


# Computational Mathematics and AI

## Lecture 8: High-Dimensional PDEs

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# Reading List

**Historical Context:** High-dimensional PDEs are abundant, curse of dimensionality coined in optimal control (Bellman 1961).

## Key Readings:

1. Han, Jentzen, and E (2018) – Solving High-Dimensional PDEs Using Deep Learning. *PNAS*  
Deep BSDE method breaking curse of dimensionality.
2. Raissi (2018) – Forward-Backward Stochastic Neural Networks. *arXiv*  
FBSNNs for high-dimensional parabolic PDEs.
3. Hu et al. (2024) – Hutchinson Trace Estimation for PINNs. *JMLR*  
Scaling PINNs to 100,000+ dimensions.
4. Li, Verma, and Ruthotto (2024) – Neural Network for Stochastic Optimal Control  
*SIAM SISC*  
Neural networks for high-dimensional control problems.

**Lecture Outline:** Model Problem  $\rightarrow$  PINNs+HTE  $\rightarrow$  FBSDE  $\rightarrow$  PMP-informed

# High-Dimensional Semilinear Parabolic PDE

# The Semilinear Parabolic PDE

We consider the **semilinear parabolic PDE** for  $u : [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}$ :

$$\frac{\partial u}{\partial t} + \mu(t, x) \cdot \nabla u + \frac{1}{2} \text{trace}(\sigma \sigma^\top \nabla^2 u) + f(t, x, u, \sigma^\top \nabla u) = 0, \quad \text{for } t \in [0, T]$$

- ▶  $u(T, x) = g(x)$  for  $x \in \mathbb{R}^d$  — **terminal condition** at time  $T$
- ▶  $\mu : [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$  — **drift coefficient**
- ▶  $\sigma : [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$  — **diffusion coefficient**
- ▶  $f$  — **nonlinear drift term**, depends on  $u$  and  $\nabla u$

## Applications:

- ▶ Stochastic optimal control (Hamilton-Jacobi-Bellman equations)
- ▶ Financial mathematics (option pricing)
- ▶ Pattern formation and reaction-diffusion systems (Allen-Cahn equation)

## Example: HJB (Han, Jentzen, and E 2018; Raissi 2018)

$$\frac{\partial u}{\partial t} + \Delta u - \|\nabla u\|^2 = 0, \quad \text{for } t \in [0, T) \quad u(T, x) = g(x)$$

Solution is the value function of the stochastic optimal control problem:

$$\begin{aligned} \min_{a \in \mathcal{A}} \mathbb{E} \left[ g(X_T) + \int_0^T L(X_s, a_s) ds \right] \\ \text{s.t. } dX_s = 2a_s ds + \sqrt{2} dW_s, \quad X_0 = x \end{aligned}$$

- ▶ **Running cost:**  $L(x, a) = \|a\|^2$
- ▶ **Terminal cost:**  $g(x) = \log \left( \frac{1}{2} (1 + \|x\|^2) \right)$
- ▶ Analytical solution (Hopf-Cole transform):  $u(t, x) = -\log (\mathbb{E} [\exp(-g(X_T)) \mid X_t = x])$
- ▶ Verify: Let  $v = e^{-u}$ . Then  $\partial_t v = -\partial_t u \cdot v$ ,  $\nabla v = -\nabla u \cdot v$ ,  $\Delta v = (\|\nabla u\|^2 - \Delta u)v$ .  
HJB  $\Rightarrow \partial_t v = \Delta v$ , i.e.,  $v$  solves the **heat equation!**
- ▶  $d = 100$  is completely intractable for grid-based methods

**Today: illustrate curse of dimensionality with four representative approaches**

# General Paradigm: NNs for High-Dimensional Control

## Offline: Learn control (high computational cost)

1. Parameterize control/value function with neural net
2. Sample state space: uniform? random walk?
3. Define loss function: PDE residual, terminal matching, control objective, ...
4. Train weights via SGD, Adam, ...

**Challenge:** Avoid curse of dimensionality in network size, sample complexity, time

## Online: Evaluate policy (very fast, real-time)

Evaluate trained policy and measure performance with control objective (can be different from loss)

**Today: Compare three neural approaches for high-D stochastic control**

# PINNs with Hutchinson Trace Estimation

# PINNs for Semilinear Parabolic PDEs

**Idea:** Parameterize  $u_\theta(t, x)$  as a neural network

**Loss function:** Minimize expected PDE residual

$$\mathcal{L}(\theta) = \mathbb{E}_{(t,x)} |\mathcal{N}[u_\theta](t, x)|^2$$

with PDE residual  $\mathcal{N}[u] = \partial_t u + \mu \cdot \nabla u + \frac{1}{2} \text{trace}(\sigma \sigma^\top \nabla^2 u) + f$

