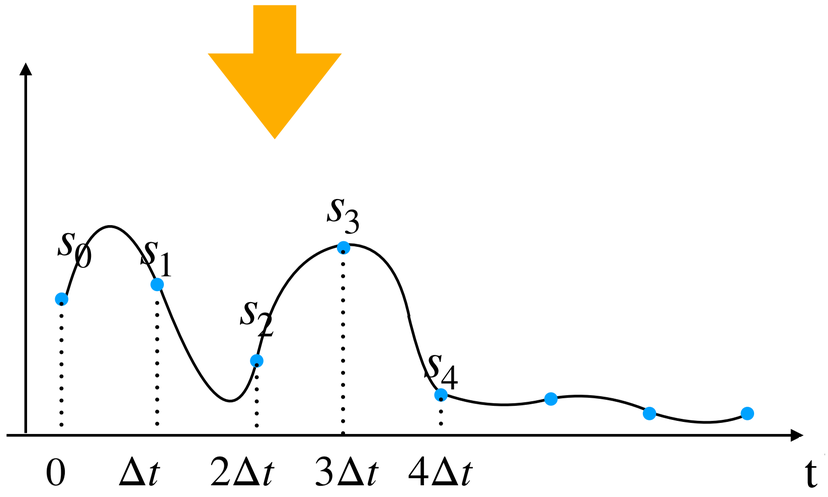

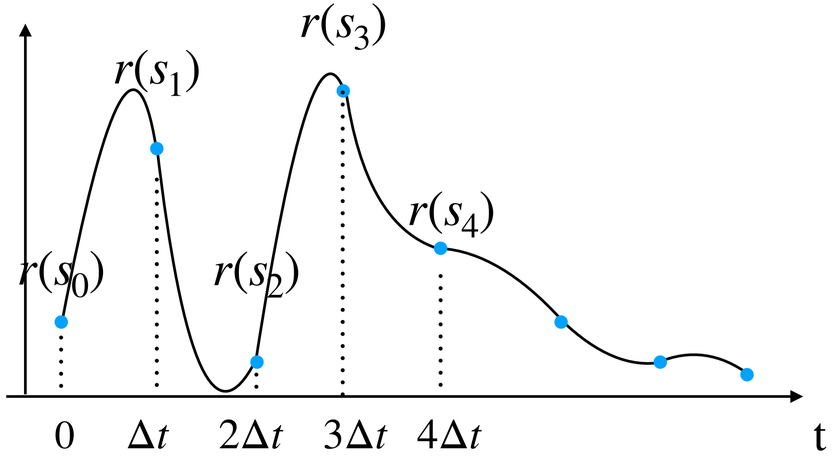

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Policy Evaluation —— A PDE view

Goal:

Estimate a function $V(s)$ related to the underlying dynamics

$$\mathscr{L}_{b,\sigma} V(s) = 0$$

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The underlying dynamics is unknown

Only discrete-time information is given

Schedule

Continuos-time RL —— Setting

Model-free RL method —— Why not the optimal, either

A PDE-based Bellman equation —— Why it is better

Algorithm

Model-free RL method

$$V(s) = \mathbb{E}\left[\int_0^\infty e^{-\beta t} r(s_t) dt \,|\, s_0 \Big| = s\right] \longrightarrow \tilde{V}(s) = \mathbb{E}\left[\sum_{i=0}^{\infty} e^{-\beta \Delta t i} r(s_{\Delta t i}) \Delta t \,|\, s_0 \Big| = s\right]$$

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Two important features about BE

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- The dynamics information is hidden in the expectation
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Two important features about BE

- The dynamics information is hidden in the expectation
  - The BE is the same for different dynamics $(b(s), \sigma(s))$
- Only depends on the current state and next state
  - Easy to plug in data directly

Least Square Temporal Difference

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LSTD in linear space

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Model-free RL method

Model-based

Model-free

- **Hard** to find an appropriate functional space $\mathcal{F}(\theta)$ for the dynamics
- **Cumulative** error (Step 1 + Step 1)
- Computationally **expensive** to solve the inverse problem
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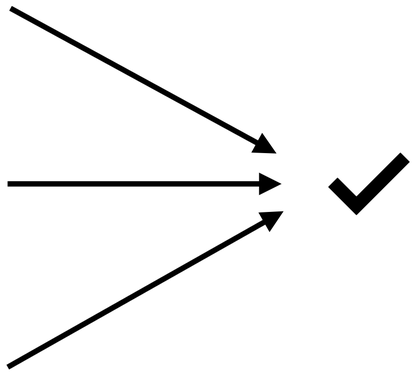

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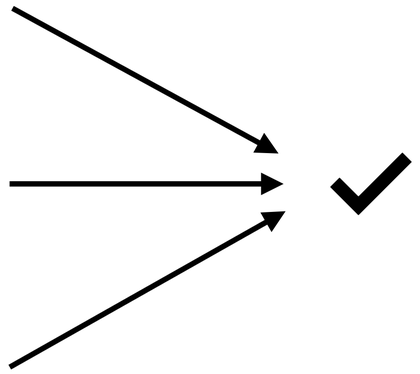

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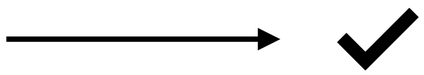

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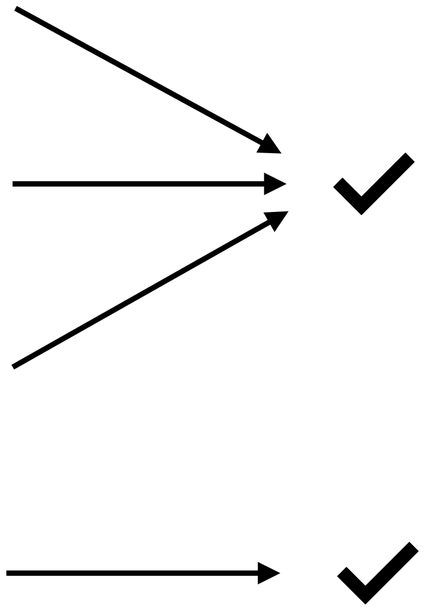

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Is it the optimal tool for continuous-time RL?

One example

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e.g.

Underlying dynamics: $\frac{d}{dt}s_t = \lambda s_t$, True value function: $V(s) = \cos^3(ks)$

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Discrete-time trajectory data: $\{s_0^j, s_{\Delta t}^j, \cdots, s_{I\Delta t}^j\}_{j=1}^{J}$

The performance of the RL algorithm

Underlying dynamics: $\frac{d}{dt}s_t = 0.05 s_t$

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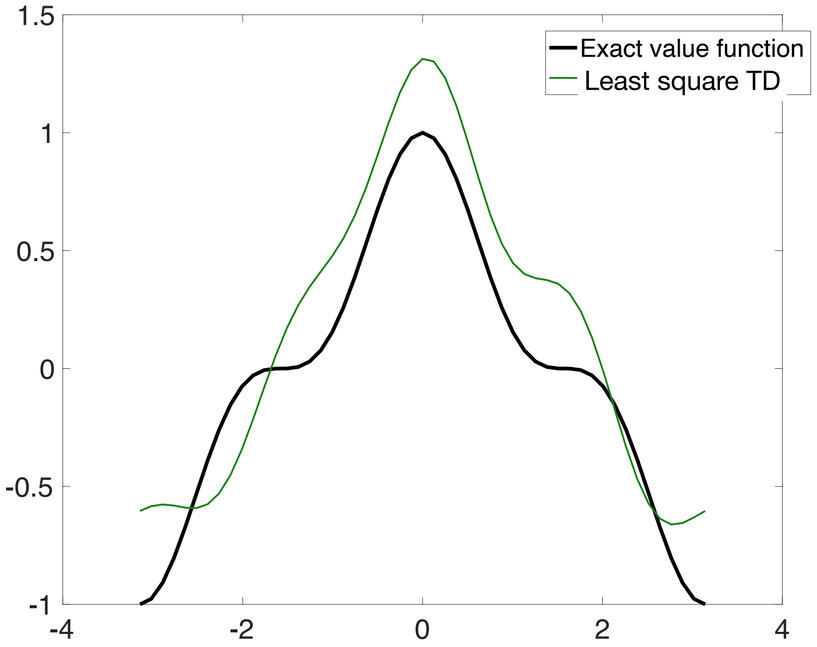

# of data: 40

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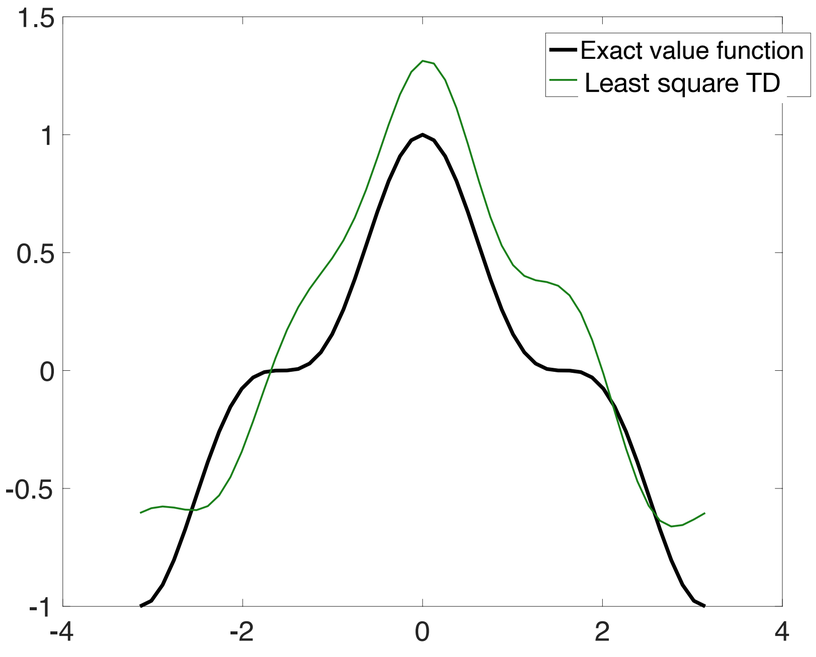

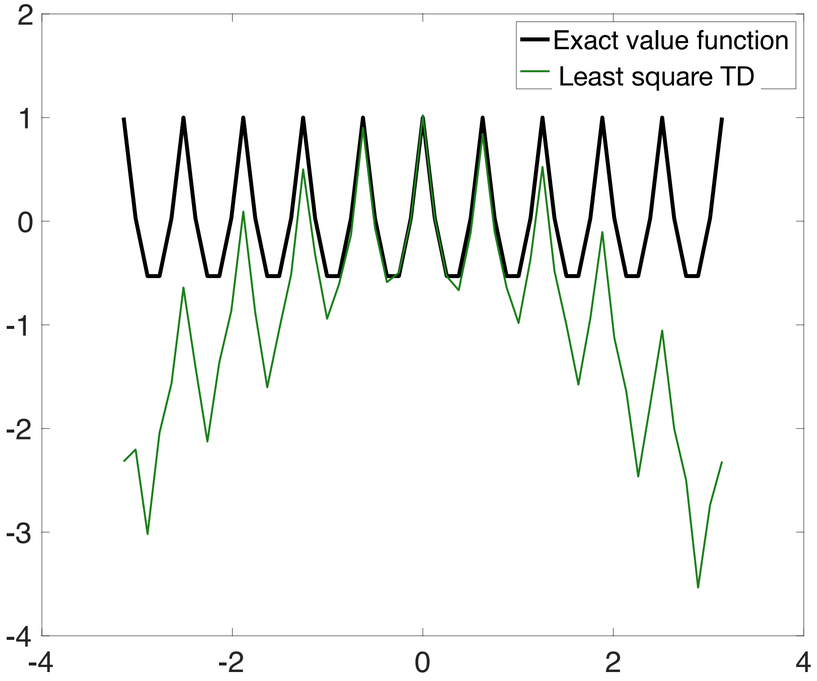

# of data: 40

# of data: 400

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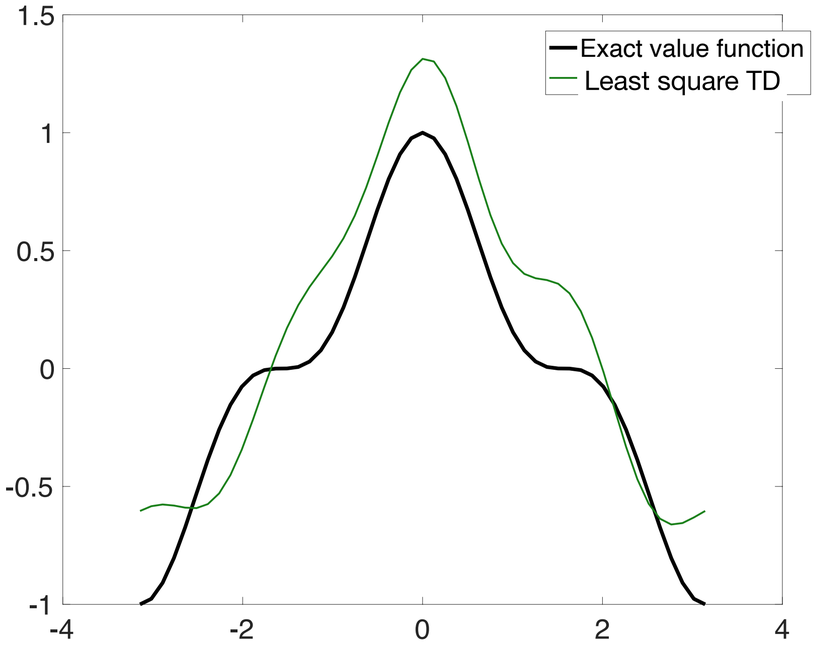

