Stochastic Optimal Control Matching

Carles Domingo-Enrich
(joint work with Jiequn Han, Brandon Amos, Joan Bruna, Ricky T.Q. Chen)

Microsoft Research New England (work done while at New York University & Meta AI)

September 5, 2024

Content of the talk

Introduction

- Stochastic optimal control: definition
- Examples: robotics, sampling unnormalized densities, importance sampling for diffusions
- Existing approaches: the adjoint method

[1] **Domingo-Enrich, C.**, Han, J., Amos, B., Bruna, J., Chen, R.T.Q. *Stochastic optimal control matching*, arXiv preprint, 2023.

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- Our algorithm: SOCM [1]
- Main features of our algorithm
- Experiments

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Key ideas

- Derivation of the SOCM loss
- The path-wise reparameterization trick
- Conclusions and future directions

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Outline

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- Diffusion models: least-squares loss to learn score function (**convex functional landscape**).
- Currently, stochastic optimal control is solved relying on the adjoint method (**highly non-convex functional landscape**).
- Our work is about developing a **least-squares loss** for stochastic optimal control.

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- **Optimal** Control: When driving from point A to B, the 'optimal' path would be the one that minimizes time and fuel.
- **Stochastic** Optimal Control: The systems or processes are random and unpredictable; we need to be robust to noise.

Example I: Robotics

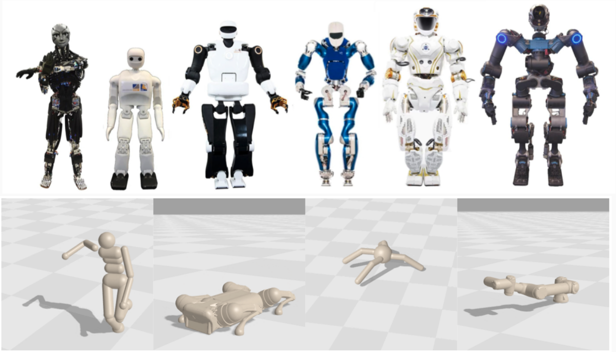

Figure 1: Sources: [FB21; Fre+21]

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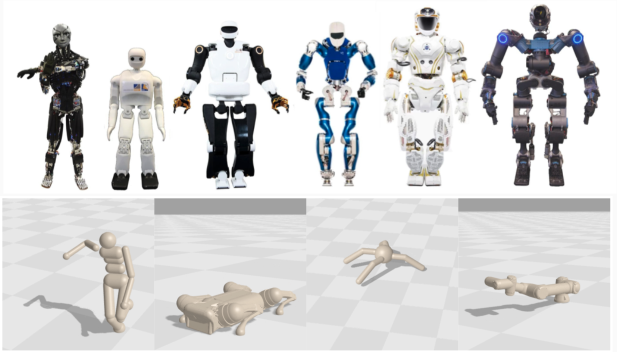

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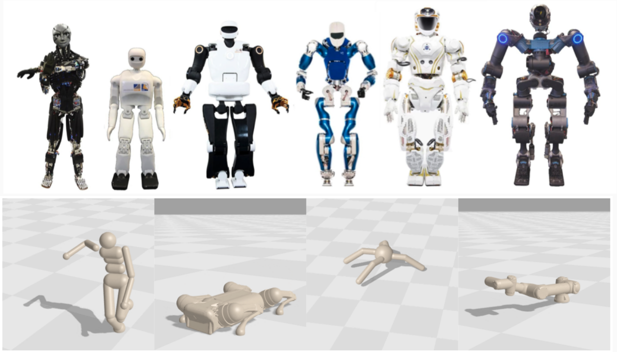

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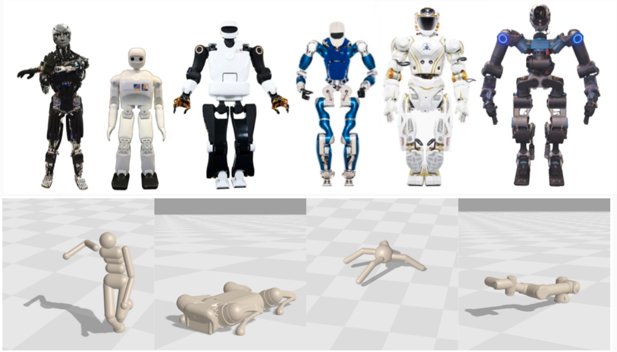

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- Stochasticity: sensor noise, unexpected user behavior, variable conditions

Uncontrolled process vs. controlled process

Uncontrolled process

$$dX_t = b(X_t, t)\, dt + \sqrt{\lambda}\sigma(t) dB_t, \qquad X_0 \sim p_0.$$

where:

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  Robot Example (RE): angles and angular velocities of each joint of the robot

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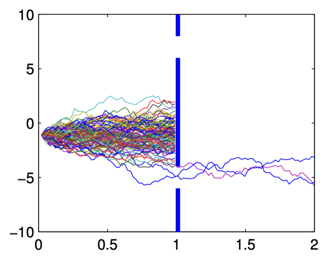