## Computational challenge: Hessian Computation

For our PDE, we need  $\text{trace}(\sigma \sigma^\top \nabla^2 u)$

- ▶ Hessian matrix:  $d \times d = 100 \times 100 = 10,000$  entries
- ▶ Computing full Hessian:  $O(d^2)$  memory,  $O(d^2)$  compute
- ▶ For  $d = 1000$ : Compute/memory becomes prohibitive

**Problem:** Standard PINNs fail at  $d > 1000$  due to Hessian cost

**Solution:** Hutchinson Trace Estimation (HTE)



# The Hutchinson Trace Estimator

For our PDE:  $\text{trace}(\sigma \sigma^\top \nabla^2 u) = \text{trace}(\sigma^\top \nabla^2 u \sigma) = \text{trace}(A)$  where  $A = \sigma^\top \nabla^2 u \sigma$

## Hutchinson's Trick (1990):

For any matrix  $A$  and random vector  $v$  with  $\mathbb{E}[vv^\top] = I$ :

$$\text{trace}(A) = \mathbb{E}[v^\top A v]$$

## Monte Carlo Approximation:

$$\text{trace}(A) \approx \frac{1}{V} \sum_{i=1}^V v_i^\top A v_i$$

where  $v_i \sim \text{Rademacher}$  (entries  $\pm 1$  with probability  $1/2$ )

## Using AD for Hessian-Vector Products (HVP)

- ▶  $v^\top \sigma^\top \nabla^2 u \sigma v$  can be computed via autodiff in  $O(1)$  memory!
- ▶ Taylor-mode AD: forward-over-reverse differentiation

**Result:**  $O(d^2) \rightarrow O(1)$  memory/compute: enables PINNs in high dimensions!

# HTE-PINN: Where Does It Sample?

## The HTE-PINN Learning Problem:

$$\min_{\theta} \mathbb{E}_{(t,x),v} \left| \partial_t u_{\theta} + \mu \cdot \nabla u_{\theta} + \frac{1}{2} v^{\top} \sigma^{\top} \nabla^2 u_{\theta} \sigma v + f \right|^2$$

where  $(t, x) \sim \text{Uniform}([0, T] \times \Omega)$  and  $v \sim \text{Rademacher}(\pm 1)$

## The Sampling Strategy:

- ▶ Sample  $(t_i, x_i)$  uniformly from  $[0, T] \times \Omega$
- ▶ Use mini-batch SGD/Adam

## Discussion:

- ▶ does the added noise from HTE impact convergence?
- ▶ uniform sampling does not beat curse of dimensionality

**Next: Exploit problem structure with relation to SDEs**

# FBSDE-Based Methods

# PDE $\rightarrow$ SDE: Forward-Backward SDE System

$$\frac{\partial u}{\partial t} + \mu(t, x) \cdot \nabla u + \frac{1}{2} \text{trace}(\sigma \sigma^\top \nabla^2 u) + f(t, x, u, \sigma^\top \nabla u) = 0, \quad \text{for } t \in [0, T), \quad u(T, x) = g(x)$$

$$\textbf{Forward SDE: } dX_t = \mu(t, X_t) dt + \sigma(t, X_t) dW_t, \quad X_0 = x_0$$

What is the evolution of  $u(t, X_t)$  along SDE trajectory? Ito's lemma gives:

$$\begin{aligned} du(t, X_t) &= \left( \frac{\partial u}{\partial t} + \mu(t, x) \cdot \nabla u + \frac{1}{2} \text{trace}(\sigma \sigma^\top \nabla^2 u) \right) dt + (\nabla_x u)^\top \sigma dW_t \\ &= -f(t, X_t, u, \sigma^\top \nabla u) dt + (\nabla_x u)^\top \sigma dW_t, \quad u(T, X_T) = g(X_T) \end{aligned}$$

$$\textbf{Backward SDE: } Y_t = g(X_T) + \int_t^T f(s, X_s, Y_s, Z_s) ds - \int_t^T Z_s^\top dW_s$$

**If  $(X_t, Y_t, Z_t)$  solves FBSDE system, then  $Y_t = u(t, X_t)$  and  $Z_t = [\sigma(t, X_t)]^\top (\nabla_x u)(t, X_t)$**

# Method 1: Deep BSDE (Han, Jentzen, and E 2018)

## Key Idea: Optimize NN Approximation $Z_\theta$ and $Y_0$ Directly

- ▶ Learnable scalar  $Y_0 \approx u(0, X_0)$
- ▶ Stack of  $N - 1$  neural networks:  $Z_k(X_k) = Z_\theta(t_k, X_k)$  for each time step
- ▶ Each subnet: 4 layers, width  $d + 10$ , BatchNorm + ReLU

