Improving Data-driven Scientific Computing

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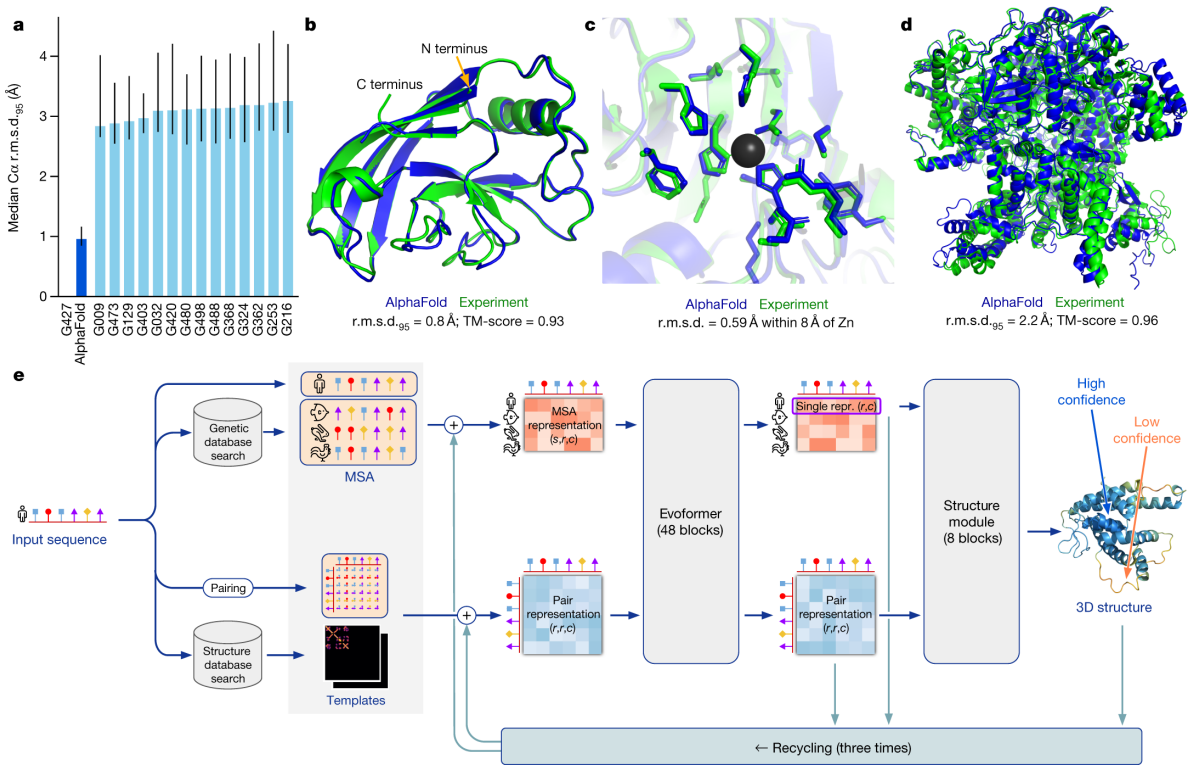
Data-driven scientific computing

Data-driven method is becoming a prevalent surrogate model in mathematical modeling and scientific computing, due to its power on approximation the data in complicated and high dimensional setting.



Data-driven scientific computing

Sometimes it is combined with traditional numerical method to improve the performance, or substitute some empirical part of the traditional method:

1. Learn the (empirical) potential function in molecular dynamics (MD).
2. Estimate the Reynolds stresses in Reynolds-averaged simulation (RAS).

Data-driven method for turbulence modeling

We briefly review the Reynolds average Navier-Stokes (RANS) equation. Denote by $\langle \mathbf{U} \rangle$ the time average of $\mathbf{U}$ and $\mathbf{u} = \mathbf{U} - \langle \mathbf{U} \rangle$:

$$\partial_t \langle \mathbf{U} \rangle + (\langle \mathbf{U} \rangle \cdot \nabla) \langle \mathbf{U} \rangle + \frac{\partial \langle \mathbf{u} u_j \rangle}{\partial x_j} = -\frac{1}{\rho} \nabla p + \nu \Delta \langle \mathbf{U} \rangle , \quad (1)$$

An extra term comes in, i.e. $\langle \mathbf{u} u_j \rangle$ Reynolds stress. The equation is no longer close!!