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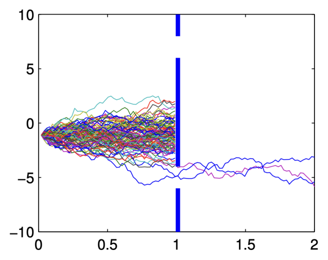

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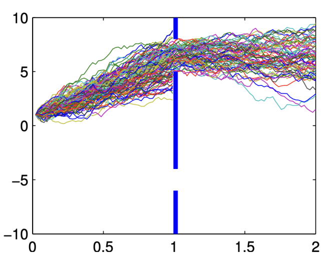

Stochastic optimal control: the problem

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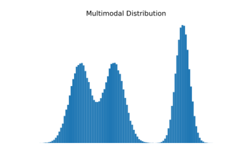

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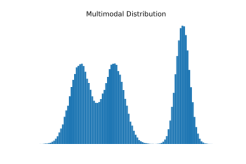

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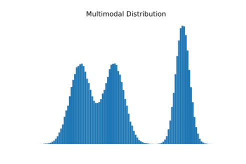

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Stochastic Optimal Control approach to sampling [BRU23]

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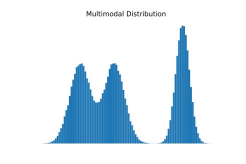

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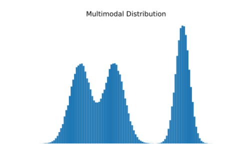

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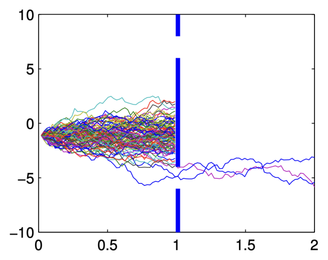

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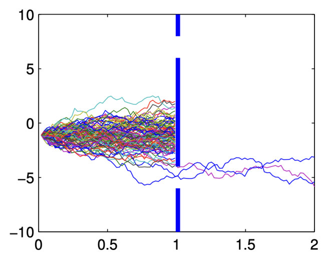

Very unlikely event! Monte Carlo estimation is high-variance.

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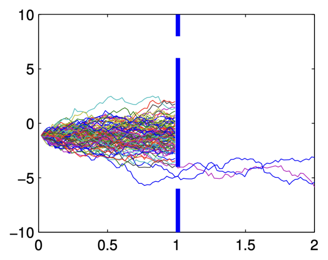

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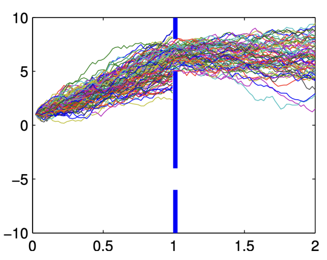

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We recover $P(X_T \in \mathcal{O})$ by setting $f(x, t) = 0$, $g(x) = -\log \mathbb{1}_{\mathcal{O}}(x)$. We need to perform importance sampling using a process that goes through the top hole often!

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Existing approaches for Stochastic Optimal Control

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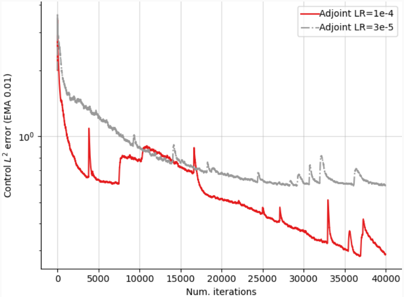
  - Update θ using a stochastic optimization algorithm (e.g. Adam)

The adjoint method has unstable training dynamics

L^2 error for control u: $\mathbb{E}_{t,X^{u^*}} \|u(X_t^{u^*}, t) - u^*(X_t^{u^*}, t)\|^2$, where u^* is the optimal control



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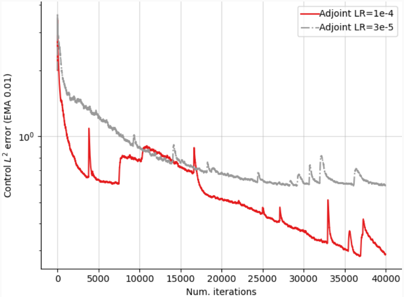

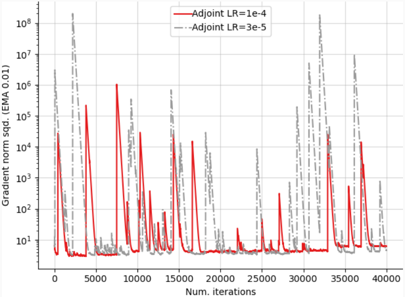

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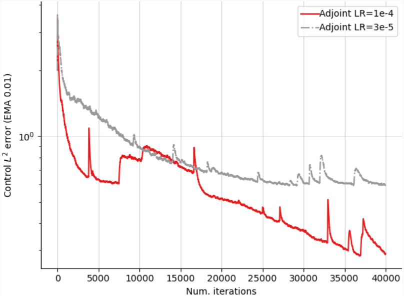

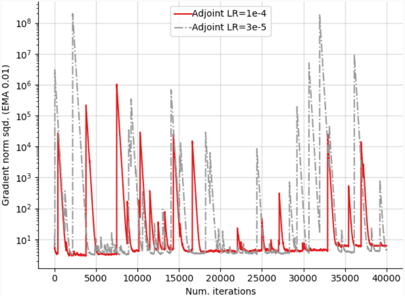

Why? Because the adjoint loss is **highly non-convex** w.r.t. the control u!