## Loss Function (Terminal Matching):

$$\mathcal{L}(\theta) = \mathbb{E} \left[ |Y_N - g(X_N)|^2 \right]$$

Where  $Y_N$  is computed by simulating the FBSDE forward in time:

$$\begin{aligned} X_{k+1} &= X_k + \mu(t, X_k) \Delta t + \sigma \Delta W_k \\ Y_{k+1} &= Y_k + f(t, X_k, u, Z_k(X_k)) \Delta t + Z_k(X_k)^\top \Delta W_k \end{aligned}$$

**Gives only pointwise estimate of  $u(0, X_0)$  at initial state!**

# Method 2: Fwd/Bwd Stochastic NN (Raissi 2018)

**Key Idea: Optimize NN approximation  $u_\theta(t, x)$  using FBSDE Residuals**

- ▶ Scalar-valued neural network  $u_\theta(t, x)$  shared across all times
- ▶ Gradient  $\nabla_x u_\theta$  via automatic differentiation
- ▶ Advantages over Deep BSDE: Parameter efficiency, can evaluate  $u_\theta$  anywhere

**Loss Function:**

$$\mathcal{L}(\theta) = \mathbb{E} \left[ |Y_N - g(X_N)|^2 + \alpha \sum_{k=0}^{N-1} |Y_{k+1} - Y_k + f_k \Delta t - Z_k^\top \Delta W_k|^2 \right]$$

where  $Y_k = u_\theta(t_k, X_k)$  and  $Z_k = \sigma^\top \nabla_x u_\theta(t_k, X_k)$

# $\Sigma$ : PINNs, Deep BSDE, and FBSNN

**PINNs:** Minimize PDE residual over domain

- ▶ In high-D: Use Hutchinson trace estimator for Hessian trace
- ▶ Sampling: Random collocation in  $[0, T] \times \Omega$

**Deep BSDE:** Learn  $Y_0$  and  $Z_k$  per time step via terminal matching

- ▶ avoids Hessian computation by working with FBSDE
- ▶ Sampling: Forward SDE  $dX = \mu_t dt + \sigma_t dW$
- ▶ Optimization: Find  $Y_0$  and  $Z_k$  to minimize  $\|Y_N - g(X_N)\|^2$

**FBSNN:** Learn  $u_\theta(t, x)$  via FBSDE residuals

- ▶ Advantage over Deep BSDE: single NN for all times, can evaluate anywhere
- ▶ Sampling: Forward SDE  $dX = \mu_t dt + \sigma_t dW$
- ▶ Optimization: Minimize residuals at each time step + terminal matching

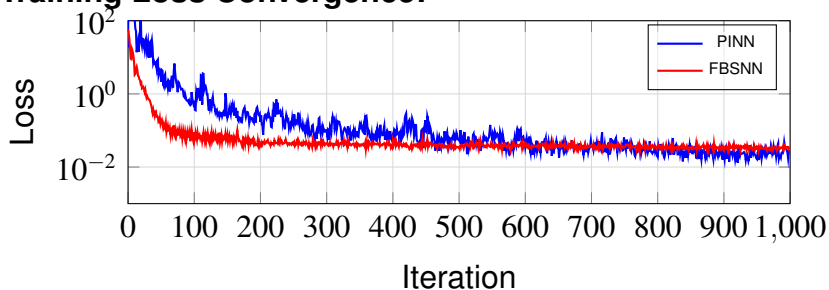
**Common disadvantage for HJB: Sampling independent of optimal control!**

# Numerical Experiments

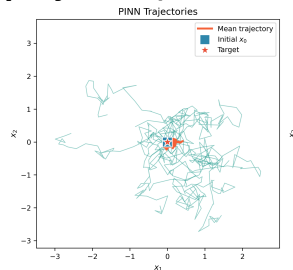


# 100D HJB Benchmark: Results (Centered Target)

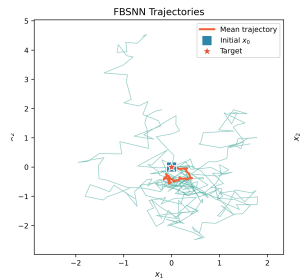
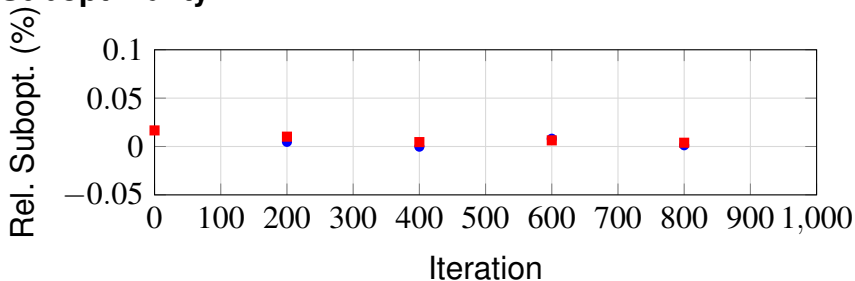
## Training Loss Convergence:



## Trajectories (2D projection):



## Suboptimality:



# 100D HJB Benchmark

$$-\frac{\partial u}{\partial t} + \Delta u - \|\nabla u\|^2 = 0, \quad \text{for } t \in [0, T) \quad u(T, x) = g(x)$$

Use terminal cost from literature:  $g(x) = \log\left(\frac{1}{2}(1 + \|x\|^2)\right)$ , i.e.,  $x_{\text{target}} = \mathbf{0} \in \mathbb{R}^{100}$ .

- ▶ Initial states:  $X_0 \sim \mathcal{N}(0, 0.1^2 I_{100})$  (near origin)
- ▶ Terminal time:  $T = 1.0$
- ▶ Ground truth: Monte Carlo with  $10^6$  samples

Method	Relative Suboptimality	Training Time	Status
PINNs + HTE	<1%	~9 min	✓ Success
FBSNN	<1%	~17 min	✓ Success

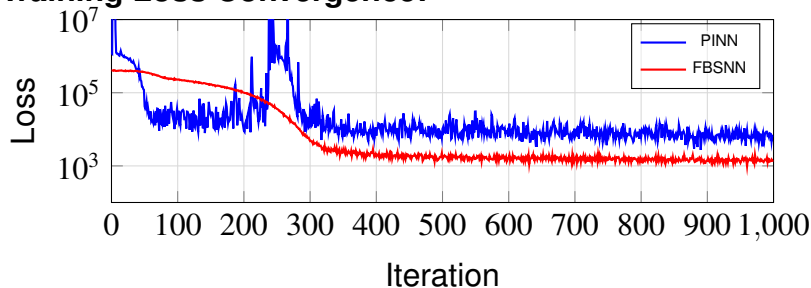
## Why It Works:

- ▶ Random samples (collocation or random walk) stay near origin
- ▶ Minimizer of terminal cost is at origin  $\Rightarrow$  samples cover the important region!
- ▶ Network learns the value function where it matters

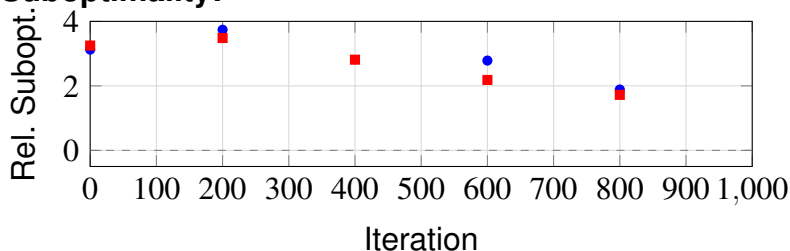
**Both methods achieve <1% suboptimality in 100 dimensions!**

# 100D HJB Benchmark: Results (Shifted Target)

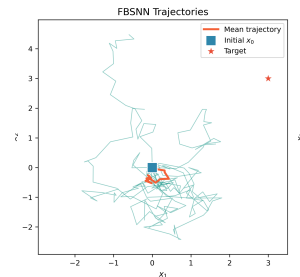
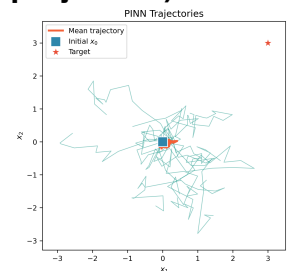
## Training Loss Convergence:



## Suboptimality:



## Trajectories (2D projection):



# Modified 100D HJB Benchmark: Shifted Target

$$-\frac{\partial u}{\partial t} + \Delta u - \|\nabla u\|^2 = 0, \quad \text{for } t \in [0, T) \quad u(T, x) = g(x)$$

Use **modified terminal cost**:  $g(x) = 1000 \log\left(\frac{1}{2} (1 + \|x - \mathbf{3}\|^2)\right)$ , i.e.,  $x_{\text{target}} = \mathbf{3} \in \mathbb{R}^{100}$ .