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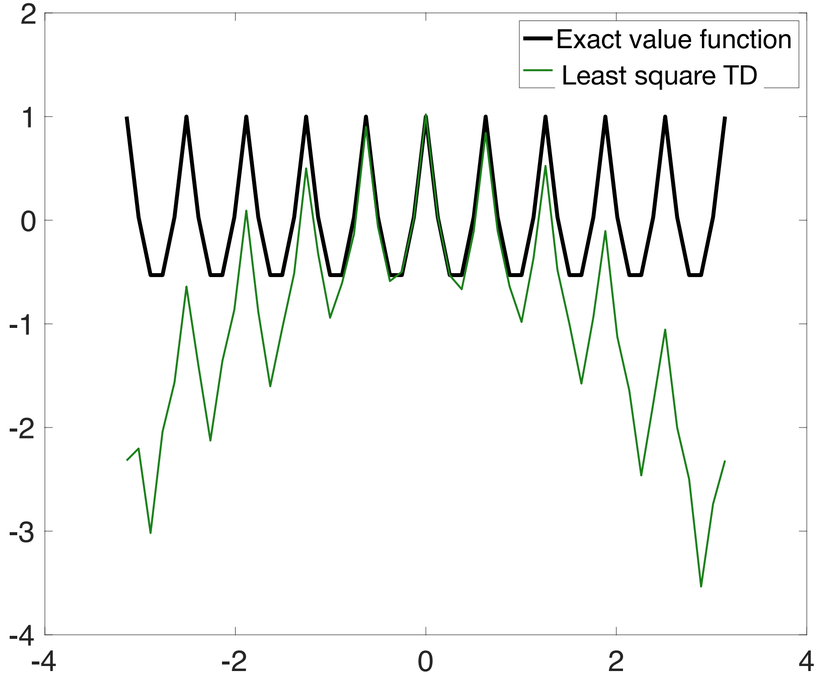

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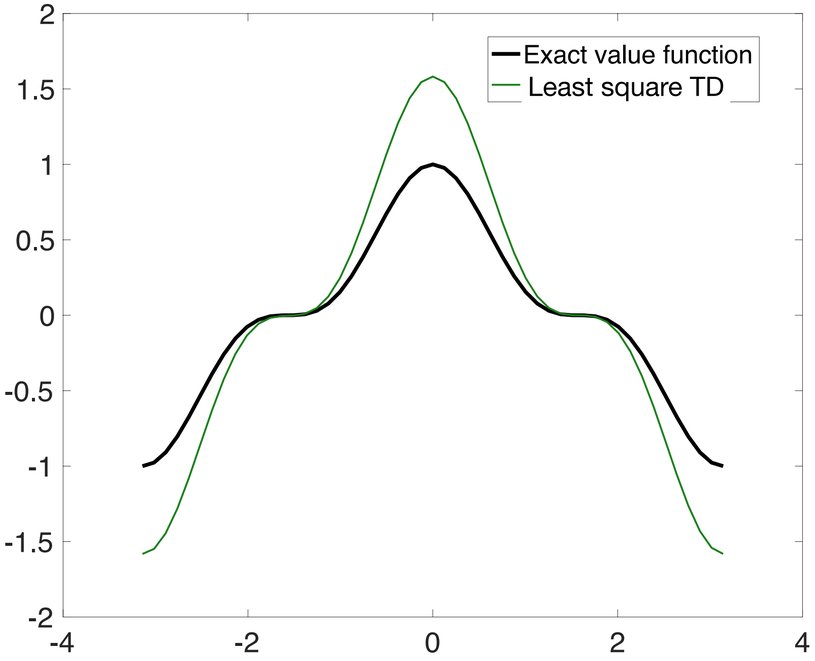

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Model-free RL algorithms

Cons

- It is not a good approximation for the continuous-time value function under certain circumstances

Pros

- Model-free
  - One can skip the inverse problem and directly compute $V(s)$
- Many well-developed RL algorithms

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Given the same information, can we do better than BE?

Schedule

Continuos-time RL —— Setting

Bellman equation ——Why it is not good

A PDE-based Model-free algorithm —— Why it is better

Algorithm

Given the same trajectory data: Our algorithm v.s. LSTD

Underlying dynamics: $\frac{d}{dt}s_t = 0.05 s_t$

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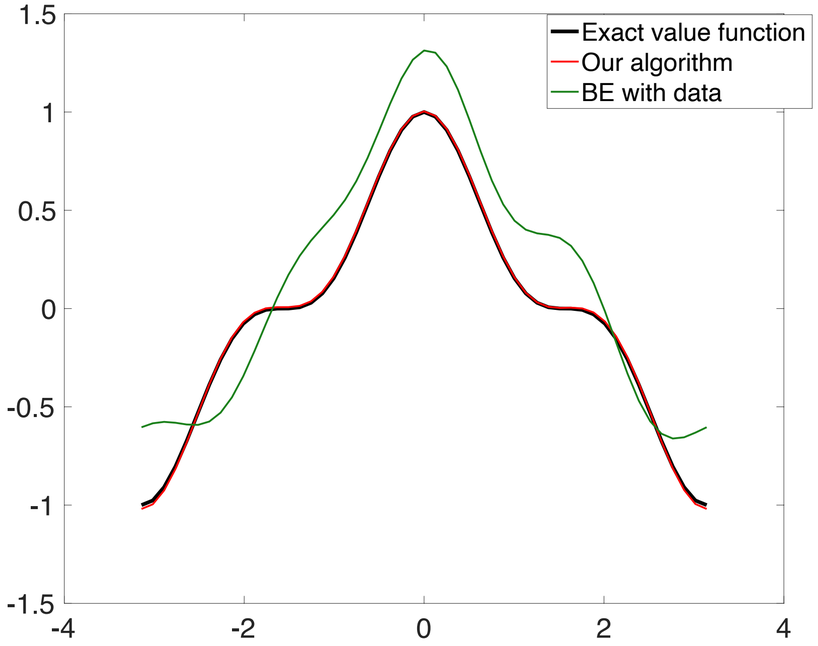

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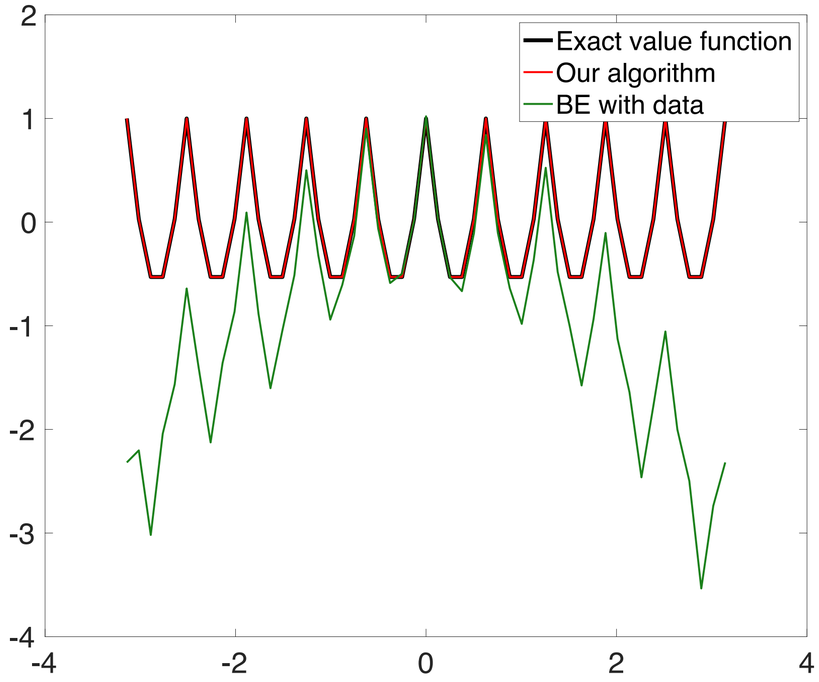
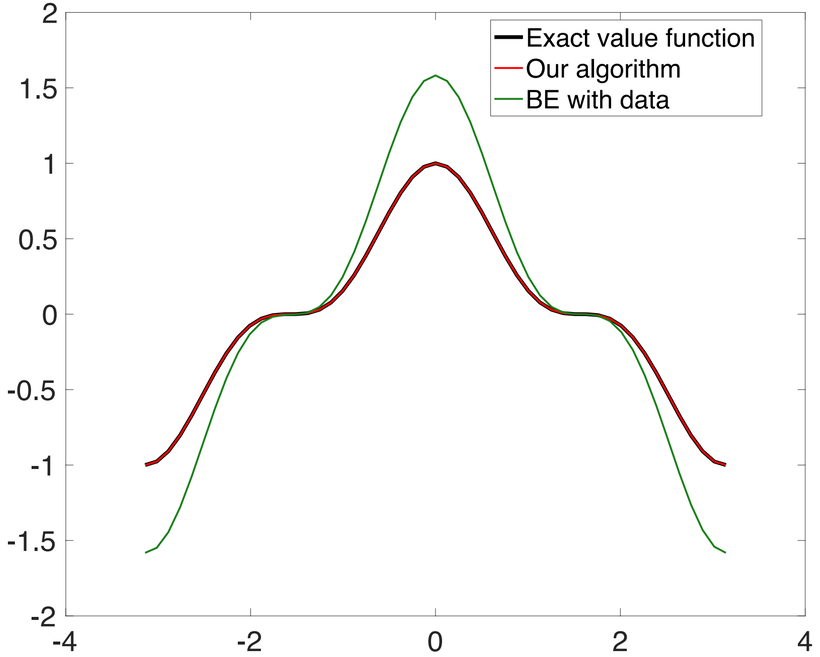


# of data: 400

$\Delta t = 0.1, \beta = 10, V(s) = \cos^3(s)$



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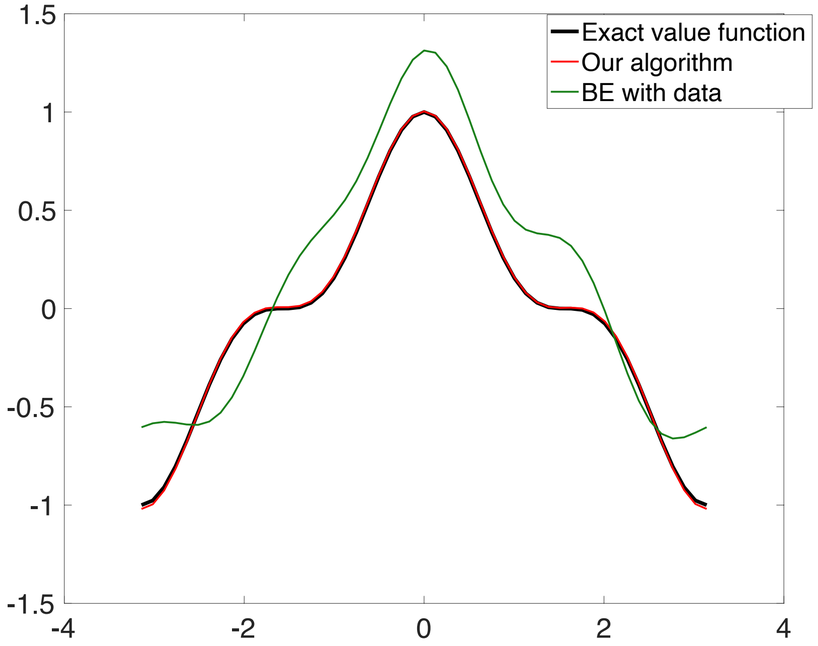

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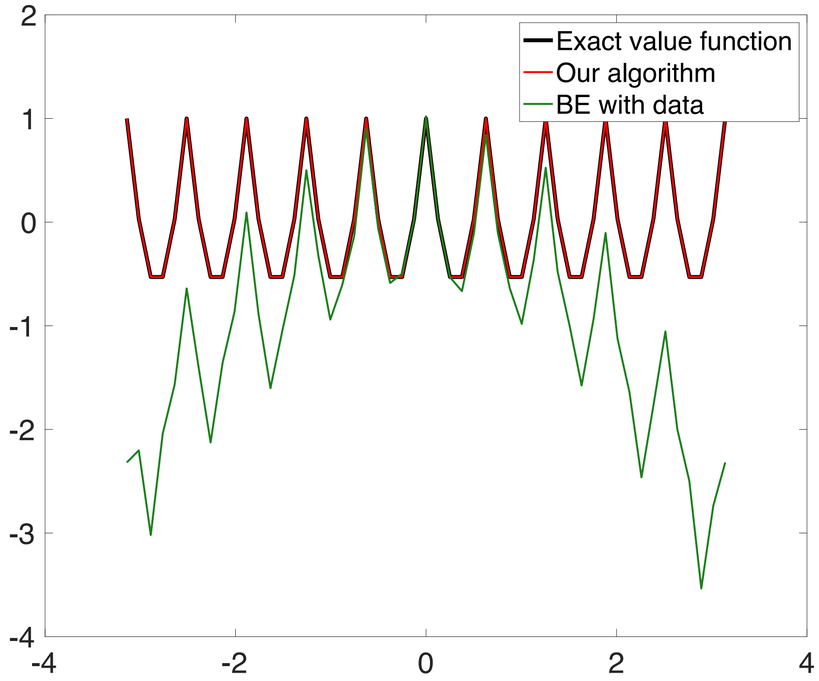

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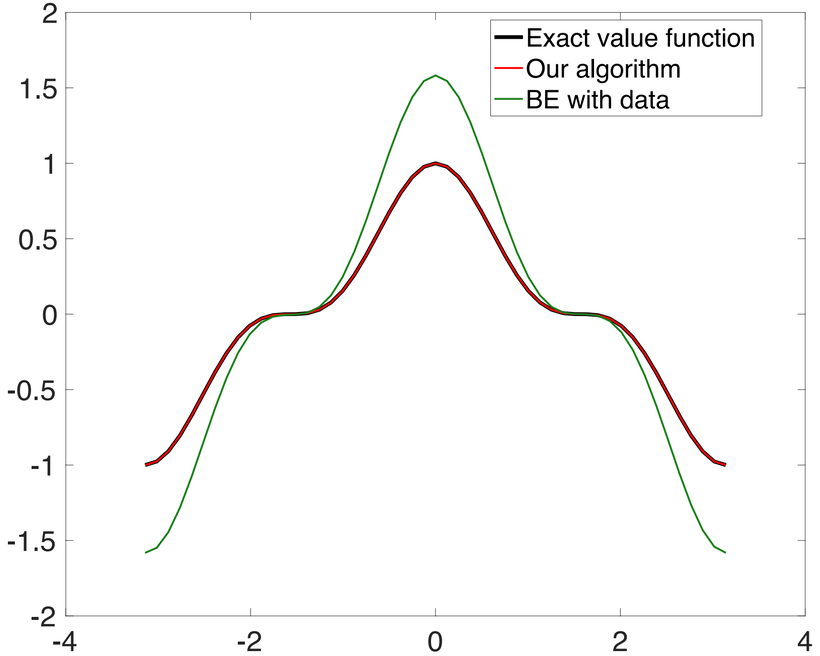

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With the same computational cost!