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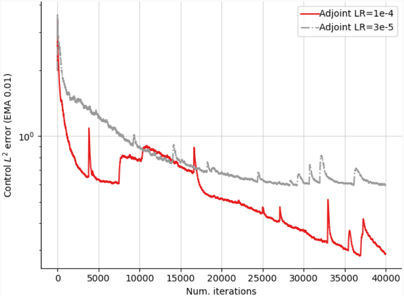

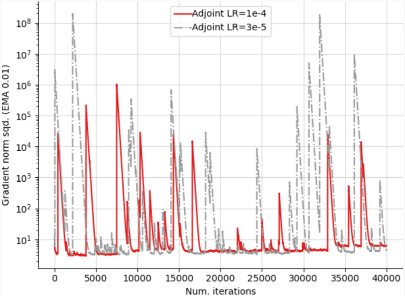

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Can we design algorithms with stable training?

Outline

Introduction

Stochastic Optimal Control Matching

Key ideas

Detour: Maximum Likelihood Normalizing Flows vs. Diffusion Models

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- *Continuous Normalizing Flows* (CNFs) [Che+18]: originally trained to maximize the log-likelihood of the generated samples, using the *adjoint method*.

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From non-convex to convex landscapes

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Generative modeling	Maximum Likelihood CNFs	Diffusion models, Flow Matching
Stochastic optimal control	Adjoint method	?

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SOCM: a least squares loss for stochastic control

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w and α depend on f, g, λ, σ (full expressions later on).

Some details on SOCM

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$$+ \underbrace{\mathbb{E}_{t,X^v}\left[\left\| w(t, v, X^v, B, M_t) - \frac{\mathbb{E}[w(t, v, X^v, B, M_t)\alpha(v, X^v, B)|t, X_t^v]}{\mathbb{E}[\alpha(v, X^v, B)|t, X_t^v]}\right\|^2 \alpha(v, X^v, B)\right]}_{\text{Conditional variance of } w}$$

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We train M to minimize the conditional variance of the matching vector field w.

- **How do we choose v?** We want v such that $\alpha(v, X^v)$ has low variance. In general, we take v to be the current learned control u.

Experiments: settings, baselines and ablations

Settings:

- Quadratic Ornstein Uhlenbeck / Linear Quadratic Regulator: Linear base drift b, quadratic state cost f, quadratic terminal cost g
- Linear Ornstein Uhlenbeck: Linear base drift b, quadratic state cost f, linear terminal cost g
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- Adjoint method [Pon62]
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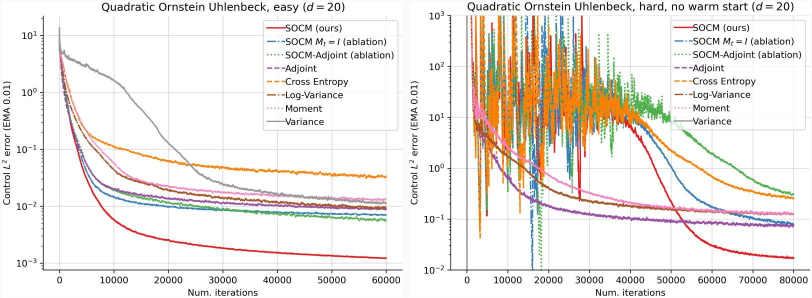
Ablations:

- SOCM with constant $M_t = \mathrm{Id}$
- SOCM-Adjoint: modification of SOCM where the adjoint method is used instead of the path-wise reparameterization trick

Experiments: Control L^2 error

Control L^2 error: $\mathbb{E}_{t,X^v}\left[\|u(X_t^v,t) - u^*(X_t^v,t)\|^2 \alpha(v,X^v,B)\right] / \mathbb{E}_{t,X^v}\left[\alpha(v,X^v,B)\right]$



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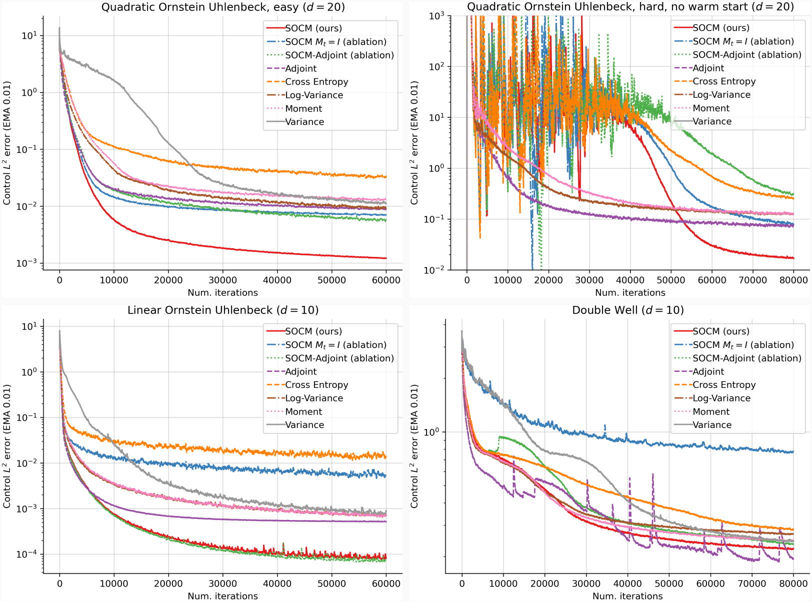