Method	Relative Suboptimality	Convergence	Status
PINNs	238%	looks good	× Fails
FBSNN	147%	looks good	× Fails

## What Happened?

- ▶ Target distance:  $\|x_{\text{target}}\| = 3\sqrt{100} = 30$
- ▶ Typical random walk distance:  $\|X_T\| \sim \sqrt{2 \cdot 100} \approx 14$
- ▶ Random collocation: uniform in bounded domain, misses far target
- ▶ **Samples rarely reach the target region!**

**As suspected: Both methods FAIL when the target shifts far away!**

# Neural SDEs for Stochastic Optimal Control

# HJB and Pontryagin Maximum Principle

Consider the value function of the stochastic optimal control problem:

$$u(t, x) = \min_a \left\{ \mathbb{E} \left[ \int_t^T L(X_s, a_s) ds + g(X_T) \right], \quad \text{s.t. } dX_s = \mu(X_s, a_s) ds + \sigma dW_s, X_t = x \right\}$$

## Key facts from optimal control theory:

1. **HJB equation:** The value function satisfies

$$-\partial_t u + \sup_a \mathcal{H}(t, x, \nabla u, \sigma \nabla^2 u, a) = 0, \quad u(T, x) = g(x)$$

where  $\mathcal{H}(t, x, p, M, a) = \frac{1}{2} \text{trace}(\sigma M) + p^\top \mu(x, a) - L(x, a)$

2. **Feedback form (PMP):** Optimal control is given by

$$a^*(t, x) \in \operatorname{argmax}_a \mathcal{H}(t, x, \nabla u(t, x), \sigma \nabla^2 u(t, x), a)$$

**For our HJB benchmark:**  $L(x, a) = \|a\|^2$ ,  $\mu(x, a) = 2a$ ,  $\sigma = \sqrt{2}$

$\Rightarrow$  Optimal control:  $a^*(t, x) = -\nabla u(t, x)$

**Challenges:** forward-backward structure, nonlinearity, high-dimensionality

# The Controlled Forward SDE

**Key Insight: Use PMP to Define the Forward SDE**

## FBSDE Methods (earlier section)

**Random walk:**

$$dX_t = \sqrt{2} dW_t$$

- ▶ Sampling independent of  $\theta$
- ▶ Trajectories don't reach target
- × **Fails when target shifts!**

## Neural SOC (This section)

**PMP-guided:**

$$dX_t = \underbrace{-2\nabla u_\theta(t, X_t)}_{2a} dt + \sqrt{2} dW_t$$

- ▶ Sampling depends on  $\theta$
- ▶ Trajectories guided toward target
- ✓ **Works for any target!**

**Consequence:** The drift  $-2\nabla u_\theta$  guides samples to low-cost regions.

**What is the backward SDE along the controlled trajectory?**

# Itô's Lemma: Deriving the Backward SDE

**Setup:** Let  $u$  solve the HJB:  $\partial_t u + \Delta u - \|\nabla u\|^2 = 0$ ,  $u(T, x) = g(x)$

Consider  $u(t, X_t)$  along the **controlled trajectory**:  $dX_t = -2\nabla u(t, X_t) dt + \sqrt{2} dW_t$

**Apply Itô's lemma:**

$$\begin{aligned} du(t, X_t) &= \partial_t u dt + \nabla u^\top dX_t + \frac{1}{2} \text{trace}(\nabla^2 u \cdot 2I) dt \\ &= \partial_t u dt + \nabla u^\top \left( -2\nabla u dt + \sqrt{2} dW_t \right) + \Delta u dt \\ &= (\partial_t u - 2\|\nabla u\|^2 + \Delta u) dt + \sqrt{2} \nabla u^\top dW_t \end{aligned}$$

Using HJB:  $\partial_t u + \Delta u = \|\nabla u\|^2$ , we get:

$$\partial_t u - 2\|\nabla u\|^2 + \Delta u = \|\nabla u\|^2 - 2\|\nabla u\|^2 = -\|\nabla u\|^2$$

With  $a^* = -\nabla u$  and running cost  $L = \|a^*\|^2 = \|\nabla u\|^2$ :

$$\boxed{du(t, X_t) = -L(X_t, a_t^*) dt + \sqrt{2} \nabla u^\top dW_t}$$

**The backward SDE has drift =  $-(\text{running cost})$ ! Terminal:  $u(T, X_T) = g(X_T)$**



# Comparing: Random Walk vs. Controlled FBSDE

## Random Walk FBSDE

**Forward:**  $dX_t = \sqrt{2} dW_t$

**Backward:**

$$dY_t = +\|\nabla u\|^2 dt + Z_t^\top dW_t$$

- ▶  $Y_t = u(t, X_t)$ ,  $Z_t = \sqrt{2}\nabla u$
- ▶ **Drift is positive!**
- ▶ Value *increases* along random paths (drifting into high-cost regions)