Algorithm

LSTD

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Our algorithm

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Why & When?

Why & When?

- Is it possible that it is the problem of LSTD? Is it possible that other RL algorithms work?
- When is BE not a good approximation to the continuous-time RL?
- What is the underlying equation behind our algorithm?
- When does our algorithm approximate work well?

Why LSTD is bad?

Most of the
RL algorithms

Why LSTD is bad?

Most of the RL algorithms $\xrightarrow[\text{to approximate}]{\text{use trajectory data}}$

Why LSTD is bad?

Most of the RL algorithms $\xrightarrow[\text{to approximate}]{\text{use trajectory data}}$ BE: $\tilde{V}(s) = \tilde{r}(s) + \gamma \mathbb{E}\left[\tilde{V}(s_{t+\Delta t}) \,|\, s_t = s\right]$

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The solution to BE a NOT good approximation for continuous-time RL

Why LSTD is bad?

Most of the RL algorithms $\xrightarrow[\text{to approximate}]{\text{use trajectory data}}$ BE: $\tilde{V}(s) = \tilde{r}(s) + \gamma \mathbb{E}\left[\tilde{V}(s_{t+\Delta t}) \,|\, s_t = s\right]$

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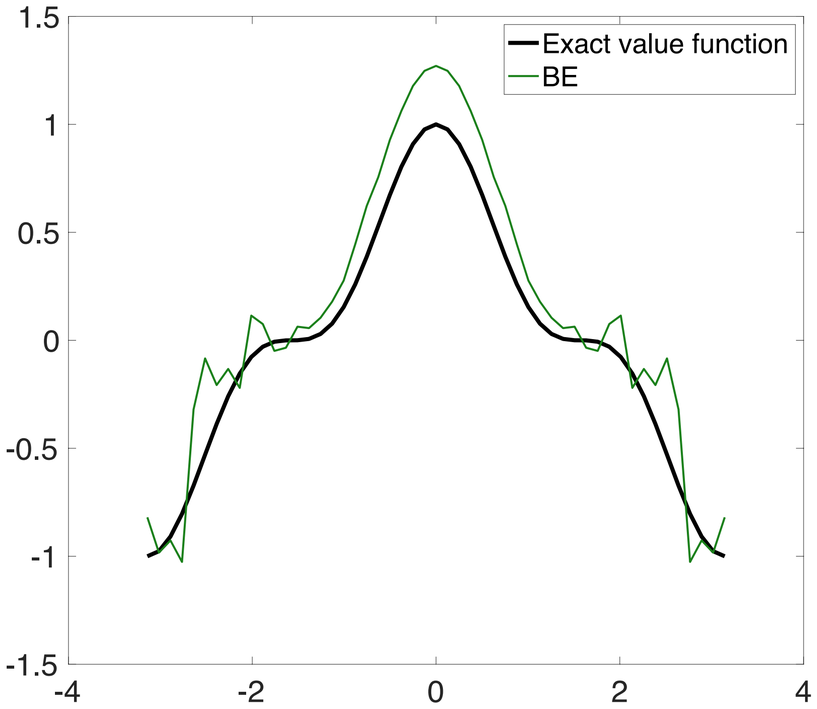
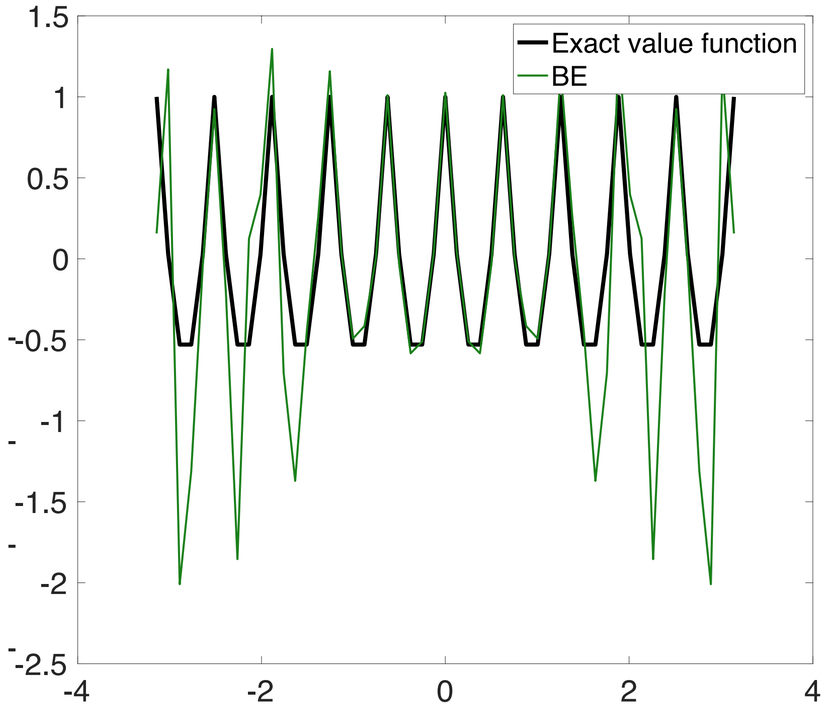
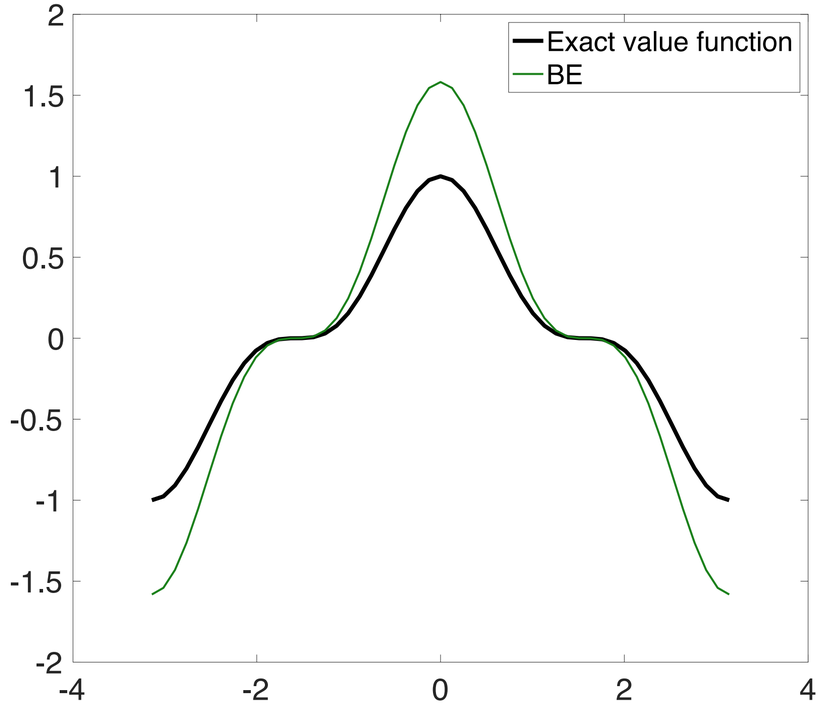
$\Delta t = 5, \beta = 0.1, V(s) = \cos^3(s)$



$\Delta t = 0.5, \beta = 0.1, V(s) = \cos^3(10s)$



$\Delta t = 0.1, \beta = 10, V(s) = \cos^3(s)$



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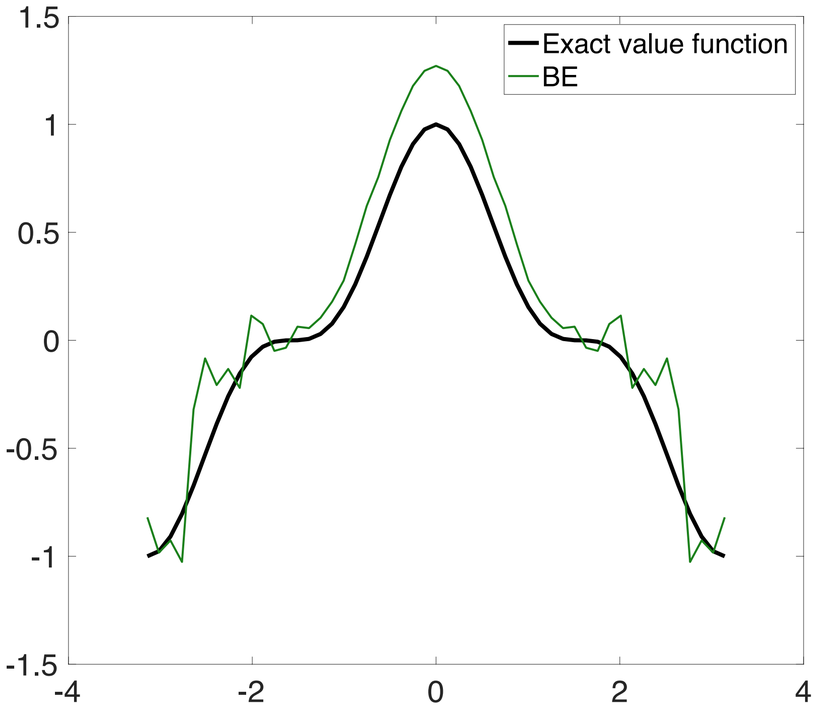

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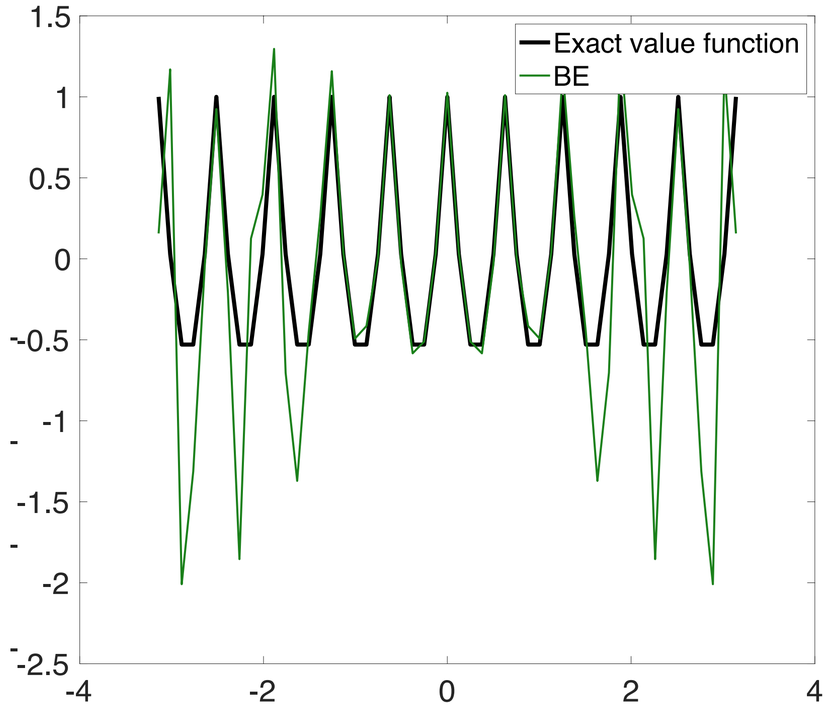

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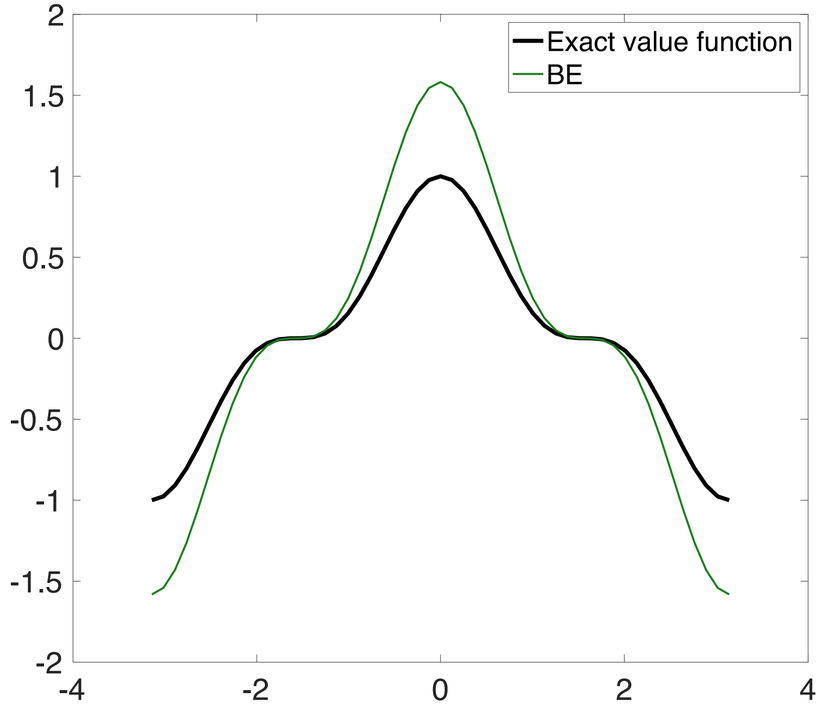

- **The RL algorithm is converging to BE solution, not the true value function**

Why & When?

