Stochastic Optimal Control Matching

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Overview

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

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.

SOC as the Foundation of Generative Models

The Core Challenge: Unnormalized Densities

Generative models must sample from complex distributions $p_{\text{data}}(x) = \frac{1}{Z}\tilde{p}_{\text{data}}(x)$ where the normalization constant $Z = \int \tilde{p}_{\text{data}}(x)dx$ is intractable to compute. This intractability arises from the curse of dimensionality when integrating over high-dimensional spaces.

SOC Connection

Key Insight:
Transform tractable distributions (Gaussian) to complex target distributions through optimal control policies.

This bridges the gap between:

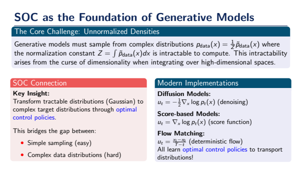
- Simple sampling (easy)
- Complex data distributions (hard)

Modern Implementations

Diffusion Models:
$u_t = -\frac{1}{2}\nabla_x \log p_t(x)$ (denoising)

Score-based Models:
$u_t = \nabla_x \log p_t(x)$ (score function)

Flow Matching:
$u_t = \frac{x_1 - x_0}{T - t}$ (deterministic flow)
All learn optimal control policies to transport distributions!



Unnormalized Densities: The fundamental challenge in generative modeling is sampling from distributions $p(x) = \frac{1}{Z}e^{-E(x)}$ where Z is unknown. SOC provides the mathematical framework to construct sampling procedures.

Historical Context: From Langevin dynamics to modern diffusion models, all major breakthroughs in generative modeling can be understood through the lens of stochastic optimal control theory.

What is a Stochastic Control Problem?

Control-Affine Stochastic Differential Equation

The general form of a controlled stochastic process:

$$dX_t^u = \big(b(X_t^u, t) + \sigma(t)u(X_t^u, t)\big)dt + \sqrt{\lambda}\sigma(t)dB_t \tag{1}$$

State Process: $X_t^u \in \mathbb{R}^d$ (system state under control u at time t)

Drift Term: $b(X_t^u, t) \in \mathbb{R}^d$ (natural evolution of the system)

Control Term: $\sigma(t)u(X_t^u, t) \in \mathbb{R}^d$ (how control influences the system)

Diffusion Coefficient: $\sigma(t) \in \mathbb{R}^{d\times d}$ (volatility matrix)

Noise Process: $B_t \in \mathbb{R}^d$ (Brownian motion, external randomness)

Noise Intensity: $\lambda > 0$ (controls the strength of stochastic perturbations)

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Control-Affine Structure: The "control-affine" property means the control u enters linearly (affinely) in the drift term. This is the most general practical form for controlled SDEs, encompassing most applications in finance, robotics, and machine learning.

J'aimerais bien mettre en context ces equations en parlant d'un steering motor pour un driverless vehicule et apres faire le lien avec les flow + diffusion models

Je dois aussi expliquer l'importance que le steering input ainsi que le noise sont tous les 2 multipliés par sigma(t) ce qui signifie que ...

The Optimal Control Objective

Cost Function to Minimize

Find the optimal control policy $u^* \in \mathcal{U}$ that minimizes:

$$\min_{u \in \mathcal{U}} \mathbb{E}\left[\int_0^T \left(\frac{1}{2}\|u(X_t^u, t)\|^2 + f(X_t^u, t)\right) dt + g(X_T^u)\right] \tag{2}$$

Control Effort: $\frac{1}{2}\|u(X_t^u, t)\|^2$ (penalizes large control actions)

Running Cost: $f(X_t^u, t)$ (ongoing cost during the process evolution)

Terminal Cost: $g(X_T^u)$ (final cost based on end state at time T)

Control Space: $\mathcal{U}$ (set of admissible control policies)

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Why dont we want to excessivly steer, this is not like overfitting but I still need to find the reason

Classic Approach to Finding Optimal Control

Optimal Control u^*

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

Hamilton-Jacobi-Bellman (HJB) Equation

The classical approach uses the HJB PDE to characterize the value function $V(x, t)$:

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

With boundary condition: $V(x, T) = \Phi(x)$ (terminal cost)

The Curse of Dimensionality

Classical numerical methods (finite differences, grid-based) become computationally intractable in high dimensions due to exponential growth in grid size: $\mathcal{O}(N^d)$ where d is dimension.