Ling et al. proposed a data-driven surrogate model to estimate the Reynolds stresses based on the averaged velocity field via neural network.

Data-driven method for turbulence modeling

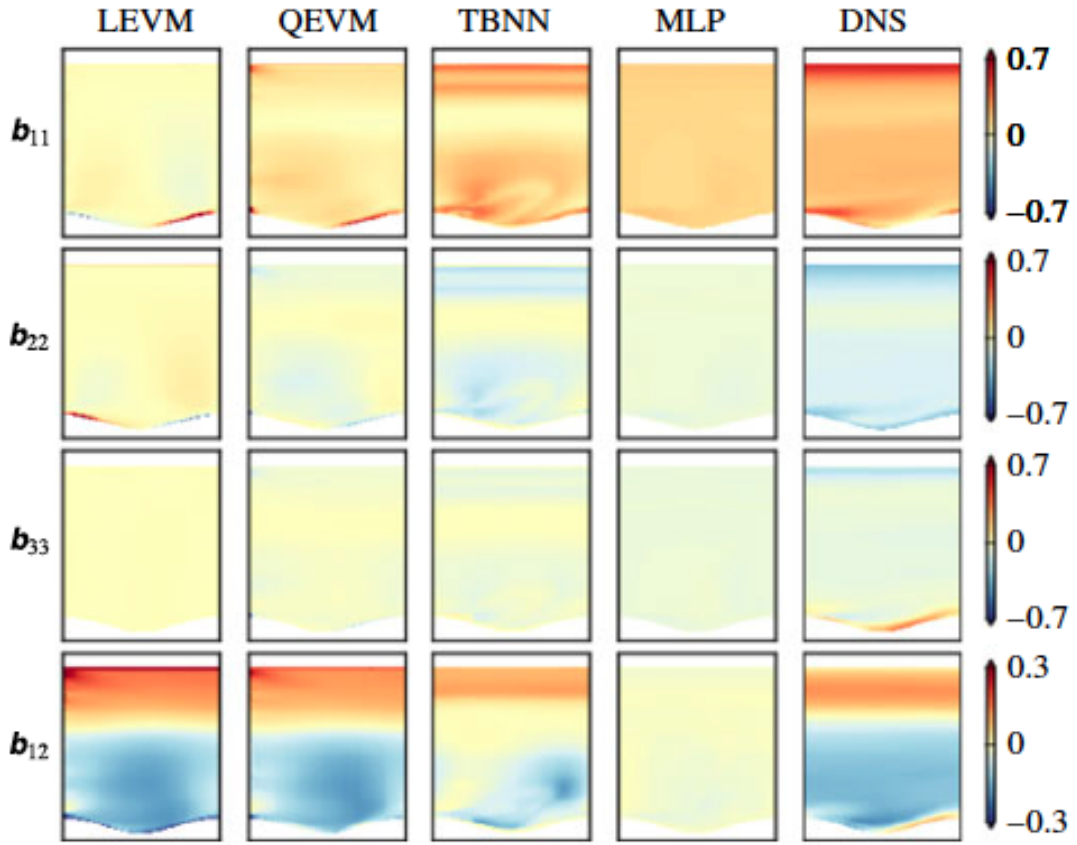


FIGURE 3. Predictions of Reynolds stress anisotropy $\boldsymbol{b}$ tensor on the wavy wall test case. The columns show the predictions of the LEVM, QEVM, TBNN and MLP models. The true DNS anisotropy values are shown in the right-most column for comparison.