- Is it possible that it is the problem of LSTD? Is it possible that other RL algorithms work?
  - As long as the algorithm is derived from BE, it won't work under these circumstances.
- When is BE not a good approximation to the continuous-time RL?
- What is the underlying equation behind our algorithm?
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When is Bellman equation bad?

True value function: $\beta V(s) = r(s) + \mu(s) \cdot \nabla V(s) + \frac{1}{2}\Sigma(s) : \nabla^2 V(s)$

BE: $\tilde{V}(s) = r(s)\Delta t + e^{-\beta \Delta t}\mathbb{E}[V(s_{\Delta t}) \,|\, s_0 = s]$

Theorem for RL approximation [Z-24]

Assume that $\|r(s)\|_{L^\infty}$, $\|\mathscr{L}_{\mu,\Sigma} r(s)\|_{L^\infty}$ are bounded, then

$$\|V(s) - \tilde{V}(s)\|_{L^\infty} \lesssim \frac{\beta \|r\|_{L^\infty} + \|\mathscr{L}_{\mu,\Sigma} r\|_{L^\infty}}{\beta} \Delta t + o(\Delta t)$$

$$\mathscr{L}_{\mu,\Sigma} = \mu(s) \cdot \nabla + \frac{1}{2}\Sigma(s) : \nabla^2, \quad \text{where } \Sigma = \sigma\sigma^\top$$

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How does reward look like in RL applications?

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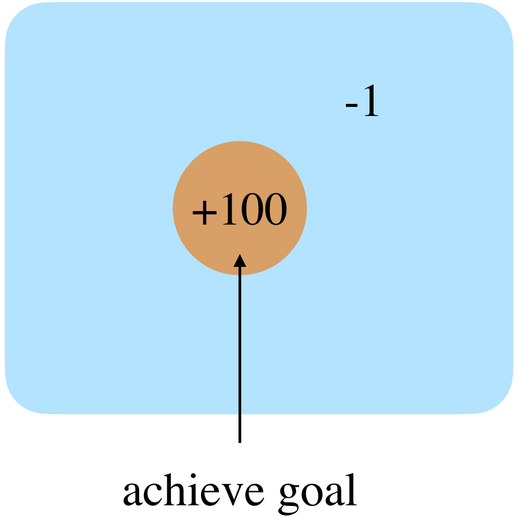

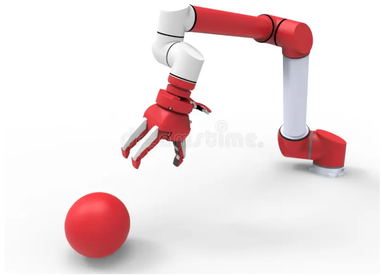

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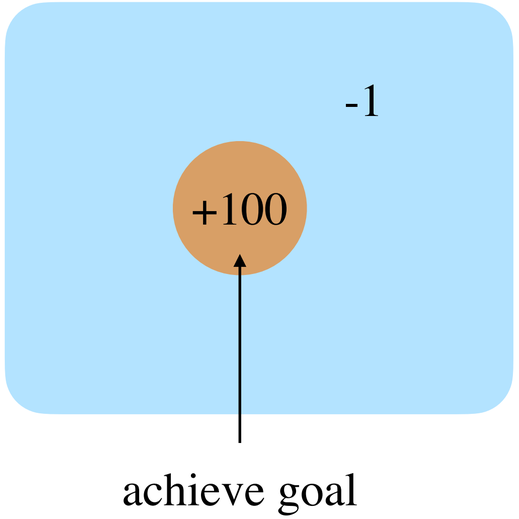

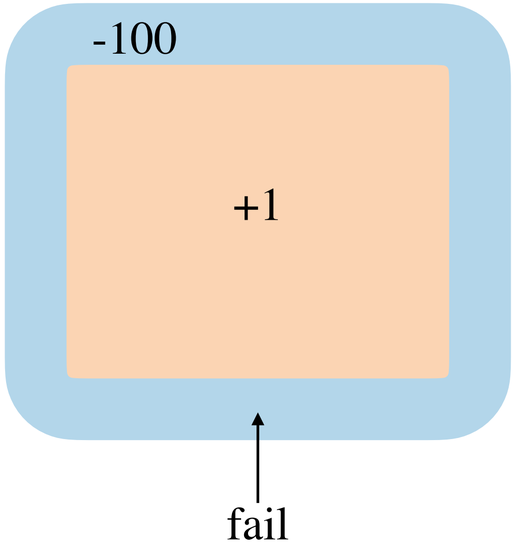

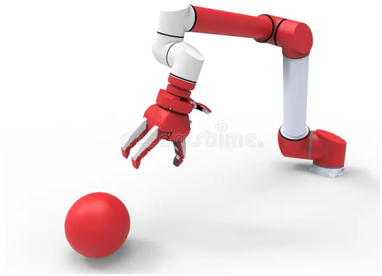

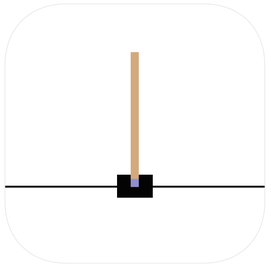

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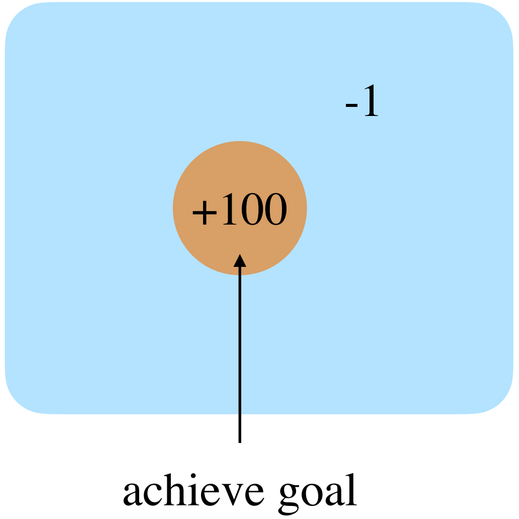

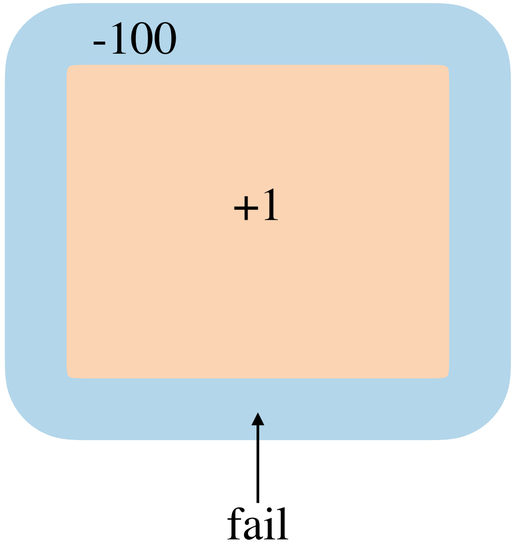

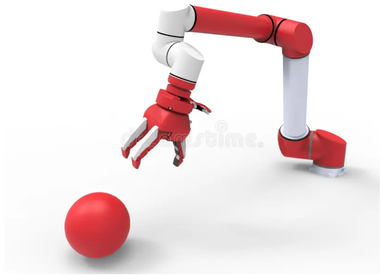

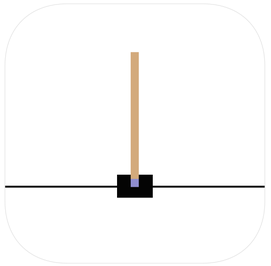

The reward often varies a lot!

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What is the underlying equation behind our algorithm

Deterministic Dynamics

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- $p_{\Delta t}(s)$ represents the state at $t + \Delta t$ given state at t is s

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- Similarity: two important features of BE

  - Same formulation for different dynamics $(b(s), \sigma(s))$
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- Difference: No smoothness infomation in continuous-time

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- Similarity: PDE, containing continuous-time information
- Difference: Only continuous information, has to estimate the dynamics first

Model-based PDE formulation

Pros

- Keep the **PDE form** to estimate $V(s)$
  - Well-developed PDE analysis tool
  - Keep the continuous-time structure

Model-free RL algorithms

Pros

- **Model-free**
  - One can skip the inverse problem and directly compute $V(s)$
  - Many practical RL algorithms

Combine the advantages of PDE formulation with model-free algorithm

PhiBE in general dynamics

PhiBE: $$\beta\hat{V}_1(s) = r(s) + \frac{1}{\Delta t}\mathbb{E}[s_{\Delta t} - s \,|\, s_0 = s] \cdot \nabla \hat{V}_1(s) + \frac{1}{2\Delta t}\mathbb{E}[(s_{\Delta t} - s)(s_{\Delta t} - s)^\top \,|\, s_0 = s] : \nabla^2 \hat{V}_1(s)$$

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similar to the Bellman equation

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The form of the PDE ↑ derived from the true continuous-time physical environment

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Contains discrete-time information ↑ similar to the Bellman equation

PhiBE, incorporating discrete-time information into continuous-time PDE

Higher-order PhiBE in deterministic dynamics

i-th order PhiBE (deterministic dynamics)

i-th order PhiBE: $\beta \hat{V}_i(s) = r(s) + \hat{\mu}_i(s) \cdot \nabla \hat{V}_i(s)$

$$\text{with} \quad \hat{\mu}_i(s) = \frac{1}{\Delta t} \left[\sum_{j=1}^{i} a_j^{(i)} (s_{j\Delta t} - s_0) \,\middle|\, s_0 = s \right]$$

Here the coefficients $(a_0^{(i)}, \cdots, a_i^{(i)})^\top = (A^{(i)})^{-1} b^{(i)}$,
where $A_{kj}^{(i)} = j^k$, $b_k^{(i)} = (0,1,0,\cdots,0)^\top$

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Different from classical numerical schemes

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Different from classical numerical schemes

Numerical schemes known dynamics ——> discrete trajectory

PhiBE known discrete trajectory ——> dynamics

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Theoretical Guarantees in general deterministic dynamics

$$\frac{d}{dt}s_t = \mu(s_t)$$

i-th order PhiBE [Z-24]

Assume that $\|\nabla r(s)\|_{L^\infty}$, $\|\mathscr{L}_\mu^i \mu(s)\|_{L^\infty}$ are bounded.
In addition, $\|\nabla \mu(s)\|_{L^\infty} < \beta$

$$\|V(s) - \hat{V}_i(s)\|_{L^\infty} \leq \frac{\|\nabla r\|_{L^\infty}\|\mathscr{L}_\mu^i \mu\|_{L^\infty}}{(\beta - \|\nabla \mu(s)\|_{L^\infty})^2}\Delta t^i$$

where $\mathscr{L}_\mu = \mu(s)\cdot\nabla$,

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The dynamics changes slowly, the error is smaller

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The dynamics changes slowly, the error is smaller

The advantage of error depending more on the dynamics instead of reward:

- More flexibility of designing the reward function
- Only need less data points to achieve the same error

Theoretical Guarantees in stochastic dynamics

Weighted L^2 norm

Define

$$\|f\|_\rho = \int f^2(s)\rho(s)ds,$$

where $\rho(s)$ is the stationary distribution of the SDE that satisfies

$$\nabla \cdot \left[\mu(s)\rho(s) + \frac{1}{2}\nabla \cdot (\Sigma(s)\rho(s))\right] = 0$$

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PhiBE [Z-24]

Assume that $\lambda_{\min}(\Sigma(s)) \geq \lambda_{\min} > 0$,

$\|\nabla^k \mu(s)\|_{L^\infty}$, $\|\nabla^k \Sigma(s)\|_{L^\infty}$, for $k = 0,\cdots,2i$ are bounded,

$\max_{k,l} \sum_i \|\partial_{s_i} \Sigma_{kl}(s)\|_{L^\infty} \leq 2\lambda_{\min}$, then

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When the dynamics changes slowly or the magnitude of the noise is large, 1st order PhiBE is better than BE.

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Theoretical Guarantees for the linear approximation

$$\beta\hat{V}(s) = r(s) + \frac{1}{\Delta t}\mathbb{E}[s_{\Delta t} - s \,|\, s_0 = s] \cdot \nabla \hat{V}(s) + \frac{1}{2\Delta t}\mathbb{E}[(s_{\Delta t} - s)(s_{\Delta t} - s)^\top \,|\, s_0 = s] : \nabla^2 \hat{V}(s)$$

Theoretical Guarantees for the linear approximation

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Model-free algorithm is using data to approximate $\hat{V}^G$

PhiBE under linear approximation [Z-24]

Under mild assumption on $b(s), \Sigma(s), r(s)$, and boundedness of $\|\nabla \log \rho\|_{L^\infty}$ or $\|\Phi\|_{L^\infty}$, $\Delta t^i \le C_{\Delta t}$, then

$$\|\hat{V}_i^G(s) - V(s)\|_\rho \le \frac{C_2}{\beta^2}\Delta t^i + C^G \min_{\hat{V}_P = \theta^\top \Phi} \|V_i(s) - \hat{V}_P(s)\|_{H^1_\rho}$$

$C_2 \,.\, C^G$ decreases as the dynamics changes slowly

Theoretical Guarantees for the linear approximation

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Open problem: sample complexity of the algorithm

Conclusion

- Is it possible that it is the problem of LSTD? Is it possible that other RL algorithms work?
  - As long as the algorithm is derived from BE, it won't work under these circumstances.