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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. The optimal control is then $u^*(x, t) = \arg\min_u[\cdots]$ from the HJB equation.

Neural PDE Solvers for SOC

Core Innovation: Neural ODEs (Chen et al., 2018)

Key Insight: Replace discrete layers with continuous-time ODEs
$\frac{dh(t)}{dt} = f_\theta(h(t), t)$ where $h(t)$ represents hidden states evolving continuously

Neural Network Approximation

Value Function:

$$V(x, t) \approx V_\theta(x, t) \tag{4}$$

Control Policy:

$$u(x, t) \approx u_\phi(x, t) \tag{5}$$

Both parameterized by deep neural networks

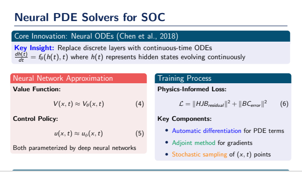
Training Process

Physics-Informed Loss:

$$\mathcal{L} = \|HJB_{residual}\|^2 + \|BC_{error}\|^2 \tag{6}$$

Key Components:

- Automatic differentiation for PDE terms
- Adjoint method for gradients
- Stochastic sampling of (x, t) points



Neural ODEs: Chen et al. (2018) showed that residual networks can be interpreted as discretizations of ODEs. This insight led to continuous-depth models and, crucially for our context, neural methods for solving differential equations.

Physics-Informed Neural Networks: The key is training networks to satisfy the HJB equation through the residual loss, making the physics constraints part of the optimization objective.

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 (1/3)

SOCM Loss Function

The Stochastic Optimal Control Matching objective is defined as:

$$\mathcal{L}_{SOCM}(u, M) := \mathbb{E}\left[\frac{1}{T}\int_0^T \|u(X_t^v, t) - w(t, v, X^v, B, M_t)\|^2 dt \times \alpha(v, X^v, B)\right] \tag{7}$$

Where:

- X^v is the process controlled by v:

$$dX_t^v = (b(X_t^v, t) + \sigma(t)v(X_t^v, t))dt + \sqrt{\lambda}\sigma(t)dB_t, \text{ with } X_0^v \sim p_0 \tag{8}$$

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

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Ici, je dois presenter en details la matrice Mt, 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 (2/3)

Reparameterization Function $w(t, v, X^v, B, M_t)$

The **target matching function** computed via path-wise reparameterization:

$$
\begin{aligned}
w(t, v, X^v, B, M_t) = \sigma(t)^\top \Bigg(& -\int_t^T M_t(s) \nabla_x f(X_s^v, s)\, ds \; - \; M_t(T) \nabla g(X_T^v) \\
& + \int_t^T \big(M_t(s) \nabla_x b(X_s^v, s) - \partial_s M_t(s) \big) (\sigma^{-1}(s))^\top v(X_s^v, s)\, ds \\
& + \sqrt{\lambda} \int_t^T \big(M_t(s) \nabla_x b(X_s^v, s) - \partial_s M_t(s) \big) (\sigma^{-1}(s))^\top dB_s \Bigg)
\end{aligned}
\tag{9}
$$

Where $M_t(s)$ is the **reparameterization matrix** (learned jointly with u)

The SOCM Framework (2/3)

Importance Weight $\alpha(v, X^v, B)$

The **importance sampling weight** for measure correction:

$$\alpha(v, X^v, B) = \exp\Bigg(-\frac{1}{\lambda}\int_0^T f(X_t^v, t)\, dt - \frac{1}{\lambda} g(X_T^v) - \frac{1}{\sqrt{\lambda}}\int_0^T \langle v(X_t^v, t), dB_t\rangle - \frac{1}{2\lambda}\int_0^T \|v(X_t^v, t)\|^2 dt \Bigg) \tag{10}$$

Incorporates running costs, terminal costs, and control effort

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Reparameterization Matrix M_t: This matrix enables path-wise reparameterization, a technique to reduce variance in gradient estimation by reparameterizing the stochastic process. It's optimized jointly with the control u to minimize the overall SOCM loss.