Imitation learning

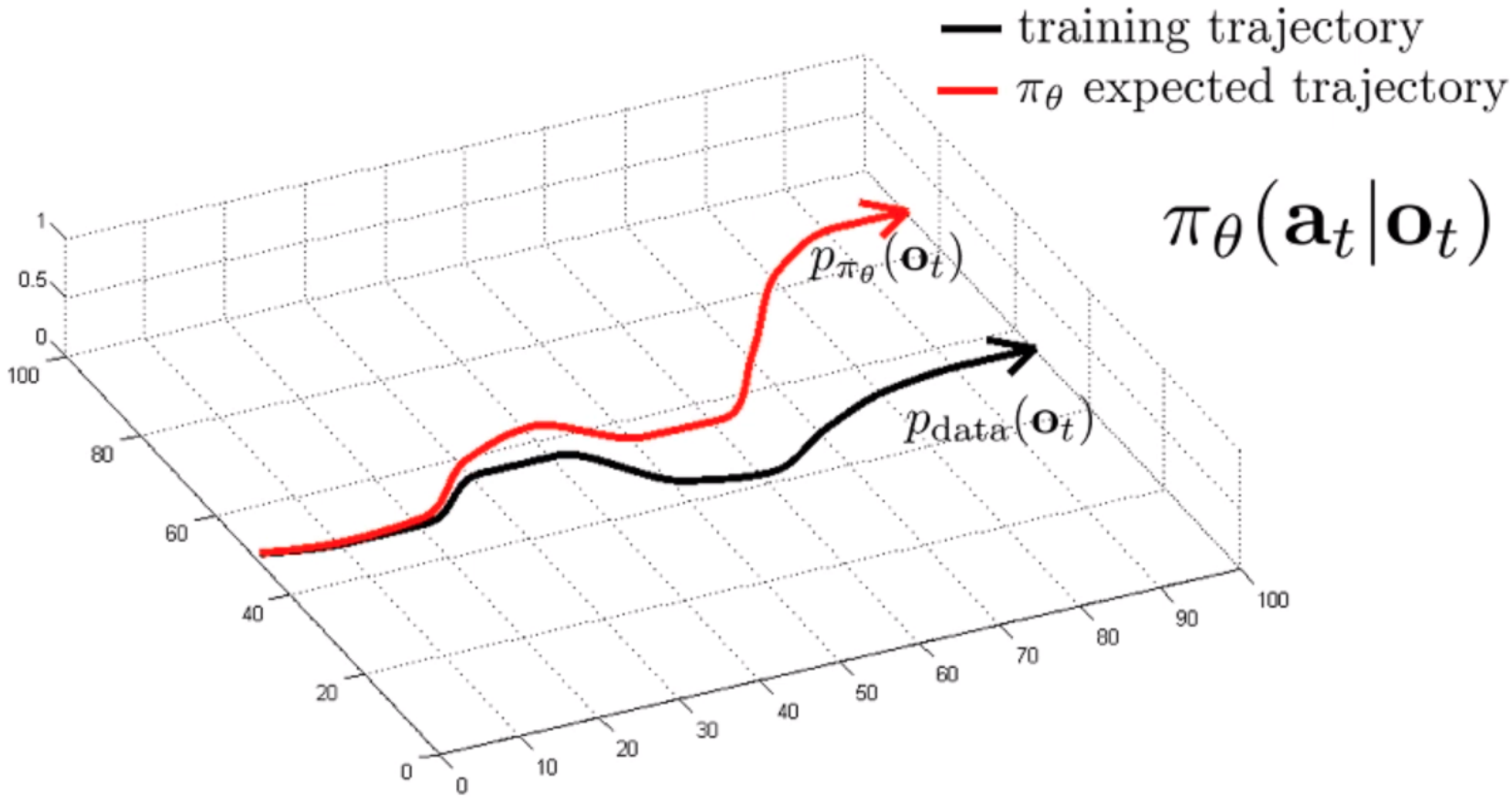
In contrast to the task in the computer science society, scientific computing is more close to reinforcement learning. In most setting that is important to us, the task belongs to the regime of imitation learning.

Definition

For a system with transition model $p(x_t|x_{t-1}, u_{t-1})$ *with states* $x \in \mathcal{X}$ *and controls* $u \in \mathcal{U}$*, the imitation learning problem is to leverage a set of demonstrations* $\Xi = \{(x_0, u_0), (x_1, u_1), \cdots\}$ *from an expert policy* π^* *to find a policy* $\widehat{\pi}$ *that imitates the expert policy.*

Dilemma of imitation learning

Basic algorithm called **behavior cloning** defines a loss function $l(\cdot,\cdot)$ and a parametrised model $\phi(\cdot,\theta)$ to learn the mapping between x and u, i.e. $\arg\min \mathbb{E}_x l(u,\phi(x,\theta))$.



the problem: $p_{\text{data}}(\mathbf{o}_t) \neq p_{\pi_\theta}(\mathbf{o}_t)$

What has been done in the imitation learning community?

Modified the training dataset to mitigate the distribution shift.