Experiments: Importance weight variance

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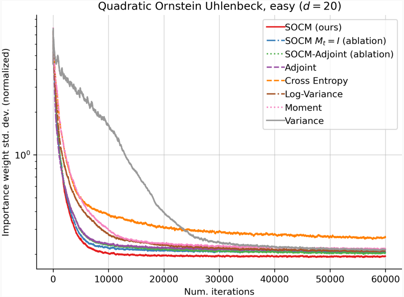

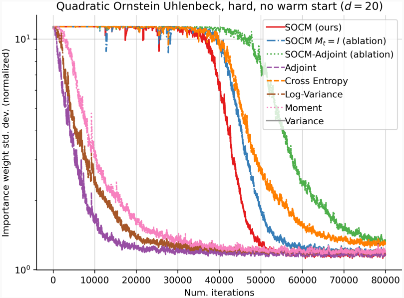

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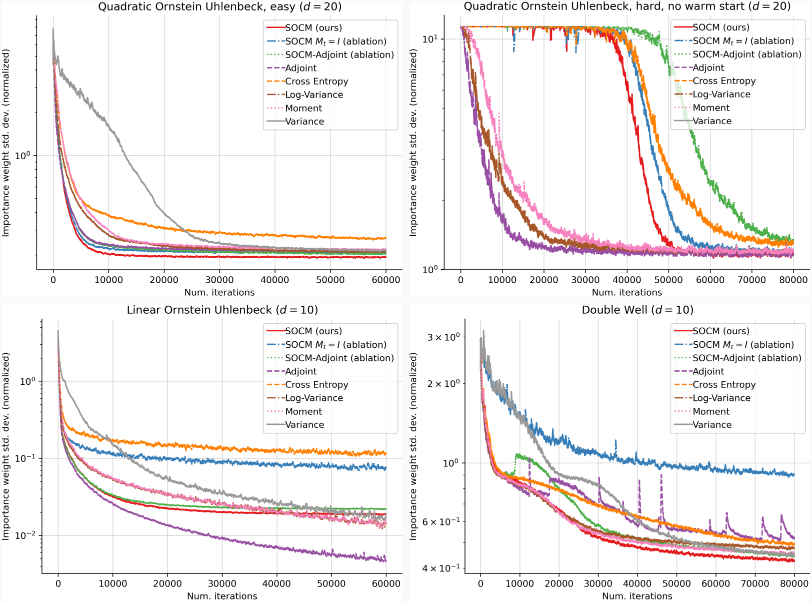
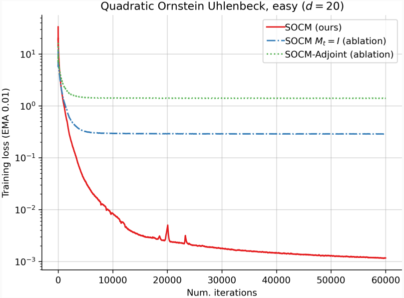
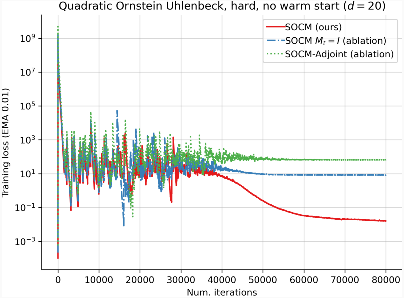


Experiments: Training loss for SOCM and ablations

$\mathcal{L}(u, M) = L^2$ error of u + Conditional variance of w





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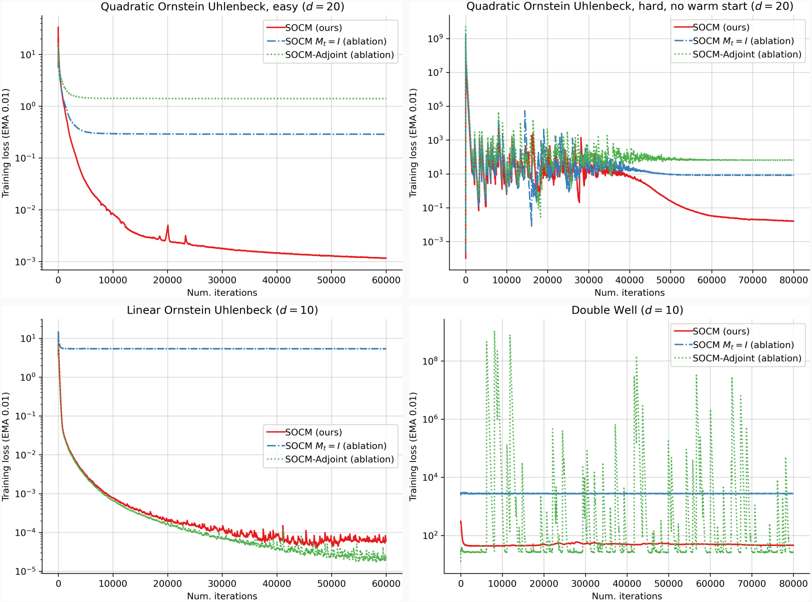