- When is BE not a good approximation to the continuous-time RL?
  - When the reward function has a large variation

- What is the underlying equation behind our algorithm?
  - PhiBE & High-order PhiBE

- When does our algorithm approximate work well?
  - When the dynamics change slowly

PhiBE in linear dynamics

Linear dynamics

Underlying dynamics: $\frac{d}{dt}s_t = \lambda s_t$

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$$s_t = e^{\lambda t} s_0$$

When $\lambda > 0$, the dynamics change exponentially fast

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PhiBE for linear dynamics [Z-24]

$$\|V(s) - \tilde{V}(s)\|_{L^\infty} \lesssim \frac{1}{\beta}\left(\beta\|r(s)\|_{L^\infty} + |\lambda|\|s \cdot \nabla r(s)\|_{L^\infty}\right)\Delta t$$

$$\|V(s) - \hat{V}_i(s)\|_{L^\infty} \lesssim \frac{1}{\beta^2}|\lambda|^{i+1}\|s\nabla r\|\Delta t^i$$

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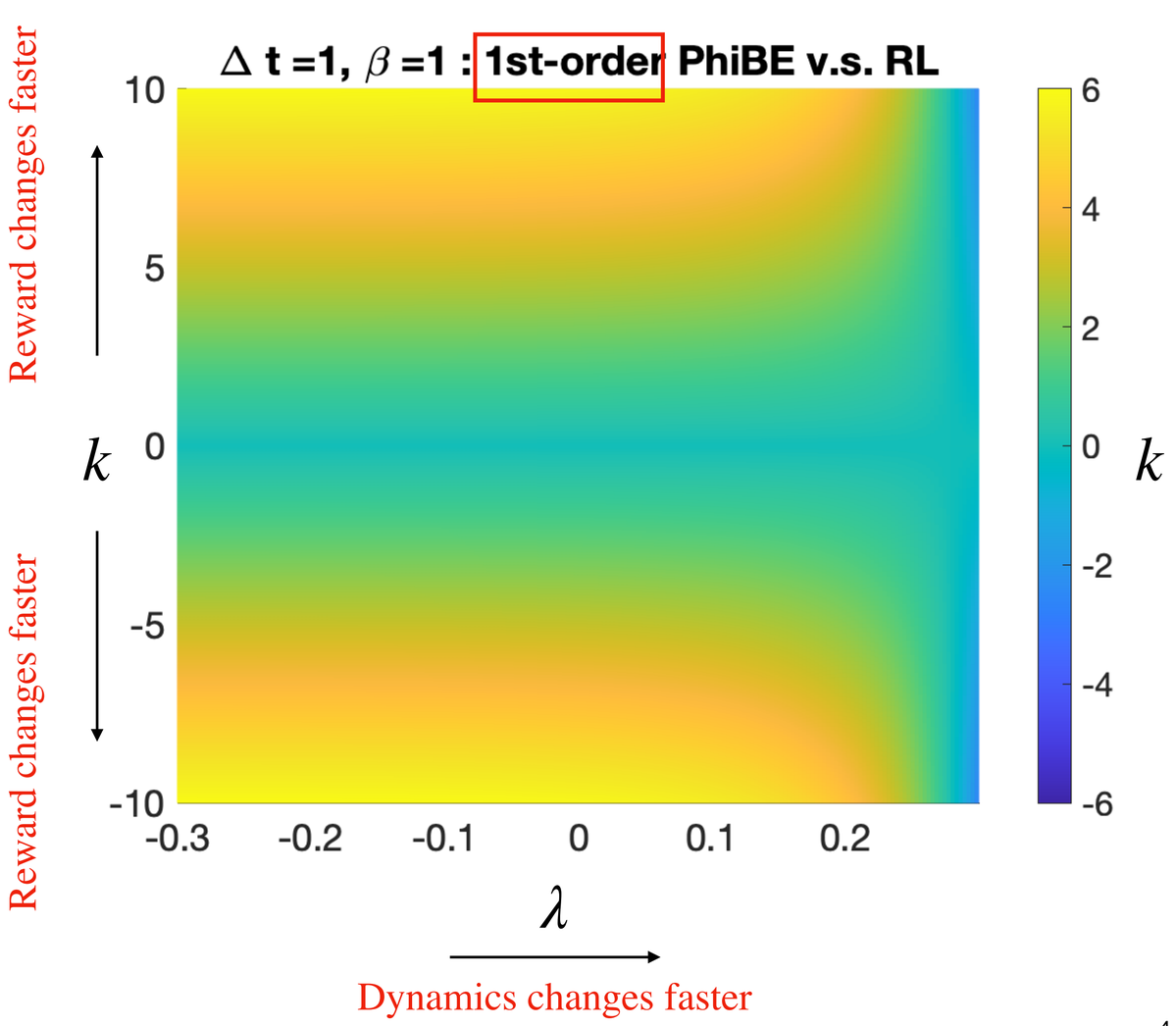
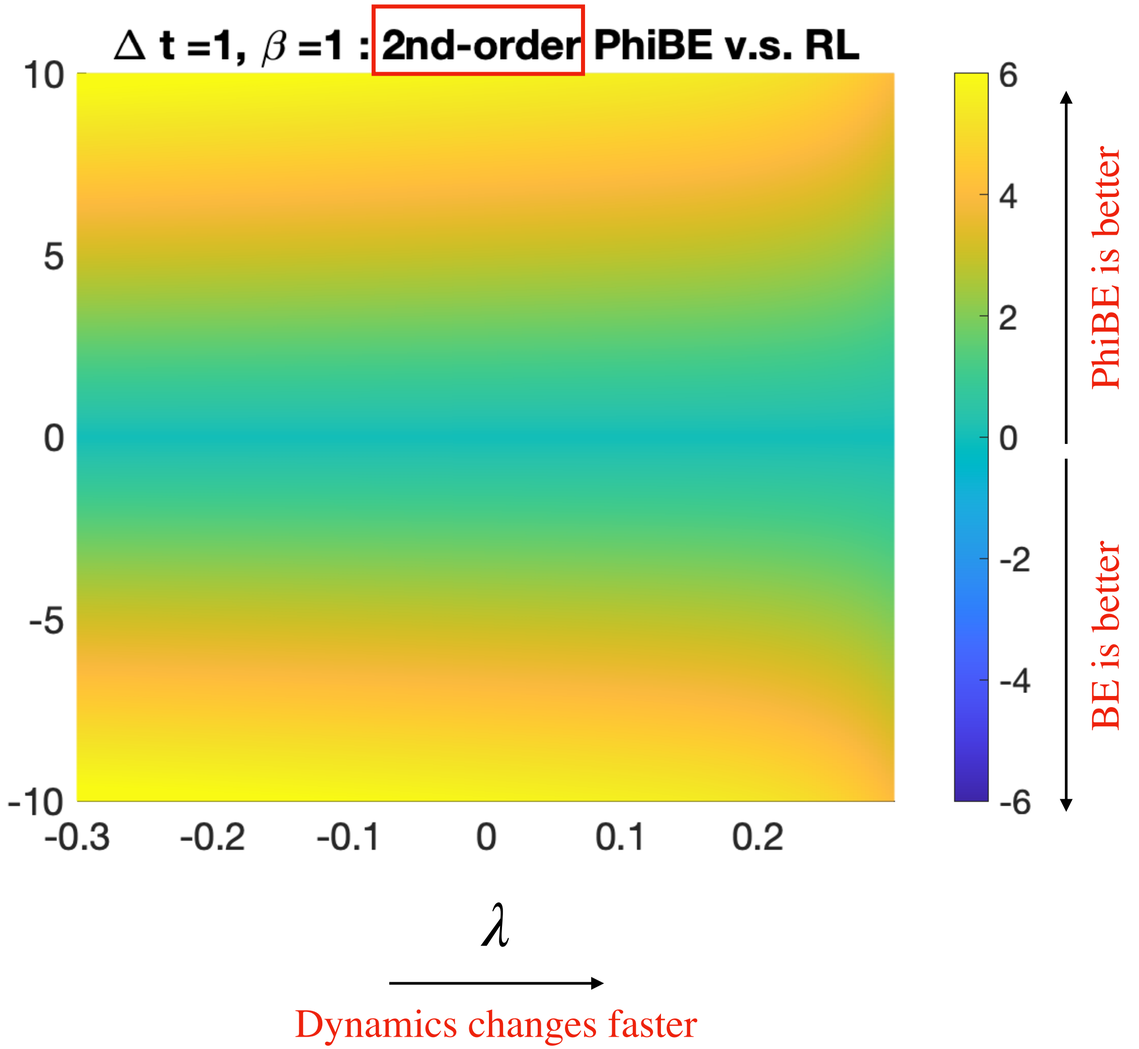
- When $|\lambda|$ is smaller, the error is smaller
- When $|\lambda|\Delta t < 1$, higher order PhiBE is better

LQR

$$V(s) = \int_0^{\infty} e^{-\beta t} k s_t^2 dt, \quad \dot{s}_t = \lambda s_t$$





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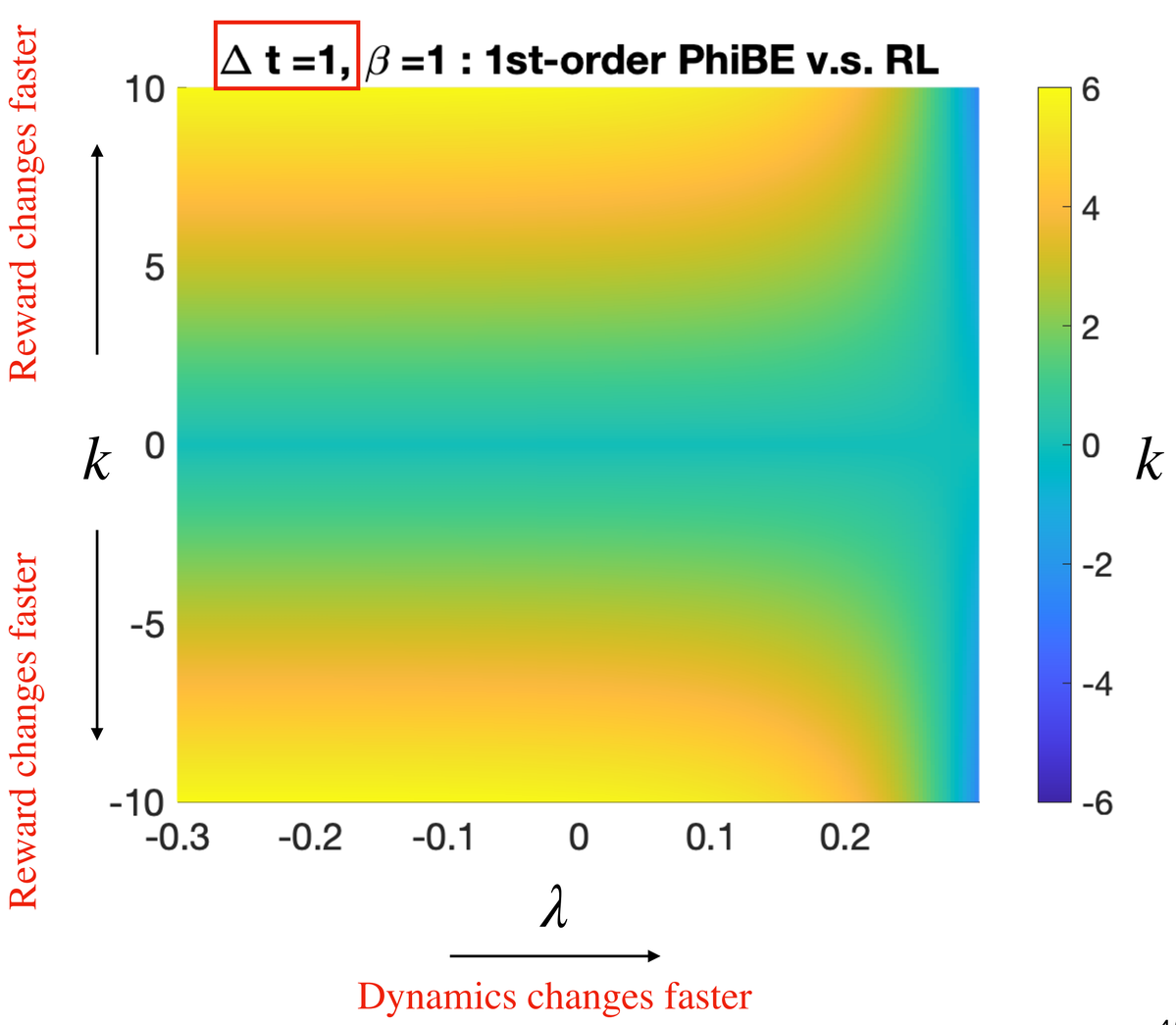