Algorithm 1: DAgger: Dataset Aggregation

Data: π^*

Result: $\hat{\pi}^*$

$\mathcal{D} \leftarrow 0$

Initialize $\hat{\pi}$

for $i = 1$ **to** N **do**

  $\pi_i = \beta_i \pi^* + (1 - \beta_i)\hat{\pi}$

  Rollout policy π_i to sample trajectory $\tau = \{x_0, x_1, \dots\}$

  Query expert to generate dataset $\mathcal{D}_i = \{(x_0, \pi^*(x_0)), (x_1, \pi^*(x_1)), \dots\}$

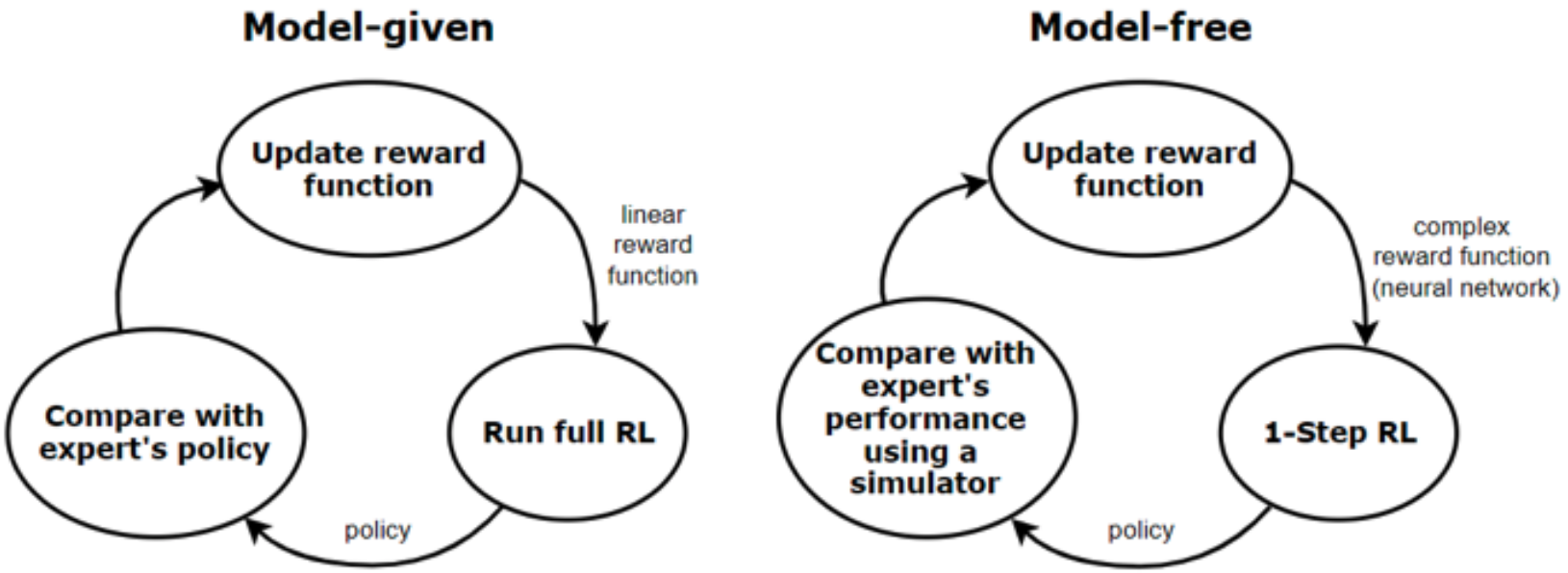
  Aggregate datsets, $\mathcal{D} \leftarrow \mathcal{D} \cup \mathcal{D}_i$

  Retrain policy $\hat{\pi}$ using aggregated dataset $\mathcal{D}$

return $\hat{\pi}$

What has been done in the imitation learning community?

Inverse reinforcement learning.



An intuition

Since the dilemma comes from the mismatch between training and test distribution, one can add regularization to the optimization step to force them become similar. In other word, one can force the test trajectories stays near the training set. This can be formed as a standard problem in manifold learning.

Inner-outer loop

A common structure in the data-driven scientific computation method: inner-outer loop:

$$\begin{aligned} \mathbf{X}_{k+1} &= A\mathbf{X}_k + B\mathbf{Z}_k, \quad \mathbf{X}_k \in \mathbb{R}^n, \mathbf{Z}_k \in \mathbb{R}^m, \\ \mathbf{Z}_k &= f(\mathbf{X}_k). \end{aligned}$$

The outer loop is known to us and usually has some good numerical properties, i.e. linear, stable, etc, while the inner loop can be complicated.