Outline

Derivation of the SOCM loss (1/3)

Reminders:

- X^u is the process controlled by u; it is the solution of
$$dX_t^u = (b(X_t^u, t) + \sigma(t)u(X_t^u, t))\, dt + \sqrt{\lambda}\sigma(t)dB_t, \qquad X_0^u \sim p_0.$$
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Lemma (Path-integral representation of the optimal control)

The optimal control u^* satisfies
$$u^*(x,t) = \lambda\sigma(t)^\top \nabla_x \log \mathbb{E}\big[\exp\big(-\lambda^{-1}\textstyle\int_t^T f(X_s, s)\,\mathrm{d}s - \lambda^{-1}g(X_T)\big)\big|X_t = x\big]. \quad (5)$$

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Consider the loss
$$\begin{aligned}\tilde{\mathcal{L}}(u) &= \mathbb{E}\big[\tfrac{1}{T}\textstyle\int_0^T \big\|u(X_t,t) - u^*(X_t,t)\big\|^2 \mathrm{d}t \exp\big(-\lambda^{-1}\int_0^T f(X_t,t)\,\mathrm{d}t - \lambda^{-1}g(X_T)\big)\big] \\ &= \mathbb{E}\big[\tfrac{1}{T}\textstyle\int_0^T \big(\big\|u(X_t,t)\big\|^2 - 2\langle u(X_t,t), u^*(X_t,t)\rangle + \big\|u^*(X_t,t)\big\|^2\big)\,\mathrm{d}t \\ &\qquad \times \exp\big(-\lambda^{-1}\textstyle\int_0^T f(X_t,t)\,\mathrm{d}t - \lambda^{-1}g(X_T)\big)\big].\end{aligned}$$

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The only optimum of this loss is u^*. Using equation (5), the cross-term can be rewritten as:
$$\begin{aligned}&\mathbb{E}\big[\tfrac{1}{T}\textstyle\int_0^T \langle u(X_t,t), u^*(X_t,t)\rangle\,\mathrm{d}t \exp\big(-\lambda^{-1}\int_0^T f(X_t,t)\,\mathrm{d}t - \lambda^{-1}g(X_T)\big)\big] \\ &= -\lambda\mathbb{E}\big[\tfrac{1}{T}\textstyle\int_0^T \big\langle u(X_t,t), \sigma(t)^\top\nabla_x\mathbb{E}\big[\exp\big(-\lambda^{-1}\int_t^T f(X_s,s)\,\mathrm{d}s - \lambda^{-1}g(X_T)\big)\big|X_t = x\big]\big\rangle\,\mathrm{d}t \\ &\qquad \times \exp\big(-\lambda^{-1}\textstyle\int_0^t f(X_s,s)\,\mathrm{d}s\big)\big].\end{aligned}$$

Derivation of the SOCM loss (2/3)

To evaluate the derivative of the conditional expectation, we use:

Proposition (Path-wise reparameterization trick for stochastic optimal control)

For each $t \in [0, T]$, let $M_t : [t, T] \to \mathbb{R}^{d \times d}$ be an arbitrary continuously differentiable function matrix-valued function such that $M_t(t) = \mathrm{Id}$. We have that

$$
\begin{aligned}
&\nabla_x \mathbb{E}\big[\exp\big(-\lambda^{-1} \textstyle\int_t^T f(X_s, s)\,\mathrm{d}s - \lambda^{-1} g(X_T)\big)\big|X_t = x\big] \\
&= \mathbb{E}\big[\big(-\lambda^{-1} \textstyle\int_t^T M_t(s)\nabla_x f(X_s, s)\,\mathrm{d}s - \lambda^{-1} M_t(T)\nabla g(X_T) \\
&\qquad + \lambda^{-1/2} \textstyle\int_t^T (M_t(s)\nabla_x b(X_s, s) - \partial_s M_t(s))(\sigma^{-1})^\top (X_s, s)\mathrm{d}B_s\big) \\
&\qquad \times \exp\big(-\lambda^{-1} \textstyle\int_t^T f(X_s, s)\,\mathrm{d}s - \lambda^{-1} g(X_T)\big)\big|X_t = x\big].
\end{aligned}
\tag{6}
$$

Using (6) and completing the square, we obtain that for some constant K independent of u,

$$
\begin{aligned}
\tilde{\mathcal{L}}(u) = \mathbb{E}\big[\tfrac{1}{T} \textstyle\int_0^T \big\| u(X_t, t) + \sigma(t)\big(\textstyle\int_t^T M_t(s)\nabla_x f(X_s, s)\,\mathrm{d}s + M_t(T)\nabla g(X_T) \\
- \lambda^{1/2} \textstyle\int_t^T (M_t(s)\nabla_x b(X_s, s) - \partial_s M_t(s))(\sigma^{-1})^\top (X_s, s)\mathrm{d}B_s\big)\big\|^2 \,\mathrm{d}t \\
\times \exp\big(-\lambda^{-1} \textstyle\int_0^T f(X_t, t)\,\mathrm{d}t - \lambda^{-1} g(X_T)\big)\big] + K.
\end{aligned}
$$

If we perform a change of process from X to X^v by applying the Girsanov theorem, where v is arbitrary, we obtain the loss $\mathcal{L}_{\mathrm{SOCM}}(u, M)$.