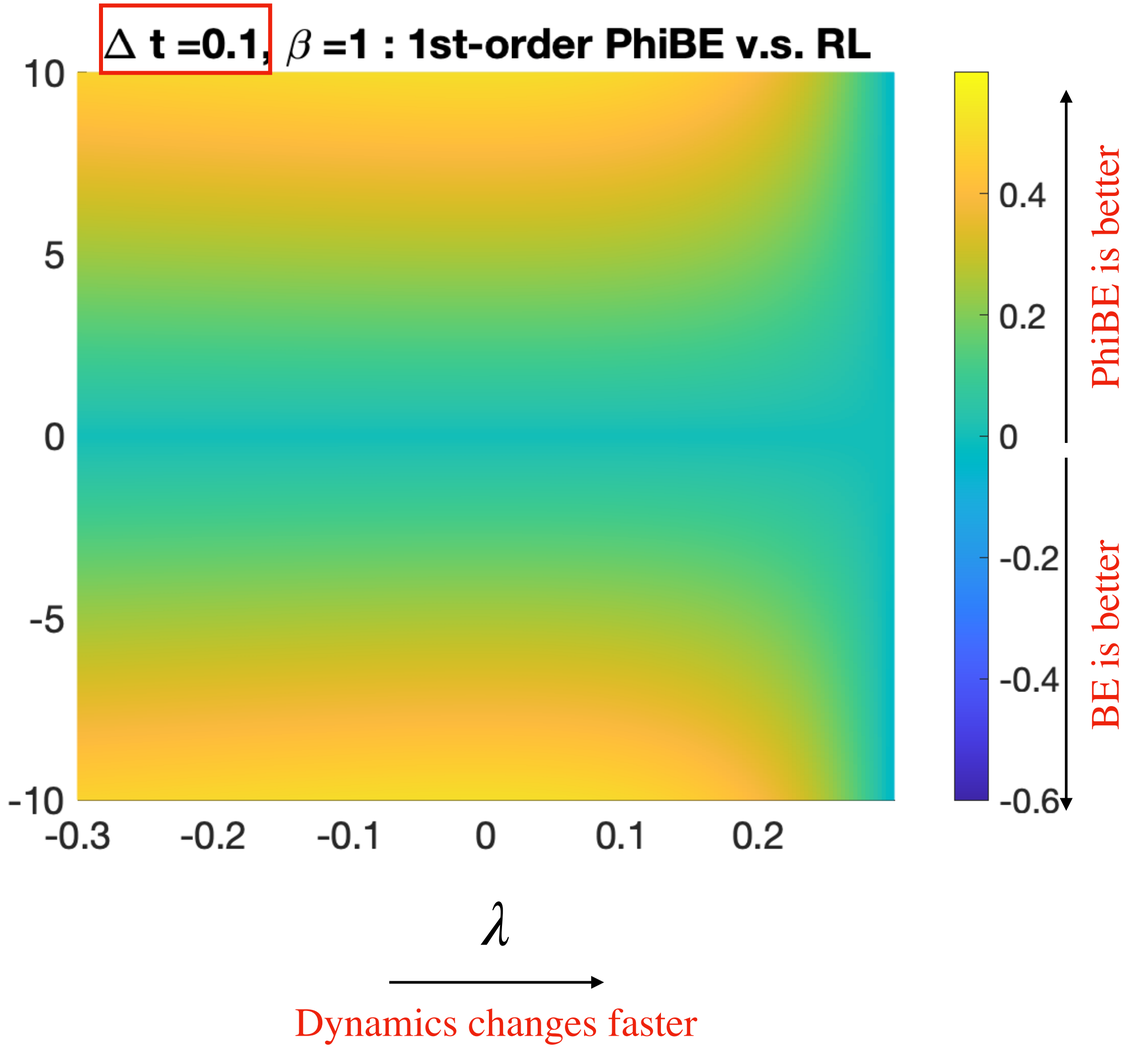

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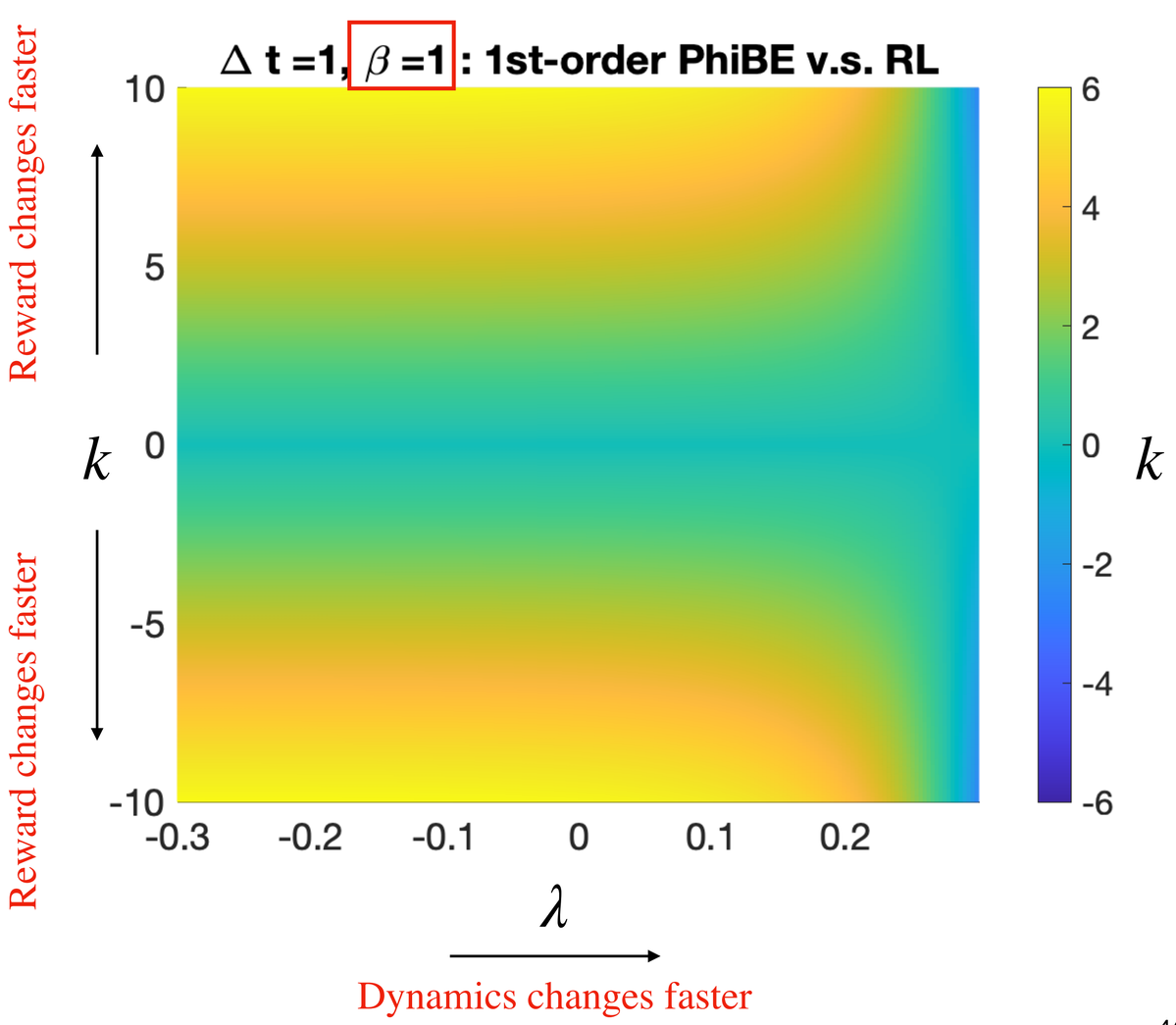

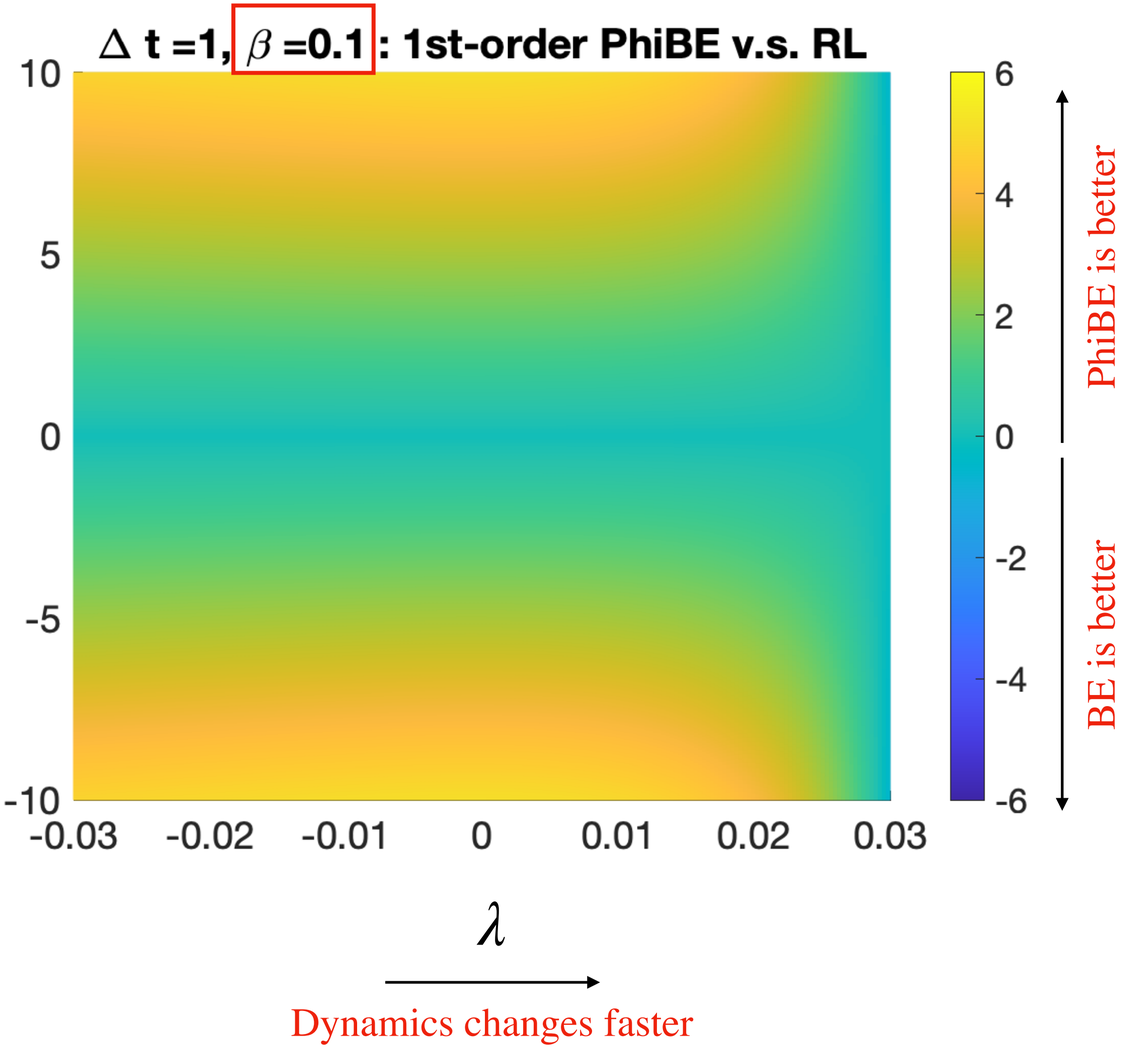

Schedule

Continuos-time RL —— Setting

Bellman equation ——Why it is not good

A PDE-based Bellman equation —— Why it is better

More numerical experiments

Given the same trajectory data: PhiBE v.s. BE

Underlying dynamics: $\frac{d}{dt}s_t = \lambda \sin(s_t)$

Given the same trajectory data: PhiBE v.s. BE

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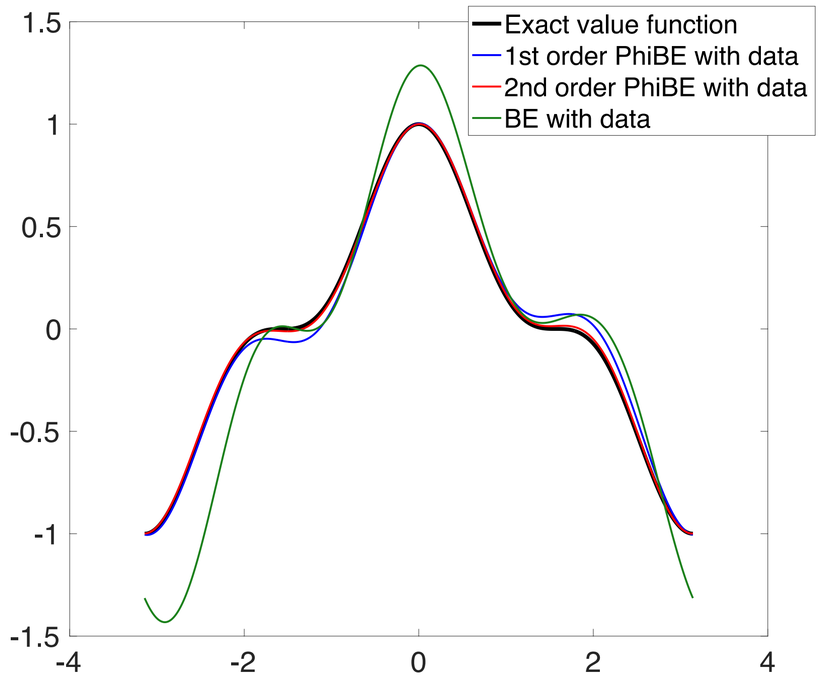
$\Delta t = 5, \beta = 0.1, \lambda = 0.05, V(s) = \cos^3(s)$