## Controlled FBSDE

**Forward:**  $dX_t = -2\nabla u_\theta dt + \sqrt{2} dW_t$

**Backward:**

$$dY_t = -\|\nabla u\|^2 dt + Z_t^\top dW_t$$

- ▶  $Y_t = u(t, X_t)$ ,  $Z_t = \sqrt{2}\nabla u$
- ▶ **Drift is negative!**
- ▶ Value *decreases* by running cost along optimal paths

**Martingale verification:** Define  $M_t = Y_t + \int_0^t L ds$ . Then  $dM_t = Z_t^\top dW_t$  (martingale!)

$$\Rightarrow u(0, x_0) = \mathbb{E} \left[ \int_0^T L(X_t, a_t^*) dt + g(X_T) \right] \quad (\text{control objective!})$$

# Why Random Sampling Methods Fail

## What Went Wrong with PINNs, Deep BSDE, FBSNN?

- ▶ **PINNs + HTE:** Random collocation points in bounded domain
- ▶ **Deep BSDE:** Random walk  $dX = \sqrt{2} dW$
- ▶ **FBSNN:** Random walk  $dX = \sqrt{2} dW$

All ignore the **optimal control structure** of the problem!

## The Solution: PMP-Informed Sampling

Instead of random sampling, use the **controlled dynamics**:

$$dX_t = -2\nabla u_\theta(t, X_t) dt + \sqrt{2} dW_t$$

## Benefits:

- ▶ Trajectories are guided toward optimal paths (even with crude initial  $u_\theta$ )
- ▶ Backward SDE becomes simple: just integrates running cost
- ▶ Loss function directly measures control objective

**We use the current network estimate to guide sampling!**

# PMP-Informed Neural SDE Solver: The Training Loop

1. **Initialize** value network  $u_\theta(t, x)$
2. **For each training iteration:**
  - (a) **Compute optimal control:**  $a_\theta^*(t, x) = -\nabla_x u_\theta(t, x)$
  - (b) **Sample trajectories with PMP-guided drift:**

$$X_{k+1} = X_k + 2a_\theta^*(t_k, X_k)\Delta t + \sqrt{2\Delta t}\xi_k, \quad \xi_k \sim \mathcal{N}(0, I)$$

- (c) **Compute loss:**

$$\mathcal{L}(\theta) = \mathbb{E} \left[ \sum_{k=0}^{N-1} L(X_k, a_k^*)\Delta t + g(X_N) \right] + \lambda_{\text{HJB}} P_{\text{HJB}} + \lambda_T P_T + \lambda_{\nabla T} P_{\nabla T}$$

(penalty terms enforce HJB and terminal conditions)

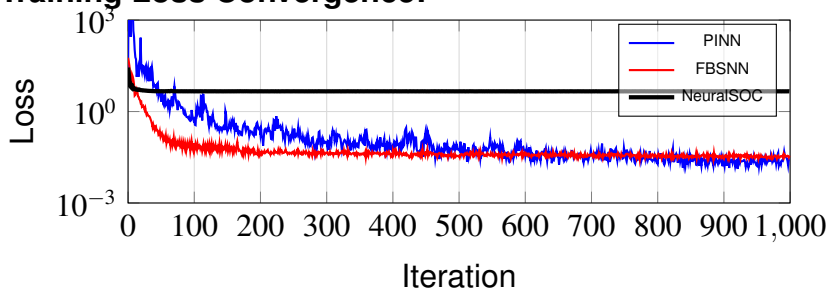
- (d) **Update**  $\theta$  via gradient descent
3. **Return** trained network  $u_\theta$

## Key Difference from Random-Sampling Methods:

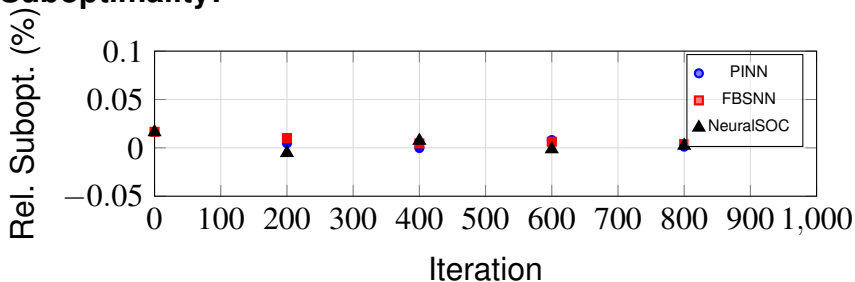
- ▶ Trajectories are **guided by current policy estimate**
- ▶ Crude estimate initially, iterations pulls trajectories toward relevant regions
- ▶ **Must backprop through the SDE!** ( $X_k$  depends on  $\theta$  via  $a_\theta^*$ )

