

Stochastic Optimal Control Matching

Carles Domingo-Enrich, Jiequn Han, Brandon Amos, Joan Bruna, Ricky T. Q.
Chen

Thomas Mousseau

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Overview

1. Setup and Preliminaries
2. Stochastic Optimal Control Matching
3. Experiments and results
4. Conclusion

Neural ODE: Continuous Normalizing Flows

Continuous Normalizing Flows (CNF)

CNFs model complex distributions by transforming a simple distribution (e.g., Gaussian) through a continuous-time ODE. The transformation is defined by a neural network that learns the dynamics of the flow.

Key Idea

Instead of discrete steps, CNFs use a continuous-time approach to model the evolution of the distribution, allowing for more flexible and expressive transformations.

Stochastic Optimal Control Matching

└ Setup and Preliminaries

└ Neural ODE: Continuous Normalizing Flows

Cette slide n'est pas complete, je voudrais ici presenter le debut de ce milieu soit le Neural ODEs, le but qu'ils combent dans le milieu et leur premiere implementation soit CNFs. De plus, je veux aussi expliquer les Adjoint Methods ici puisque elles sont recurrente dans tous le reste du SOCM papier

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Evolution of Generative Models

- 2020** **DDPM:** Denoising Diffusion Probabilistic Models interpret generation as reversing a discrete noise-adding process, learning to denoise at each step. They produced high-quality samples but required thousands of slow sampling steps.
- 2021** **Score-based Models:** Score-based generative models extended diffusion to continuous-time SDEs, learning the score function ($\nabla_x \log p_t(x)$) to reverse a stochastic diffusion process. This unified diffusion with stochastic control, allowed probability flow ODEs, and sped up sampling.
- 2023** **Flow Matching:** Flow matching views generation as learning a deterministic ODE vector field that directly transports a simple distribution (e.g., Gaussian) to data. This removed stochasticity and significantly improved efficiency compared to diffusion/score methods.

What is a Stochastic Control Problem?

Dynamics (SDE)

$$dx_t = \underbrace{u_t dt}_{\text{drift coefficient}} + \underbrace{dw_t}_{\text{diffusion coefficient}} \quad (1)$$

Cost Function

$$J(u) = \mathbb{E} \left[\int_0^T L(x_t, u_t, t) dt + \Phi(x_T) \right] \quad (2)$$

Key Components

- **State Process:** $x_t \in \mathbb{R}^d$ (position in state space at time t)
- **Control Process:** $u_t \in \mathbb{R}^d$ (action/decision at time t)
- **Noise Process:** w_t (random disturbances, typically Brownian motion)
- **Running Cost:** $L(x_t, u_t, t)$ (cost accumulated over time)
- **Terminal Cost:** $\Phi(x_T)$ (cost at the final time T)

Stochastic Optimal Control Matching

└ Setup and Preliminaries

└ What is a Stochastic Control Problem?

A stochastic control problem involves finding an optimal control policy to steer a dynamical system under uncertainty while minimizing the expected cost.

A voir si je rajouter une autre slide qui presente la solution avec HJB + Feynman-Kac approche.

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The Goal: Finding Optimal Control

Optimal Control u^*

Find the control policy u^* that minimizes the expected cost: $u^* = \arg \min_u J(u)$

Classical Approaches

- **Hamilton-Jacobi-Bellman (HJB) equation:** Partial differential equation approach
- **Pontryagin's Maximum Principle:** Necessary conditions for optimality
- **Dynamic Programming:** Discrete-time recursive approach

Challenge

These classical methods become computationally intractable in high dimensions due to the *curse of dimensionality*.

Classical vs Neural Solutions

Classical: HJB PDE

Hamilton-Jacobi-Bellman Equation:

$$\frac{\partial V}{\partial t} + \min_u \left[L(x, u, t) + \frac{\partial V}{\partial x} f(x, u, t) + \frac{1}{2} \text{tr}(\sigma^T \nabla^2 V \sigma) \right] = 0 \quad (3)$$

Solution Process:

- Discretize state space on grid
- Use finite difference methods
- Solve backward in time from $V(x, T) = \Phi(x)$

Modern: Neural PDE Solvers

Neural Network Approximation:

$$V(x, t) \approx V_\theta(x, t) \quad (4)$$

Solution Process:

- Parameterize value function with NN
- **Physics-informed loss**: HJB residual
- **Automatic differentiation** for gradients
- Train end-to-end with SGD

Key Differences

Stochastic Optimal Control Matching

└ Setup and Preliminaries

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Key Differences

HJB Equation: The Hamilton-Jacobi-Bellman equation provides the theoretical foundation for solving stochastic optimal control problems by characterizing the value function $V(x, t)$ as the solution to a nonlinear PDE.

Neural PDE Solvers: Modern approaches use neural networks to approximate the value function directly, avoiding discretization and enabling high-dimensional problems. The network is trained to satisfy the HJB equation through physics-informed loss functions.