# of data: 40

Given the same trajectory data: PhiBE v.s. BE

Underlying dynamics: $\frac{d}{dt}s_t = \lambda \sin(s_t)$

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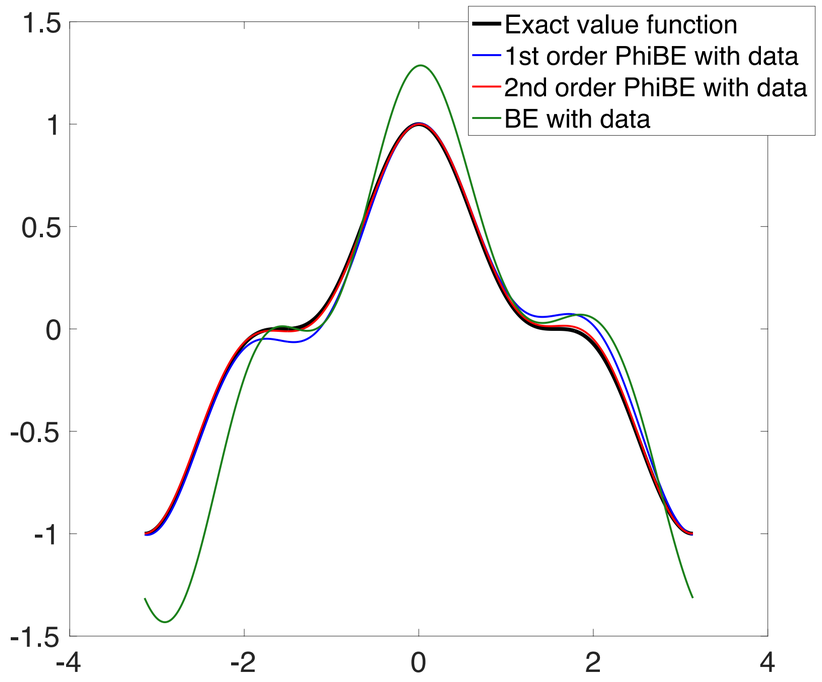
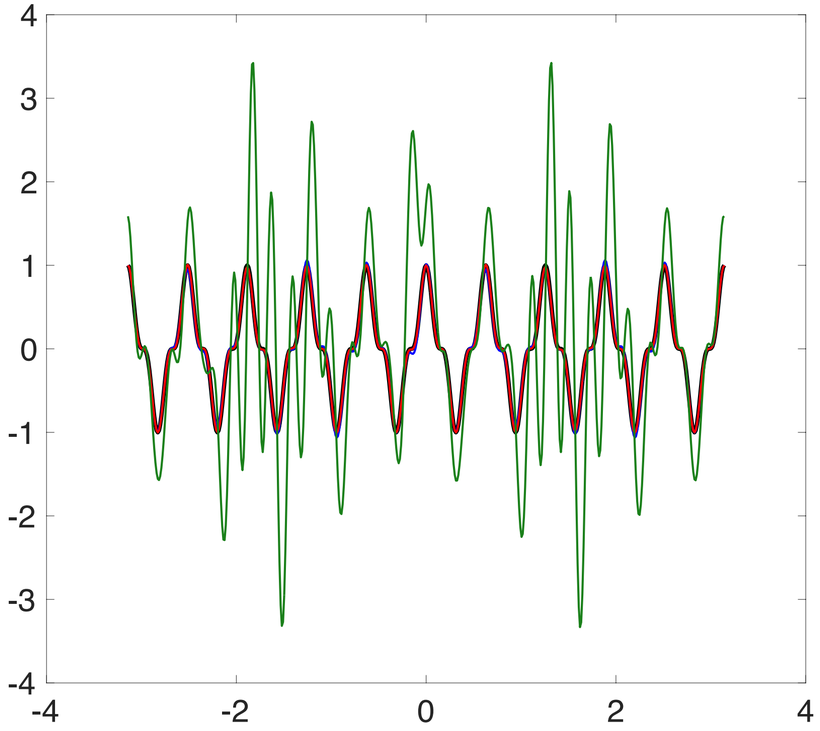


# of data: 40

$\Delta t = 0.1, \beta = 10, \lambda = 2, V(s) = \cos^3(10s)$



# of data: 400

Given the same trajectory data: PhiBE v.s. BE

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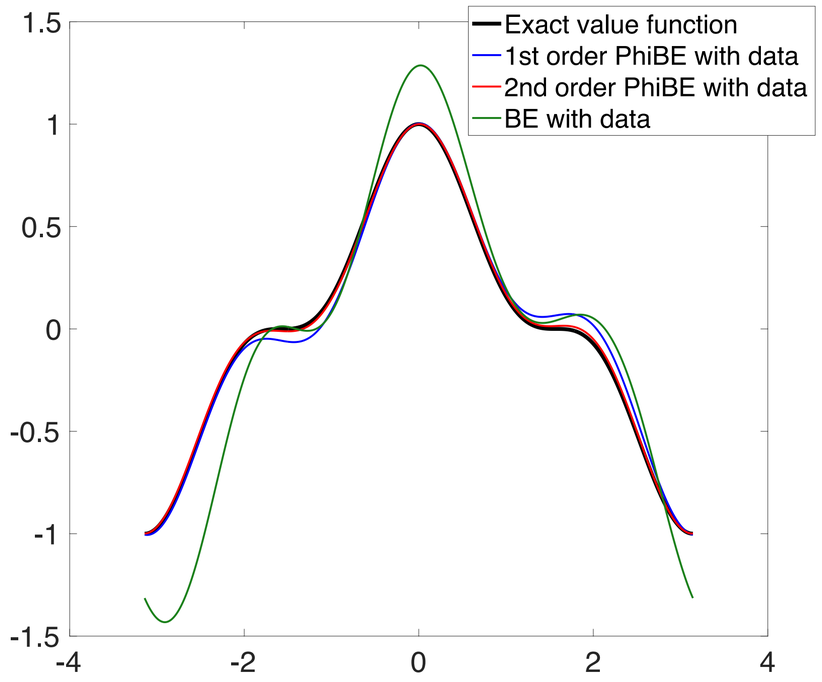

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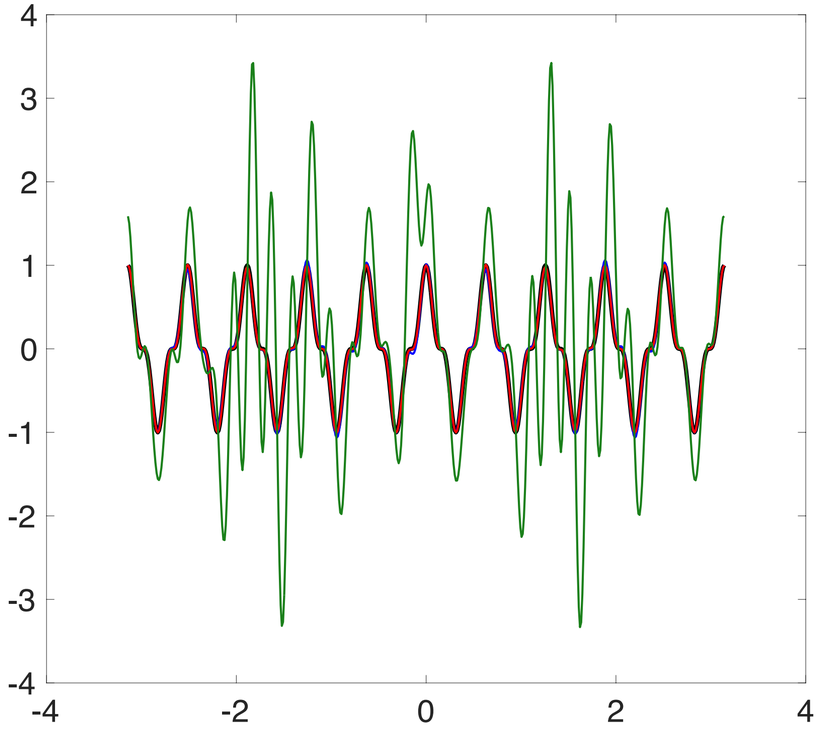

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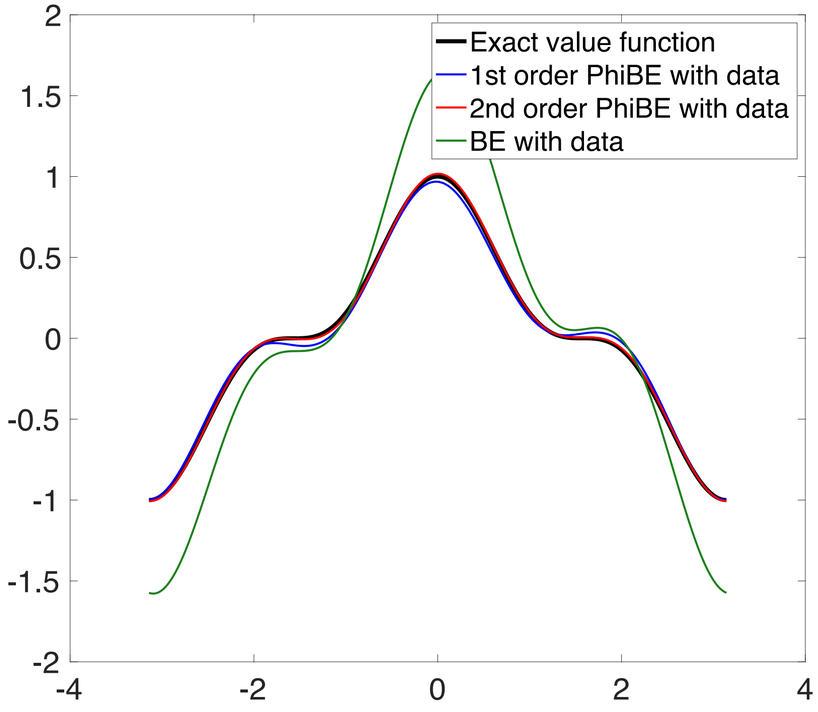
$\Delta t = 0.1, \beta = 10, \lambda = 5, V(s) = \cos^3(s)$



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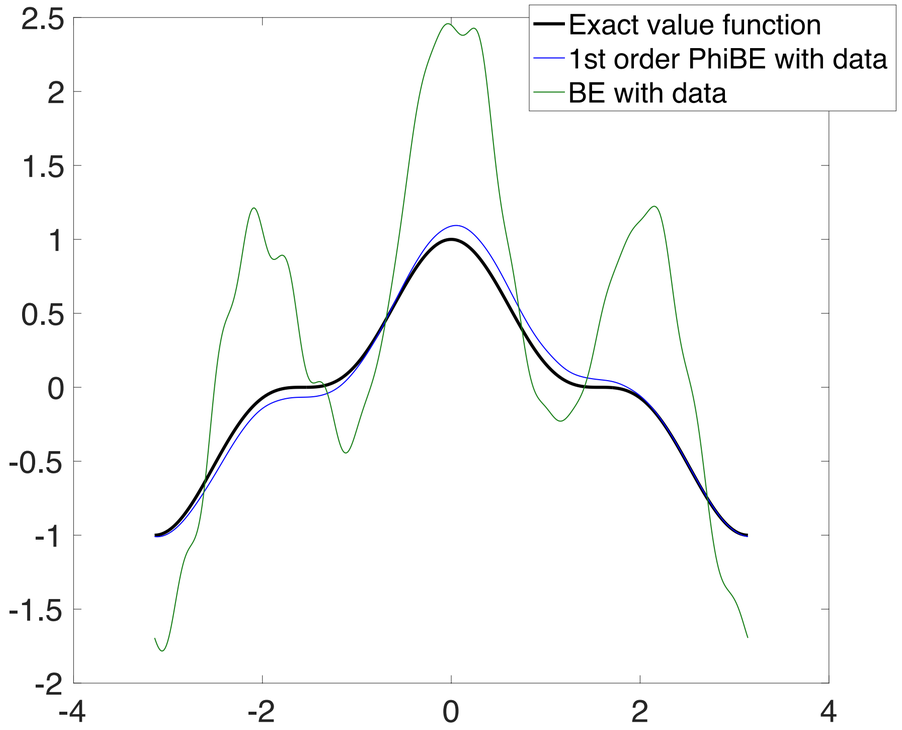
Given the same trajectory data: PhiBE v.s. BE

Underlying dynamics: $ds_t = 0.05 s_t + dB_t$

Given the same trajectory data: PhiBE v.s. BE

Underlying dynamics: $ds_t = 0.05 s_t + dB_t$

$\Delta t = 1, \ \beta = 0.1, V(s) = \cos^3(s)$



# of data: 4×10^3

Given the same trajectory data: PhiBE v.s. BE

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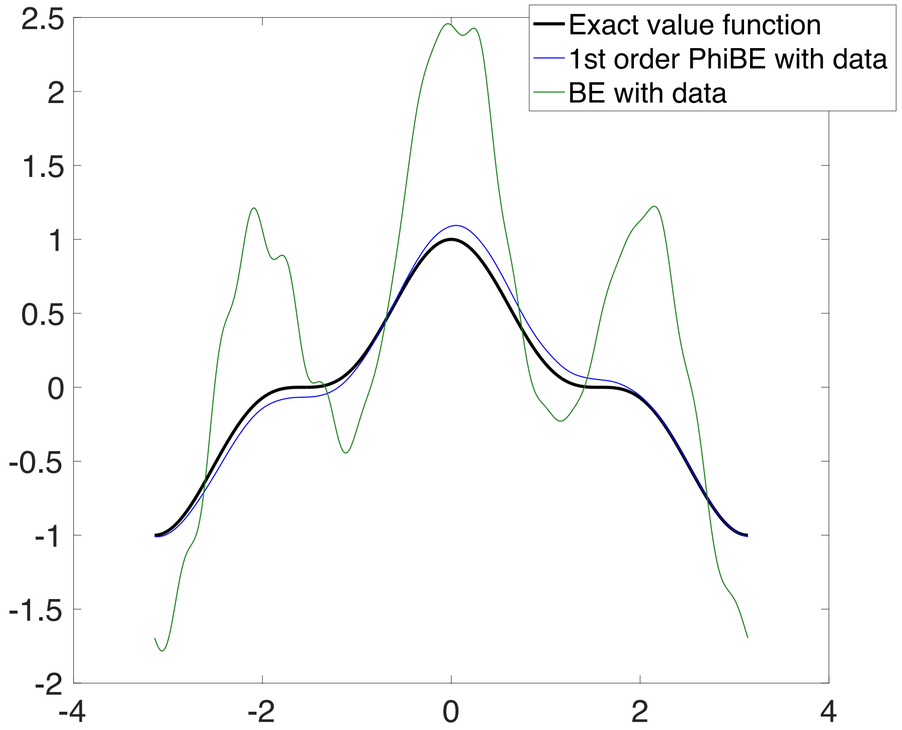
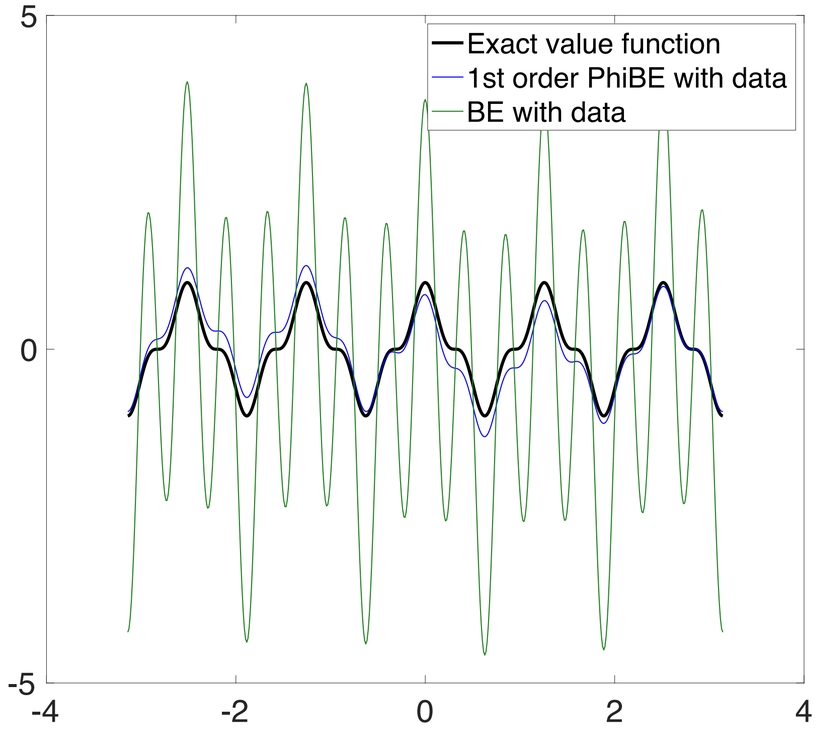