Derivation of the SOCM loss (3/3)

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$$\begin{aligned}
w(t, v, X^v, M) = &- \int_t^T M(t, s)\nabla_x f(X_s^v, s)\, ds - M(t, T)\nabla g(X_T^v) \\
&- \int_t^T (M(t, s)\nabla_x b(X_s^v, s) - \partial_s M(t, s)) v(X_s^v, s)\, ds \\
&- \sqrt{\lambda} \int_t^T (M(t, s)\nabla_x b(X_s^v, s) - \partial_s M(t, s))\, dB_s, \\
\alpha(v, X^v) = \exp\Bigg(&- \frac{1}{\lambda}\int_0^T f(X_t^v, t)\, ds - \frac{1}{\lambda} g(X_T^v) \\
&- \frac{1}{\sqrt{\lambda}} \int_0^T \langle v(X_t^v, t), dB_t\rangle - \frac{1}{2\lambda}\int_0^T \|v(X_t^v, t)\|^2\, dt \Bigg)
\end{aligned}$$

Future directions within stochastic optimal control

Applications of SOCM

- Test and benchmark SOCM as an algorithm to sample from unnormalized densities

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Technical improvements of SOCM

- Make reparameterization matrix M depend to the controlled process X^v.
- Test alternative way to use Girsanov theorem to lower the gradient variance when learning controls: explicit perturbations ψ. It can be combined with the path-wise reparameterization trick and also applied to other methods like the adjoint, cross-entropy, log-variance...

Future applications of the path-wise reparameterization trick

PWRT for diffusion processes

- The PWRT can be used to *generalize conditional score matching* to diffusion processes with generic drifts.

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- Reminder: Neural SDEs are the SDE analog of Neural ODEs, they use the adjoint method.
- We can replace the adjoint method by PWRT.

Informal derivation of the path-wise reparameterization trick (1/2)

Consider the Euler-Maruyama discretization $\hat{X} = (\hat{X}_k)_{k=0:K}$ of the uncontrolled process X with $K+1$ time steps (let $\delta = T/K$ be the step size):

$$\hat{X}_0 \sim p_0, \qquad \hat{X}_{k+1} = \hat{X}_k + \delta b(\hat{X}_k, k\delta) + \sqrt{\delta\lambda}\sigma(k\delta)\varepsilon_k, \qquad \varepsilon_k \sim N(0, I).$$

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We can approximate

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$$\begin{aligned}&\mathbb{E}\big[\exp\big(-\lambda^{-1}\int_t^T f(X_s, s)\,\mathrm{d}s - \lambda^{-1}g(X_T)\big)\big|X_t = x\big] \\ &\approx \mathbb{E}\big[\exp\big(-\lambda^{-1}\delta\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1}g(\hat{X}_K)\big)\big|\hat{X}_0 = x\big],\end{aligned}$$

Remark that for $k \in \{0, \dots, K-1\}$, $\hat{X}_{k+1}|\hat{X}_k \sim N(\hat{X}_k + \delta b(\hat{X}_k, k\delta), \delta\lambda(\sigma\sigma^\top)(k\delta))$. Hence,

$$\begin{aligned}&\mathbb{E}\big[\exp\big(-\lambda^{-1}\delta\textstyle\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1}g(\hat{X}_K)\big)\big|\hat{X}_0 = x\big] \\ &= C^{-1}\textstyle\iint_{(\mathbb{R}^d)^K} \exp\big(-\lambda^{-1}\delta\sum_{k=0}^{K-1} f(\hat{x}_k, s) - \lambda^{-1}g(\hat{x}_K) \\ &\qquad -\frac{1}{2\delta\lambda}\textstyle\sum_{k=1}^{K-1}\|\sigma^{-1}(k\delta)(\hat{x}_{k+1} - \hat{x}_k - \delta b(\hat{x}_k, k\delta))\|^2 \\ &\qquad -\frac{1}{2\delta\lambda}\|\sigma^{-1}(0)(\hat{x}_1 - x - \delta b(x, 0))\|^2\big)\,\mathrm{d}\hat{x}_1\cdots\mathrm{d}\hat{x}_K,\end{aligned} \tag{7}$$

where $C = \sqrt{(2\pi\delta\lambda)^K\prod_{k=0}^{K-1}\det((\sigma\sigma^\top)(k\delta))}$.

