# **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.
- **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.
- **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!

Stochastic Optimal Control Matching —Setup and Preliminaries

-SOC as the Foundation of Generative Models

Consection models were awards from complex distributions  $\mu_{A(i)}() = \mu_{A(i)}()$  when homoralization contract  $\mathcal{F} = \mu_{A(i)}()$  which is restricted to complex. The interaction is the case of dimensionally when integrating one high dimensional quasar. We plantless that called distributions (Canasca) to the contract of the contrac

SOC as the Foundation of Generative Models

**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:

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

**State Process:**  $X^u_t \in \mathbb{R}^d$  (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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What is a Stochastic Control Problem?

**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.

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:

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

Gen Exercises & Monose 
First the optimal control of  $y \in \mathcal{U}$  that minimizes  $\min_{x \in \mathcal{X}} \left[ \int_{x}^{x} \left( \frac{1}{2} \|u(\mathcal{X}_{i}^{x}, t)\|^{2} + (U_{i}^{x}, t_{i}^{x}) \right) \, dt + g(X_{i}^{x}) \right]$ Control Effect  $\frac{1}{2} \|u(X_{i}^{x}, t_{i}^{x})\|^{2}$  (smalless large control actions)
Removing Costs  $I(X_{i}^{x}, t_{i}^{x})$  ((negative can during the process evolution)
Terminal Costs  $I(X_{i}^{x}, t_{i}^{x})$  (for our bands on one dataset these T)

Control Space: U (set of admissible control policies)

# **SOC** in Practice

Aspect	Steering Actuator	Diffusion Models	Flow Models
State $X_t$	Vehicle position, velocity	Noisy data sample	Clean data sample
Control $u_t$	Steering angle, throttle	Denoising direction	Flow velocity field
Dynamics Source	Classical physics (vehicle dynamics)	Forward noising process	No natural drift (learnable)
Drift $b(X_t, t)$	Kinematic equations	Predetermined schedule	b=0 (control learned drift)
Control Goal	Reach target safely	Reverse noise process	Transport distributions
Noise $\sqrt{\lambda}\sigma dB_t$	Road disturbances	Brownian motion	Optional stochasticity

Stochastic Optimal Control Matching —Setup and Preliminaries
└─SOC in Practice

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SOC in Practice

**Steering Actuator:** The dynamics come from well-established physics - Newton's laws, kinematics, and vehicle dynamics. The control optimizes safety and efficiency.

**Diffusion Models:** The drift is determined by the forward noising process (e.g.,  $\beta(t)$ ), and control learns to reverse this predetermined corruption.

Flow Models: No natural drift exists - the control  $u_t$  directly becomes the drift term, learning the entire velocity field that transports distributions.

# **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):

$$\frac{\partial V}{\partial t} + \min_{u} \left[ L(x, u, t) + \frac{\partial V}{\partial x} f(x, u, t) + \frac{1}{2} tr(\sigma^{T} \nabla^{2} V \sigma) \right] = 0$$
 (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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Classic Approach to Finding Optimal Control

**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:**

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

### **Control Policy:**

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

Both parameterized by deep neural networks

### Training Process

#### **Physics-Informed Loss:**

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

#### **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
Stochastic Optimal Control	Adjoint Methods	Matching 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:

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

#### Where:

•  $X^{v}$  is the process controlled by v:

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

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:

$$w(t, v, X^{v}, B, M_{t}) = \sigma(t)^{\top} \left( -\int_{t}^{T} M_{t}(s) \nabla_{x} f(X_{s}^{v}, s) ds - M_{t}(T) \nabla g(X_{T}^{v}) \right)$$

$$+ \int_{t}^{T} \left( M_{t}(s) \nabla_{x} b(X_{s}^{v}, s) - \partial_{s} M_{t}(s) \right) (\sigma^{-1}(s))^{\top} v(X_{s}^{v}, s) ds \qquad (9)$$

$$+ \sqrt{\lambda} \int_{t}^{T} \left( M_{t}(s) \nabla_{x} b(X_{s}^{v}, s) - \partial_{s} M_{t}(s) \right) (\sigma^{-1}(s))^{\top} dB_{s}$$

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:

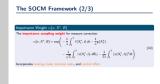
$$\alpha(v, X^{v}, B) = \exp\left(-\frac{1}{\lambda} \int_{0}^{T} f(X_{t}^{v}, t) dt - \frac{1}{\lambda} g(X_{T}^{v})\right)$$

$$-\frac{1}{\sqrt{\lambda}} \int_{0}^{T} \langle v(X_{t}^{v}, t), dB_{t} \rangle - \frac{1}{2\lambda} \int_{0}^{T} \|v(X_{t}^{v}, t)\|^{2} dt$$

$$(10)$$

Incorporates running costs, terminal costs, and control effort

☐ The SOCM Framework (2/3)



**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  $\alpha$ : 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**

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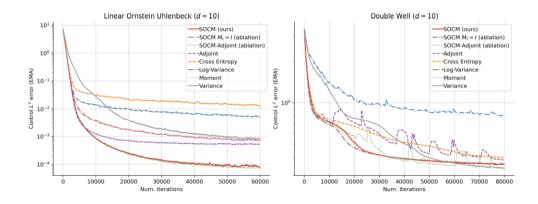
4

6

```
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 \lambda, number of iterations
           N, batch size m, number of time steps K, initial control parameters \theta_0, initial matrix parameters \omega_0, loss
           \mathcal{L}_{\text{SOCM}} in (125)
1 for n \in \{0, ..., 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}}_{SOCM}(u_{\theta_n}, M_{\omega_n}) of the loss
         \mathcal{L}_{SOCM}(u_{\theta_n}, M_{\omega_n}) in (125)
       Compute the gradients \nabla_{(\theta,\omega)}\hat{\mathcal{L}}_{SOCM}(u_{\theta_n},M_{\omega_n}) of \hat{\mathcal{L}}_{SOCM}(u_{\theta_n},M_{\omega_n}) at (\theta_n,\omega_n)
       Obtain \theta_{n+1}, \omega_{n+1} with via an Adam update on \theta_n, \omega_n, resp.
7 end
  Output: Learned control u_{\theta}.
```

Figure: Stochastic Optimal Control Matching (SOCM) Algorithm

# Experimental Results (1/2)



# Experimental Results (2/2)

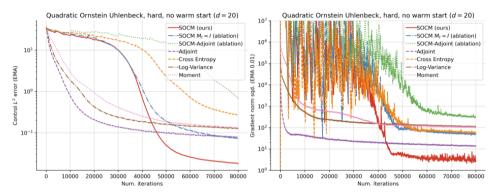
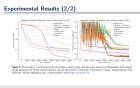


Figure 3 Plots of the  $L^2$  error incurred by the learned control (top), and the norm squared of the gradient with respect to the parameters  $\theta$  of the control (bottom), for the QUADRATIC ORNSTEIN UHLENBECK (HARD) setting and for each IDO loss. All the algorithms use a warm-started control (see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

Stochastic Optimal Control Matching Experiments and results

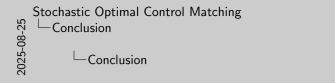
Experimental Results (2/2)



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

# **Conclusion**



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