# 100D HJB Benchmark: Results Neural SOC (Centered)

## Training Loss Convergence:

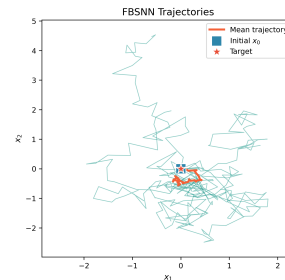


## Suboptimality:

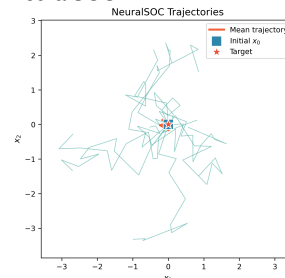


## Trajectories:

### FBSNN:

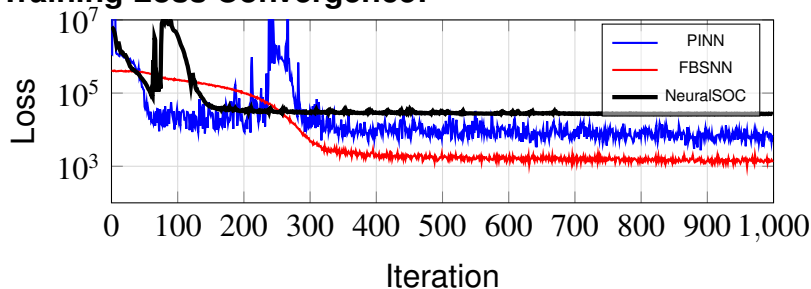


### NeuralSOC:

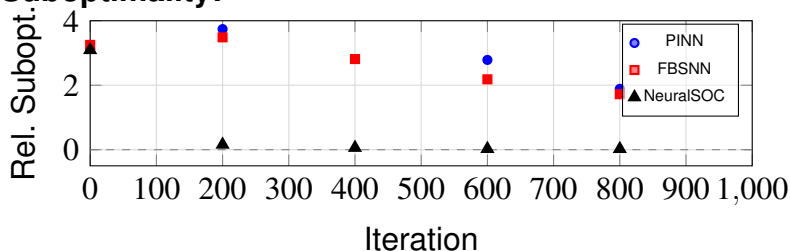


# 100D HJB Benchmark: Results with Neural SOC (Shifted)

## Training Loss Convergence:

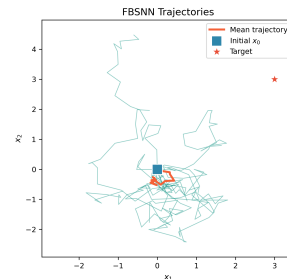


## Suboptimality:

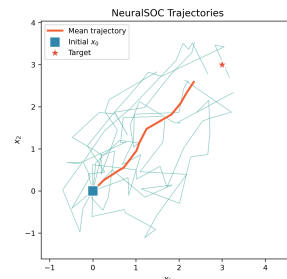


## Trajectories:

### FBSNN:



### NeuralSOC:



# Results: PMP-Informed Succeeds Where Others Fail

**The Hard Case:**  $x_{\text{target}} = (3, \dots, 3)^\top \in \mathbb{R}^{100}$

Method	Sampling	Rel. Suboptimality	Status
PINNs	Random collocation	238%	× Fails
FBSNN	$dX = \sigma dW$	147%	× Fails
<b>Neural SOC</b>	$dX = -2\nabla u_\theta dt + \sigma dW$	1.2%	✓ Success!

Three ingredients for solving high-dimensional HJB:

1. FBSDE reformulation (continuous-time dynamics)
2. Neural network approximation (meshfree representation)
3. Smart sampling (guided by current policy)

# Local vs. Global vs. Semi-global Solutions

## Different types of solutions for optimal control:

- ▶ **Local solution:** Find optimal trajectory for one given initial state  $x_0$ 
  - ▶ Standard shooting methods, adjoint methods
  - ▶ Must resolve for each new initial condition
- ▶ **Global solution:** Find optimal policy for all states  $(t, x) \in [0, T] \times \Omega$ 
  - ▶ Requires solving HJB on full domain
  - ▶ **Curse of dimensionality: impossible for  $d \gg 1$ !**
- ▶ **Semi-global solution:** Find policy that is optimal in *the subset of state space likely to be visited*
  - ▶ **Realistic goal for high-dimensional problems**
  - ▶ Learn  $u_\theta$  along (approximately) optimal trajectories
  - ▶ Generalizes to nearby initial conditions

**Key insight:** PMP-informed sampling gives semi-global solutions!  
You get good policies **where you sample**  $\Rightarrow$  sample where it matters!