Informal derivation of the path-wise reparameterization trick (2/2)

We can write
$\nabla_x \mathbb{E}\big[\exp\big(-\lambda^{-1}\delta\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1} g(\hat{X}_K)\big)|\hat{X}_0 = x\big]$

Informal derivation of the path-wise reparameterization trick (2/2)

We can write

$$\nabla_x \mathbb{E}\big[\exp\big(-\lambda^{-1}\delta \textstyle\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1} g(\hat{X}_K)\big) | \hat{X}_0 = x\big]$$
$$= \nabla_{z} \mathbb{E}\big[\exp\big(-\lambda^{-1}\delta \textstyle\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1} g(\hat{X}_K)\big) | \hat{X}_0 = x + z\big]|_{z=0}$$

Informal derivation of the path-wise reparameterization trick (2/2)

We can write

$$
\begin{aligned}
&\nabla_x \mathbb{E}\big[\exp\big(-\lambda^{-1}\delta\textstyle\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1} g(\hat{X}_K)\big)\big|\hat{X}_0 = x\big] \\
&= \nabla_z \mathbb{E}\big[\exp\big(-\lambda^{-1}\delta\textstyle\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1} g(\hat{X}_K)\big)\big|\hat{X}_0 = x + z\big]\big|_{z=0} \\
&= C^{-1}\nabla_z\big(\textstyle\iint_{(\mathbb{R}^d)^K} \exp\big(-\lambda^{-1}\delta\sum_{k=0}^{K-1} f(\hat{x}_k, s) - \lambda^{-1} g(\hat{x}_K) \\
&\qquad\qquad - \tfrac{1}{2\delta\lambda}\textstyle\sum_{k=1}^{K-1} \|\sigma^{-1}(k\delta)(\hat{x}_{k+1} - \hat{x}_k - \delta b(\hat{x}_k, k\delta))\|^2 \\
&\qquad\qquad - \tfrac{1}{2\delta\lambda}\|\sigma^{-1}(0)(\hat{x}_1 - (x+z) - \delta b(x+z, 0))\|^2\big)\, \mathrm{d}\hat{x}_1 \cdots \mathrm{d}\hat{x}_K\big)\big|_{z=0}
\end{aligned}
$$

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&= C^{-1}\nabla_z \big(\textstyle\iint_{(\mathbb{R}^d)^K} \exp\big(-\lambda^{-1}\delta \sum_{k=0}^{K-1} f(\hat{x}_k + \psi(z, k\delta), s) - \lambda^{-1} g(\hat{x}_K + \psi(z, K\delta)) \\
&\quad - \tfrac{1}{2\delta\lambda} \textstyle\sum_{k=1}^{K-1} \|\sigma^{-1}(k\delta)(\hat{x}_{k+1} + \psi(z, (k+1)\delta) - \hat{x}_k - \psi(z, k\delta) - \delta b(\hat{x}_k + \psi(z, k\delta), k\delta))\|^2 \\
&\quad - \tfrac{1}{2\delta\lambda} \|\sigma^{-1}(0)(\hat{x}_1 + \psi(z, \delta) - (x + \psi(z, 0)) - \delta b(x + \psi(z, 0), 0))\|^2\big) \, \mathrm{d}\hat{x}_1 \cdots \mathrm{d}\hat{x}_K \big)\big|_{z=0},
\end{aligned}
$$

- In the last equality, $\psi : \mathbb{R}^d \times [0, T] \to \mathbb{R}^d$ is an arbitrary twice differentiable function such that $\psi(z, 0) = z$ for all $z \in \mathbb{R}^d$, and $\psi(0, s) = 0$ for all $s \in [0, T]$.

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&\qquad\qquad - \tfrac{1}{2\delta\lambda}\textstyle\sum_{k=1}^{K-1} \|\sigma^{-1}(k\delta)(\hat{x}_{k+1} - \hat{x}_k - \delta b(\hat{x}_k, k\delta))\|^2 \\
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- We used that for $k \in \{1, \dots, K\}$, the variables $\hat{x}_k$ are integrated over $\mathbb{R}^d$, which means that adding an offset $\psi(z, k\delta)$ does not change the value of the integral. We also used that $\psi(z, 0) = z$.

Informal derivation of the path-wise reparameterization trick (2/2)

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$$
\begin{aligned}
&\nabla_x \mathbb{E}\big[\exp\big(-\lambda^{-1}\delta \textstyle\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1} g(\hat{X}_K)\big) | \hat{X}_0 = x\big] \\
&= \nabla_z \mathbb{E}\big[\exp\big(-\lambda^{-1}\delta \textstyle\sum_{k=0}^{K-1} f(\hat{X}_k, s) - \lambda^{-1} g(\hat{X}_K)\big) | \hat{X}_0 = x + z\big]|_{z=0} \\
&= C^{-1}\nabla_z \big(\textstyle\iint_{(\mathbb{R}^d)^K} \exp\big(-\lambda^{-1}\delta \sum_{k=0}^{K-1} f(\hat{x}_k, s) - \lambda^{-1} g(\hat{x}_K) \\
&\qquad - \tfrac{1}{2\delta\lambda} \textstyle\sum_{k=1}^{K-1} \|\sigma^{-1}(k\delta)(\hat{x}_{k+1} - \hat{x}_k - \delta b(\hat{x}_k, k\delta))\|^2 \\
&\qquad - \tfrac{1}{2\delta\lambda} \|\sigma^{-1}(0)(\hat{x}_1 - (x+z) - \delta b(x+z, 0))\|^2\big) \, \mathrm{d}\hat{x}_1 \cdots \mathrm{d}\hat{x}_K \big)|_{z=0} \\
&= C^{-1}\nabla_z \big(\textstyle\iint_{(\mathbb{R}^d)^K} \exp\big(-\lambda^{-1}\delta \sum_{k=0}^{K-1} f(\hat{x}_k + \psi(z, k\delta), s) - \lambda^{-1} g(\hat{x}_K + \psi(z, K\delta)) \\
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&\qquad - \tfrac{1}{2\delta\lambda} \|\sigma^{-1}(0)(\hat{x}_1 + \psi(z, \delta) - (x + \psi(z, 0)) - \delta b(x + \psi(z, 0), 0))\|^2\big) \, \mathrm{d}\hat{x}_1 \cdots \mathrm{d}\hat{x}_K \big)|_{z=0},
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- In the last equality, $\psi : \mathbb{R}^d \times [0, T] \to \mathbb{R}^d$ is an arbitrary twice differentiable function such that $\psi(z, 0) = z$ for all $z \in \mathbb{R}^d$, and $\psi(0, s) = 0$ for all $s \in [0, T]$.
- We used that for $k \in \{1, \dots, K\}$, the variables $\hat{x}_k$ are integrated over $\mathbb{R}^d$, which means that adding an offset $\psi(z, k\delta)$ does not change the value of the integral. We also used that $\psi(z, 0) = z$.
- To conclude the proof, we differentiate with respect to z under the integral sign, and define $M(s) = \nabla\psi(z, s)|_{z=0}$.