Reasons behind SOCM (1/2)

Many fundamental tasks in machine learning can be naturally cast as stochastic optimal control problems, highlighting the importance of efficient SOC methods.

Key ML Applications of SOC

- **Reward fine-tuning of diffusion and flow models:** Optimizing generation quality using reward signals
- **Conditional sampling on diffusion and flow models:** Steering generation towards specific conditions or constraints
- **Sampling from unnormalized densities:** Efficiently drawing samples from complex, intractable distributions
- **Importance sampling of rare events in SDEs:** Computing probabilities of low-probability but critical events

Reasons behind SOCM (2/2)

Current SOC methods suffer from optimization challenges that limit their effectiveness.

Current SOC Methods

- Use **adjoint methods** (like CNFs)
- Yield **non-convex** function landscapes
- Difficult optimization with local minima
- Unstable training dynamics

Diffusion Models Success

- Use **least-squares loss**
- Create **convex** functional landscapes
- Stable and reliable optimization
- Excellent empirical performance

SOCM's Innovation

Goal: Develop least-squares loss formulations for SOC problems, combining the expressiveness of stochastic control with the optimization stability of diffusion models.

SOCM in Context: Optimization Landscapes

Task	Non-convex	Least Squares
Generative Modeling	Maximum Likelihood CNFs	Diffusion models and Flow Matching
Stochastic Optimal Control	Adjoint Methods	Stochastic Optimal Control Matching

Introducing Stochastic Optimal Control Matching

SOCM offers a more principled, stable, and accurate way to learn generative dynamics by blending stochastic control theory with modern matching-based generative modeling.

Key Novel Contributions

1. **Controlled Stochastic Process:** Views the generation process as a controlled stochastic process bridging a simple distribution to data.
2. **Least-Squares Matching:** Learning the control via least-squares matching, a stable and convex regression objective.
3. **Joint Optimization:** Optimizing control and variance-reducing reparameterization matrices simultaneously, for efficient learning.
4. **Path-wise Reparameterization:** Introducing a path-wise reparameterization trick, boosting gradient estimation quality.

The SOCM Framework

SOCM Loss Function

The Stochastic Optimal Control Matching objective is defined as:

$$\mathcal{L}_{SOCM}(u, M) := \mathbb{E} \left[\frac{1}{T} \int_0^T \|u(X_t^\nu, t) - w(t, \nu, X^\nu, B, M_t)\|^2 dt \times \alpha(\nu, X^\nu, B) \right] \quad (5)$$

Where:

- X^ν is the process controlled by ν :

$$dX_t^\nu = (b(X_t^\nu, t) + \sigma(t)\nu(X_t^\nu, t))dt + \sqrt{\lambda}\sigma(t)dB_t, \text{ with } X_0^\nu \sim p_0 \quad (6)$$

- $u(X_t^\nu, t)$ is the control policy being learned
- $w(t, \nu, X^\nu, B, M_t)$ is the target matching function
- $\alpha(\nu, X^\nu, B)$ is a weighting function

Stochastic Optimal Control Matching

└ Stochastic Optimal Control Matching

└ The SOCM Framework

Ici, je dois presenter en details la matrice M_t , B ainsi que w . De plus, je veux expliquer l'intuition du path-wise reparameterization trick, a novel technique to obtain low-variance estimates of the gradient of the conditional expectation of a functional of a random process with respect to its initial value

The SOCM Framework

SOCM Loss Function

The Stochastic Optimal Control Matching objective is defined as:

$$\mathcal{L}_{\text{SOCM}}(u, M) := \mathbb{E} \left[\frac{1}{T} \int_0^T \|u(X_t^*, t) - w(t, v, X^*, B, M_t)\|^2 dt \times \alpha(v, X^*, B) \right] \quad (5)$$

Where:

- X^* is the process controlled by v :

$$dX_t^* = \{h(X_t^*, t) + \sigma(t)v(X_t^*, t)\}dt + \sqrt{\Sigma} \sigma(t)dB_t, \text{ with } X_0^* \sim p_0 \quad (6)$$

- $u(X_t^*, t)$ is the control policy being learned
- $w(t, v, X^*, B, M_t)$ is the target matching function
- $\alpha(v, X^*, B)$ is a weighting function

SOCM Algorithm

Algorithm 2 Stochastic Optimal Control Matching (SOCM)