# Outlook and Summary



# Outlook: Reinforcement Learning and HJBs

## Reinforcement Learning for Control

- ▶ Alternative approach for solving (stochastic) optimal control problems
- ▶ Example: Actor-critic methods for games
- ▶ Only observations needed (of system and objective)
- ▶ Attractive when model is complex, incomplete, or unavailable
- ▶ Challenge: Sample efficiency (**Scientific ML is not an Atari game!**)

## RL + HJB: Best of Both Worlds?

- ▶ Exploit that objective function is **known** (unlike pure RL)
- ▶ Learn control-affine dynamics model:

$$dX_t = f_\mu(t, X_t) dt + B_\mu(t, X_t) a_t dt + \sigma dW_t$$

with learnable parameters  $\mu$

- ▶ Use model to estimate  $u$  and guide sampling  $\rightarrow$  reduce sample complexity

**HJB RL: Use structure when available, see Verma et al. 2024**

# Outlook: HJB in Global Optimization

**Goal:** Find global minimum of non-convex  $f(x)$

**Algorithm:**

1. Compute Moreau envelope:

$$\varphi(t, x) = \min_y f(y) + \frac{1}{2t} \|x - y\|^2$$

2. Gradient descent:  $x_{k+1} = x_k - \alpha_k \nabla \varphi(t_k, x_k)$

3. Increase  $t$  (smoothing parameter)

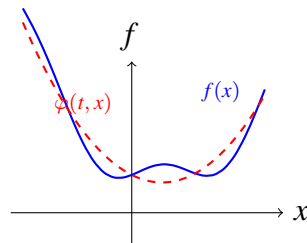
**Key observation:**  $\varphi$  solves Burgers-type HJB!

$$\partial_t \varphi(t, x) + \|\nabla \varphi(t, x)\|^2 = 0, \quad \varphi(0, x) = f(x)$$

**Connection to this lecture:** Add viscosity  $\delta > 0$ , use Cole-Hopf transform:

$$\nabla \varphi(t, x) = -\delta \nabla \log v^\delta(t, x)$$

**Same sampling ideas apply. See Heaton, Fung, and Osher 2022**



# Outlook: Mean Field Games and Control

**Setup:** Large population of interacting agents, each solving optimal control

## Individual Agent:

- ▶ State  $X_t \in \mathbb{R}^d$ , control  $a_t$
- ▶ Dynamics depend on population density  $\rho$
- ▶ Cost depends on  $\rho$  (congestion, competition)

## Population Level:

- ▶ Density  $\rho(t, x)$  evolves via Fokker-Planck
- ▶ Nash equilibrium: no agent wants to deviate
- ▶ Limit of  $N$ -player game as  $N \rightarrow \infty$

## Coupled PDE System:

$$\text{HJB (backward): } -\partial_t u + H(x, \nabla u, \rho) = 0, \quad u(T, x) = g(x, \rho_T)$$

$$\text{Fokker-Planck (forward): } \partial_t \rho + \nabla \cdot (\rho v^*(x, \nabla u)) = \Delta \rho, \quad \rho(0) = \rho_0$$

**Neural Approaches:** Similar ideas from today! (Ruthotto et al. 2020)

- ▶ Parameterize  $u_\theta(t, x)$  and  $\rho_\varphi(t, x)$  with neural networks
- ▶ Avoid spatial grids  $\rightarrow$  handle  $d = 100+$  dimensions

**Applications: crowd motion, traffic, finance, multi-agent RL, generative models**

# $\Sigma$ : High-Dimensional Optimal Control






## Key Takeaways

- ▶ **Three common approaches:** PINNs+HTE, Deep BSDE, FBSNN
  - ▶ All use neural approximation, no spatial grid, polynomial cost in  $d$
- ▶ **All succeed on “easy” problems** (centered targets)
  - ▶ Random sampling happens to cover the important region
- ▶ **All fail when the target shifts!**
  - ▶ Random sampling misses the important region in high-D
- ▶ **PMP-informed sampling succeeds** where others fail
  - ▶ Use optimal control structure; feedback loop improves sampling



## Open Research Challenges

- ▶ **Sampling for general semilinear PDEs**
  - ▶ HJB structure enables PMP-guided sampling — what about non-HJB?
- ▶ **Avoiding time integration**
  - ▶ Flow matching: learn velocity field directly, skip SDE simulation?

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