Content of the talk

Introduction

- Stochastic optimal control: definition
- Examples: robotics, sampling unnormalized densities, importance sampling for diffusions
- Existing approaches: the adjoint method

Stochastic Optimal Control Matching

- Comparing stochastic optimal control with normalizing flows
- Our algorithm: SOCM [2]
- Main features of our algorithm
- Experiments

Key ideas

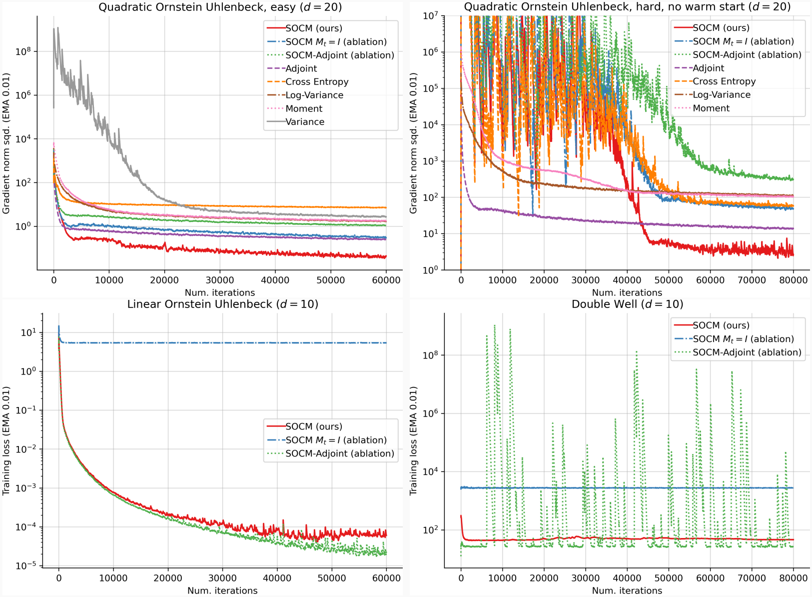
- Derivation of the SOCM loss
- The path-wise reparameterization trick
- Conclusions and future directions

[2] **Domingo-Enrich, C.**, Han, J., Amos, B., Bruna, J., Chen, R.T.Q. *Stochastic optimal control matching*, arXiv preprint, 2023.

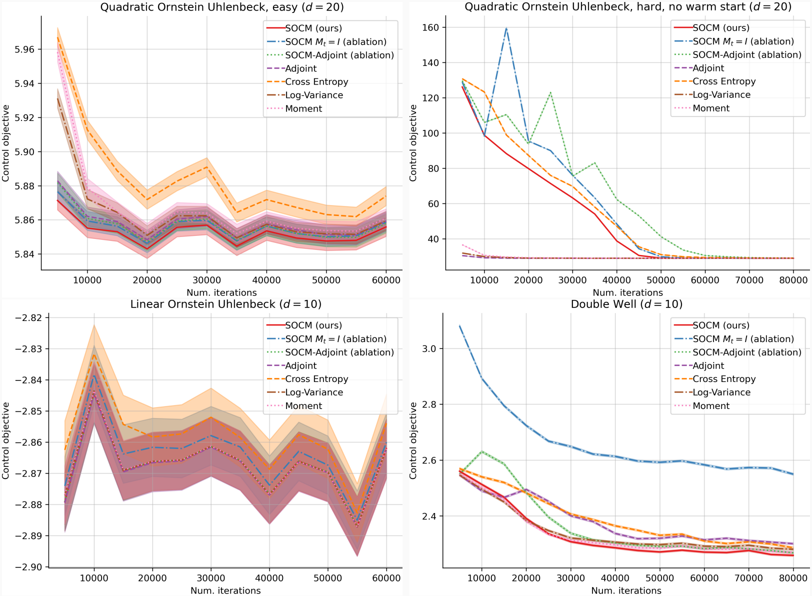
Thank you!

Contact: *cd2754@nyu.edu*

Experiments: Gradient norm



Experiments: Control objective



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