Inner-outer loop: examples

Example (RANS)

$$\begin{cases} \mathbf{u}\cdot\nabla\mathbf{u} - \nu\nabla^2\mathbf{u} + \nabla p - \nabla\cdot\tau = \mathbf{0}, \\ \nabla\cdot\mathbf{u} = 0. \end{cases}$$

$$\tau = R(\mathbf{u}).$$

Example (Quasi-potential)

$$\begin{aligned} \mathbf{X}_{k+1} &= \mathbf{X}_k - \Delta t \mathbf{Z}_k, \\ \mathbf{Z}_k &= \nabla V_\theta(\mathbf{X}_k) + g_\theta(\mathbf{X}_k). \end{aligned} \tag{2}$$

Algorithms and numerical experiments

We test different methods in a toy model of linear control.

$$\begin{aligned} \dot{x}_t &= v_t, \\ \dot{v}_t &= -\alpha(t) v_t + u_t, \end{aligned} \tag{3}$$

The initial value is given by $x_0 = 1, v_0 = 0$ and the goal is that $x_1 = 0$. u_t is the control variable to be determined. There are two different kinds of the time-dependent condition $\alpha(t) = t^2$ and $\alpha(t) = \sin 10t$.

In fact, u obey the Ricatti equation. And we use a neural network with 2 hidden layer to parameterize the mapping from (x_k, v_k, t_k) to u_k. Hence the neurons in each layer is given by $3, n, n, 1$ where n can be varied in the experiments.

Algorithms and numerical experiments

Inner-Outer loop structure of this linear control:

$$\begin{aligned} \begin{pmatrix} x_{k+1} \\ v_{k+1} \end{pmatrix} &= \begin{pmatrix} 1 & dt \\ 0 & 1-\alpha_k dt \end{pmatrix} \begin{pmatrix} x_k \\ v_k \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} u_k, \\ u_k &= \phi_{NN}(x_k, v_k, t_k). \end{aligned} \tag{4}$$

And behavior cloning method simply solve the model by minimizing the following function:

$$l(\phi_{NN}(x_k, v_k, t_k), u_k) = \|\phi_{NN}(x_k, v_k, t_k) - u_k\|_2^2 .$$

Ordinary least square

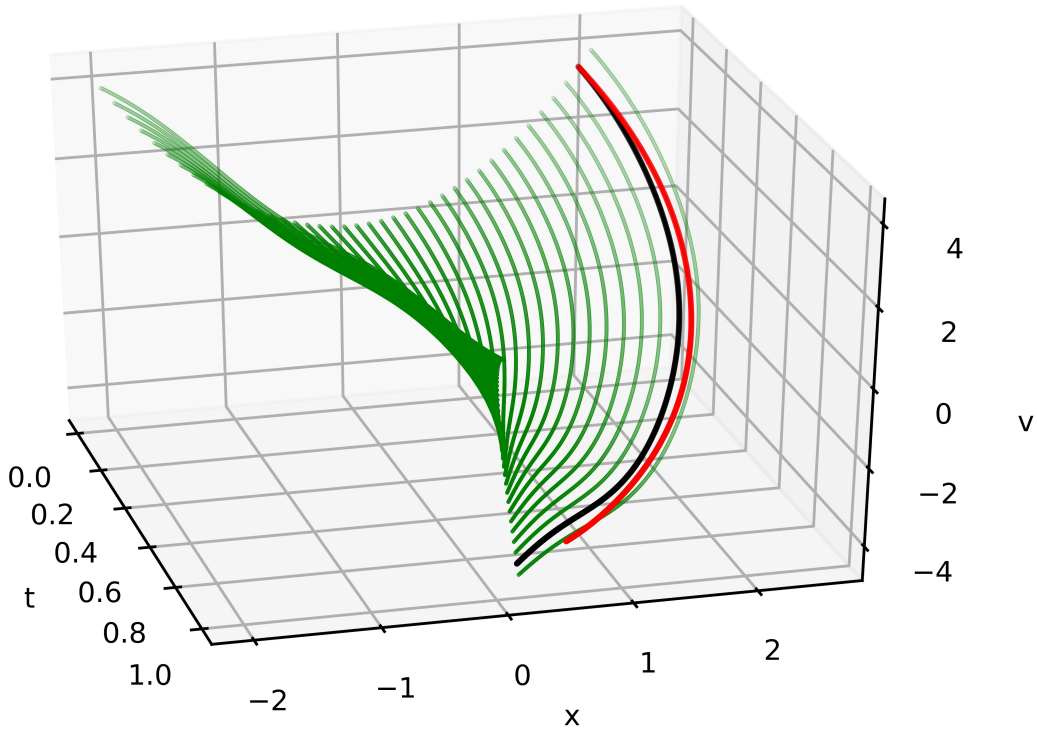


Figure: Sampled training trajectory of an estimator with underlying net of 10 hidden neurons.