Importance Weight α: This exponential weight corrects for the mismatch between the learned control measure and the optimal control measure. However, it can have high variance when costs are large or in high dimensions, which is the main limitation of SOCM.

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 $\mathcal{L}_{\mathrm{SOCM}}$ in (125)

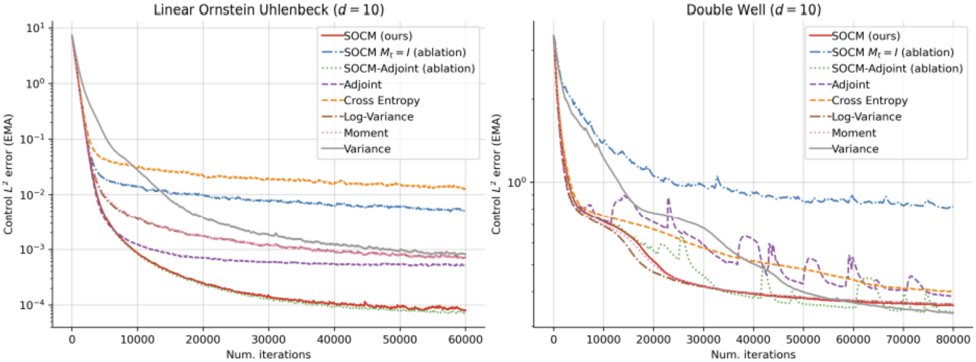
for $n \in \{0, \dots, N-1\}$ **do**
- Simulate m trajectories of the process X^v controlled by $v = u_{\theta_n}$, e.g., using Euler-Maruyama updates
- Detach the m trajectories from the computational graph, so that gradients do not backpropagate
- Using the m trajectories, compute an m-sample Monte-Carlo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

end

Output: Learned control u_{θ_N}

Figure: Stochastic Optimal Control Matching (SOCM) Algorithm

Experimental Results (1/2)



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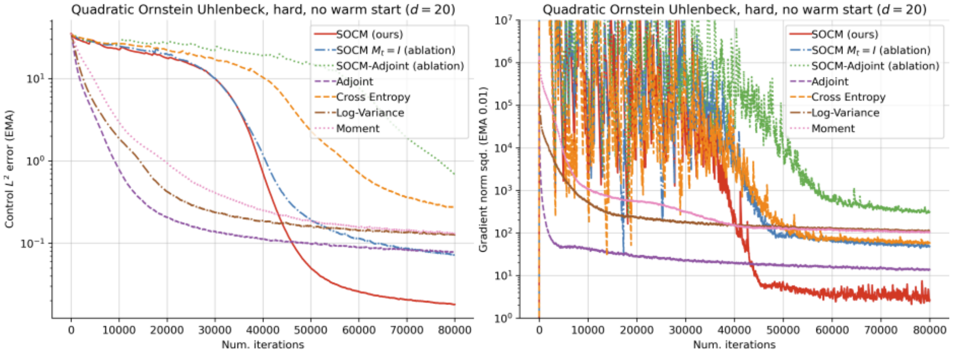
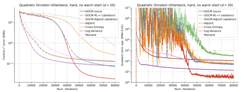


Figure 3 Plots of the L^2 error incurred by the learned control (*top*), and the norm squared of the gradient with respect to the parameters θ of the control (*bottom*), for the Quadratic Ornstein Uhlenbeck (hard) setting and for each IDO loss. All the algorithms use a warm-started control (see Appendix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

Experimental Results (2/2)



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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

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 alpha The large variance of alpha 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