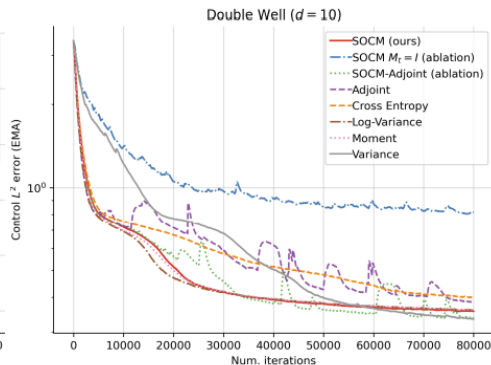
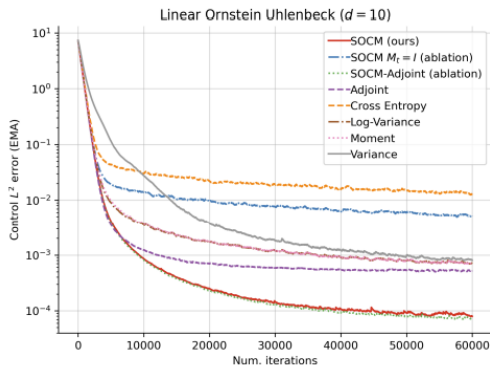
Input: State cost $f(x, t)$, terminal cost $g(x)$, diffusion coeff. $\sigma(t)$, base drift $b(x, t)$, noise level λ , number of iterations N , batch size m , number of time steps K , initial control parameters θ_0 , initial matrix parameters ω_0 , loss $\mathcal{L}_{\text{SOCM}}$ in (125)

```
1 for  $n \in \{0, \dots, N-1\}$  do
2   Simulate  $m$  trajectories of the process  $X^v$  controlled by  $v = u_{\theta_n}$ , e.g., using Euler-Maruyama updates
3   Detach the  $m$  trajectories from the computational graph, so that gradients do not backpropagate
4   Using the  $m$  trajectories, compute an  $m$ -sample Monte-Carlo approximation  $\hat{\mathcal{L}}_{\text{SOCM}}(u_{\theta_n}, M_{\omega_n})$  of the loss
       $\mathcal{L}_{\text{SOCM}}(u_{\theta_n}, M_{\omega_n})$  in (125)
5   Compute the gradients  $\nabla_{(\theta, \omega)} \hat{\mathcal{L}}_{\text{SOCM}}(u_{\theta_n}, M_{\omega_n})$  of  $\hat{\mathcal{L}}_{\text{SOCM}}(u_{\theta_n}, M_{\omega_n})$  at  $(\theta_n, \omega_n)$ 
6   Obtain  $\theta_{n+1}, \omega_{n+1}$  with via an Adam update on  $\theta_n, \omega_n$ , resp.
7 end
```

Output: Learned control u_{θ_N}

Figure: Stochastic Optimal Control Matching (SOCM) Algorithm

Experimental Results (1/2)



Experimental Results (2/2)

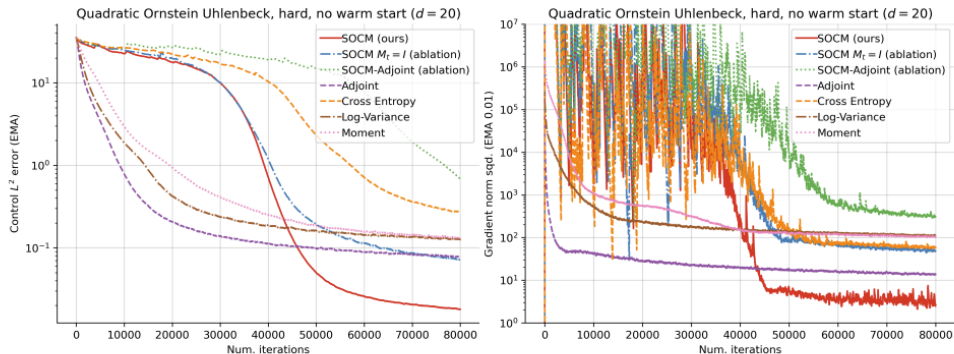


Figure 3 Plots of the L^2 error incurred by the learned control (*top*), and the norm squared of the gradient with respect to the parameters θ of the control (*bottom*), for the QUADRATIC ORNSTEIN UHLENBECK (HARD) setting and for each IDO loss. All the algorithms use a warm-started control (see [Appendix D](#)).

Stochastic Optimal Control Matching

└ Experiments and results

└ Experimental Results (2/2)

At the end of training, SOCM obtains the lowest L2 error, improving over all existing methods by a factor of around ten. The two SOCM ablations come in second and third by a substantial difference, which underlines the importance of the path-wise reparameterization trick.

JE DOIS COMPRENDRE CE QUE EST UN ORNSTEIN UHLENBECK PROCESS

Experimental Results (2/2)

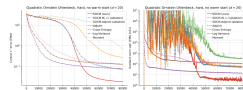


Figure 3: Plots of the L^2 error (top), and the norm squared of the gradient with respect to the parameters θ of the control (bottom), for the QG-solver: Quadratic Ornstein-Uhlenbeck (brown) setting and for each DSD line. All the algorithms use a reparameterized control (see Appendix D).

Conclusion

The main roadblock when we try to apply SOCM to more challenging problems is that the variance of the factor $\alpha(v, Xv, B)$ explodes when f and/or g are large, or when the dimension d is high. The control L2 error for the SOCM and cross-entropy losses remains high and fluctuates heavily due to the large variance of α . The large variance of α is due to the mismatch between the probability measures induced by the learned control and the optimal control. Similar problems are encountered in out-of-distribution generalization for reinforcement learning, and some approaches may be carried over from that area (Munos et al., 2016).

References