Ordinary least square

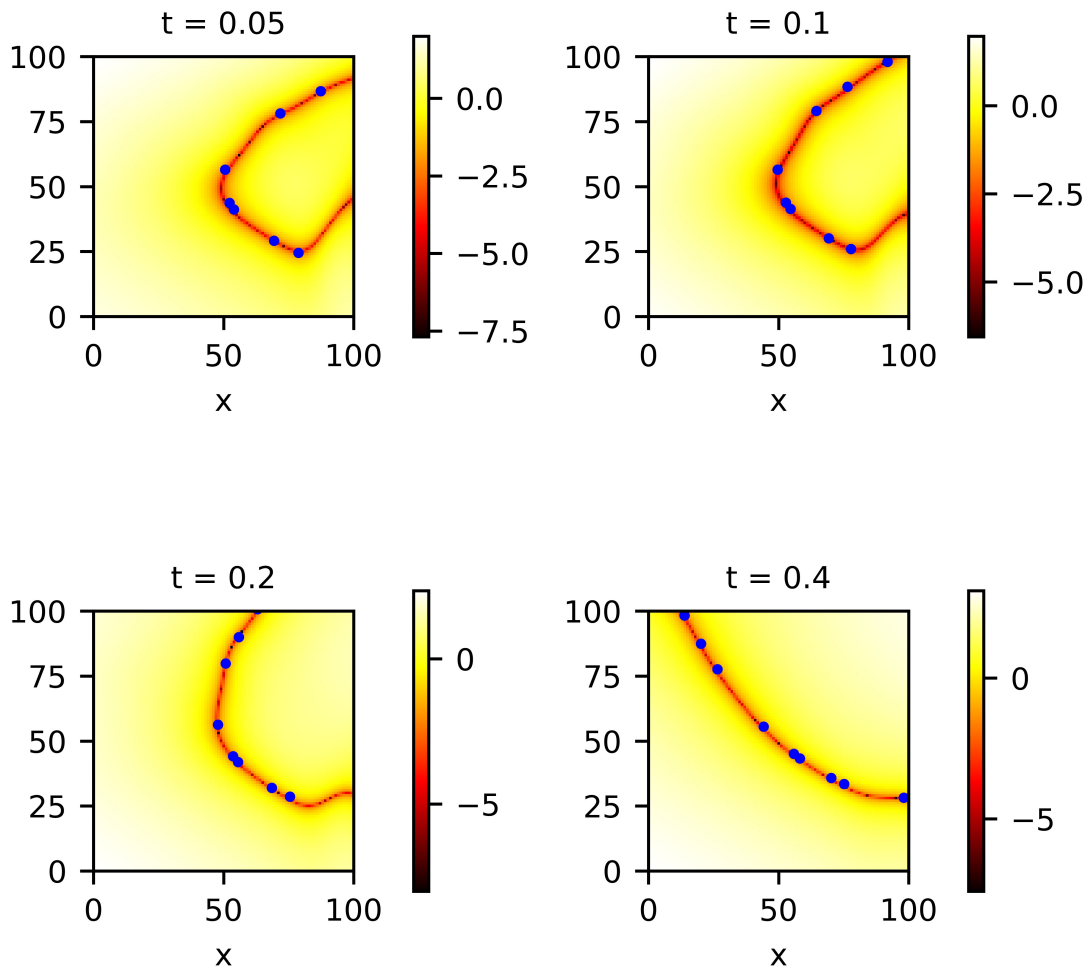


Figure: Sampled training trajectory of an estimator with underlying net of 50 hidden neurons.