# of data: 4×10^3

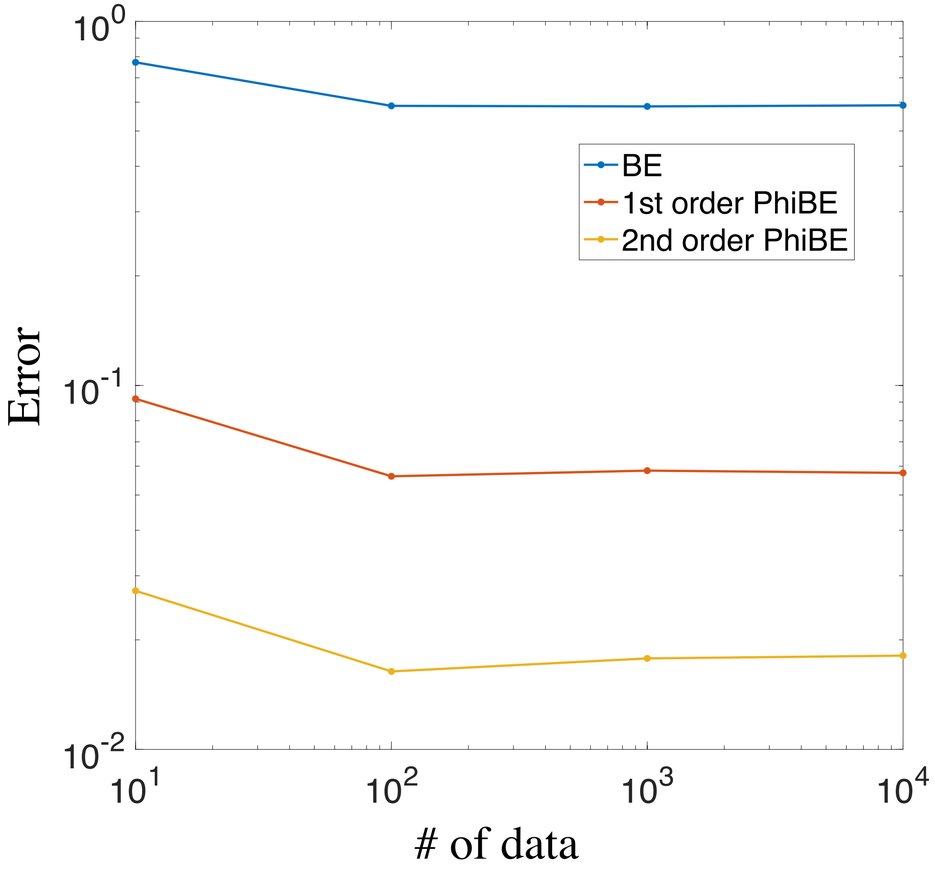
$\Delta t = 0.1,\ \beta = 0.1,\ V(s) = \cos^3(5s)$



# of data: 4×10^5

Decrease of error as # of data increases

Underlying dynamics: $\frac{d}{dt}s_t = 0.05 s_t$



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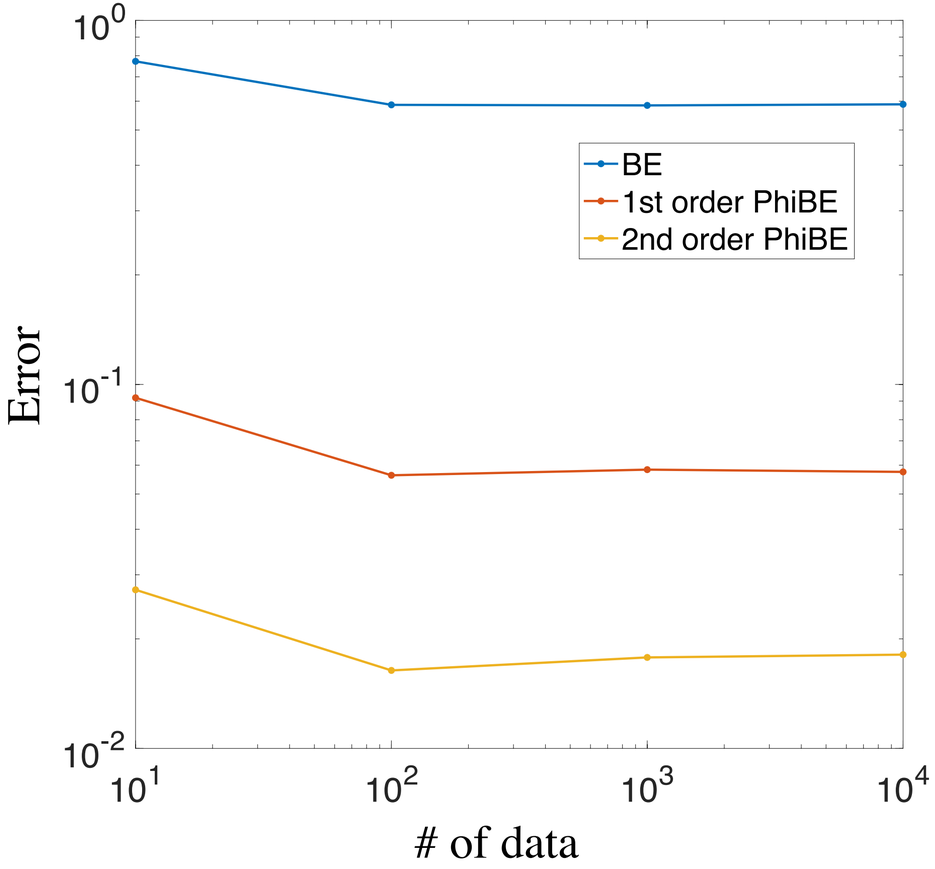
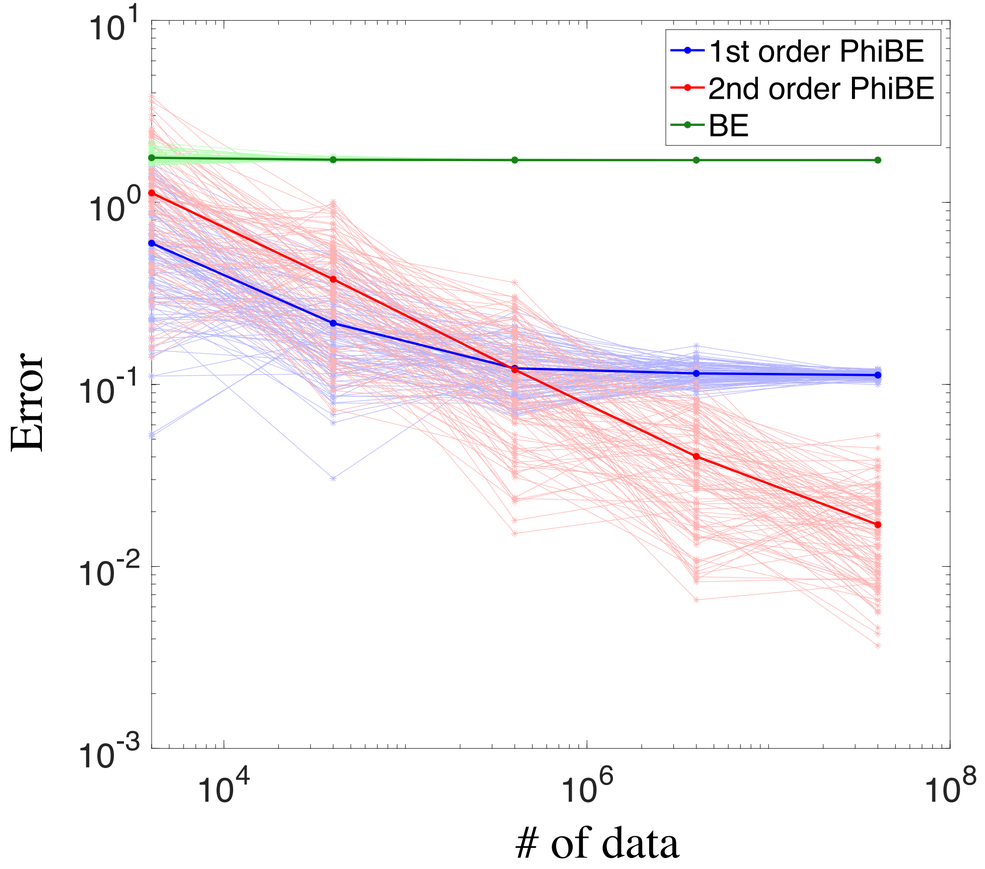


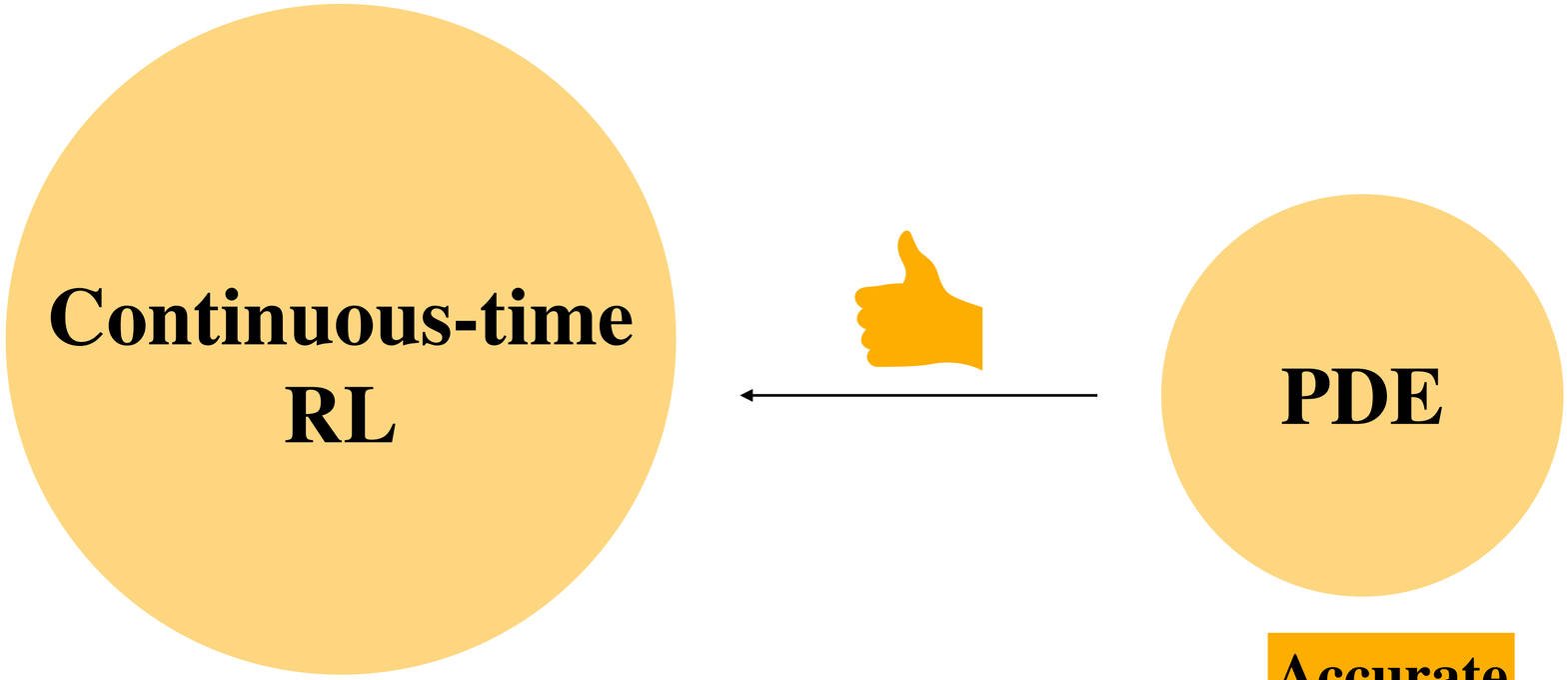
Underlying dynamics: $ds_t = 0.05 s_t + dB_t$



Conclusion

Continuous-time RL

Conclusion



Conclusion

Reference

Yuhua Zhu, 2024, PhiBE: A PDE-based Bellman Equation for Continuous-Time Policy Evaluation

Ongoing work

- Generalize to continuous-time RL
- Nonlinear approximation
- Time dependent dynamics
- Finite Horizon problems

Future work

- Multi-agent RL
- Mean-field game
- Application in robotics, autonomous driving and finance
- …