Manifold regularization

Following our intuition, we introduce manifold regularization to the loss function. Several choices of empirical manifold is listed:

Formed by the sample trajectories in the training data, i.e.

$$\mathcal{M}_t := \{(x(t), v(t), t) \quad t \in [0, 1]\},$$

The other empirical manifold related to the data-driven surrogate model and can be defined as following set:

$$\widehat{\mathcal{M}}_t := \left\{(x, v, t) \middle| \, \|\phi_{NN}(x_k, v_k, t_k) - u_k\|_2 < \epsilon \right\}.$$

Manifold regularization

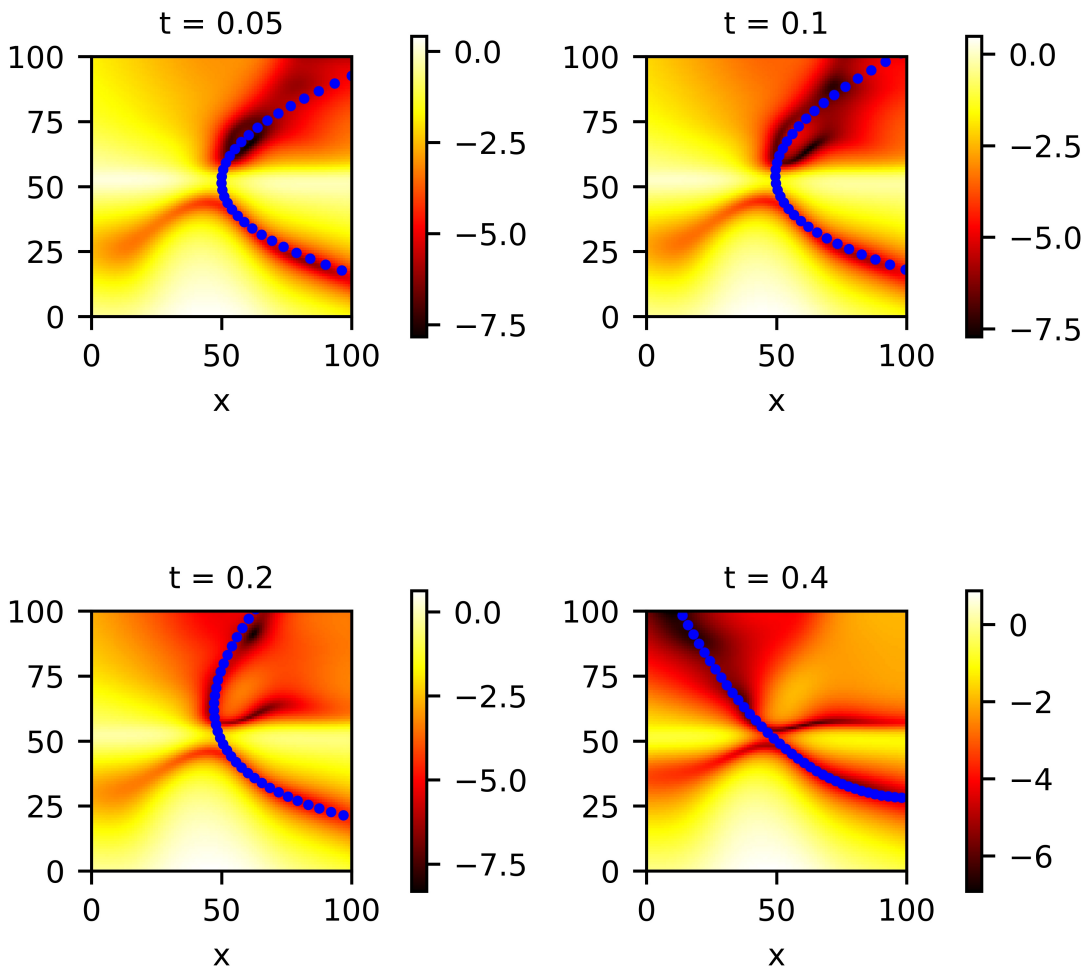


Figure: Sampled training trajectory of an estimator with underlying net of 50 hidden neurons.

Manifold regularization

The manifold related to the data-driven surrogate model characterizes the underlying manifold structure better than the manifold encoded by the training dataset, and it also outperform this latter one in sampling new trajectories.

Future work

We will further investigate the following thing:

1. Understand the success and failure of different methods in the simple setting.

2. Apply proposed methods to more practical problem to test their performance and further improve them.

Reference

1. Imitation Learning Tutorial ICML 2018.
2.