# An optimal control perspective on diffusion-based generative modeling

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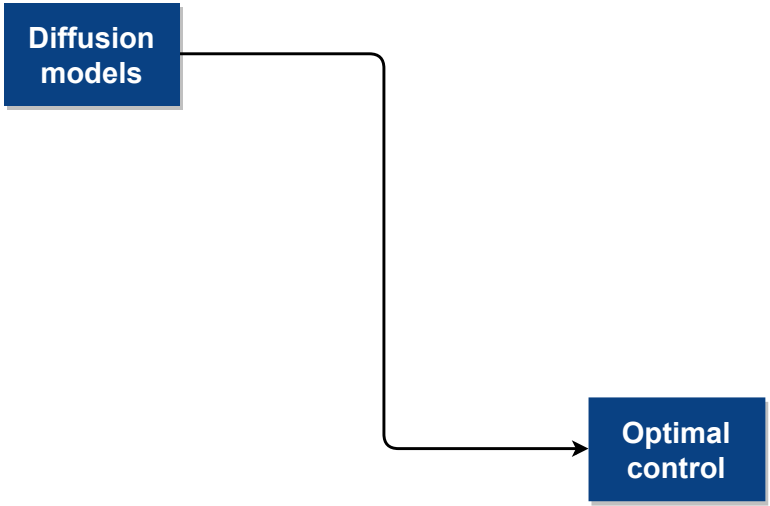
(*equal contribution)

NeurIPS 2022

December, 2022




# Overview



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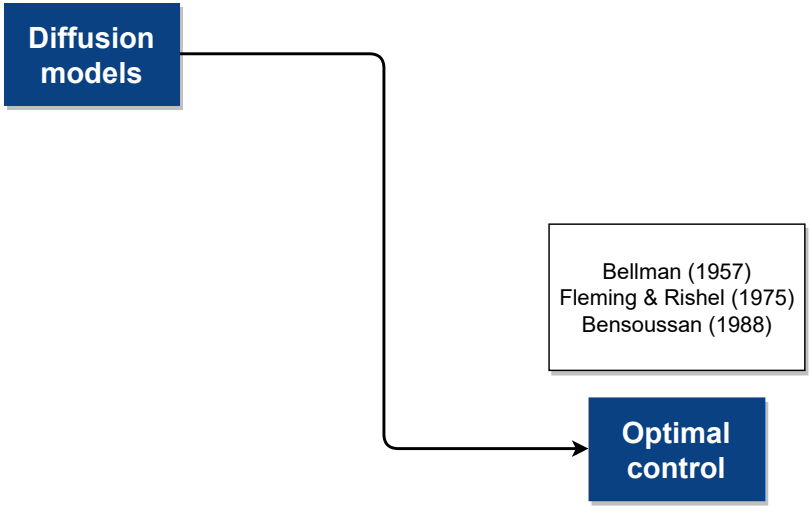
Diffusion models
Bellman (1957)
Fleming & Rishel (1975)
Bensoussan (1988)
Optimal control

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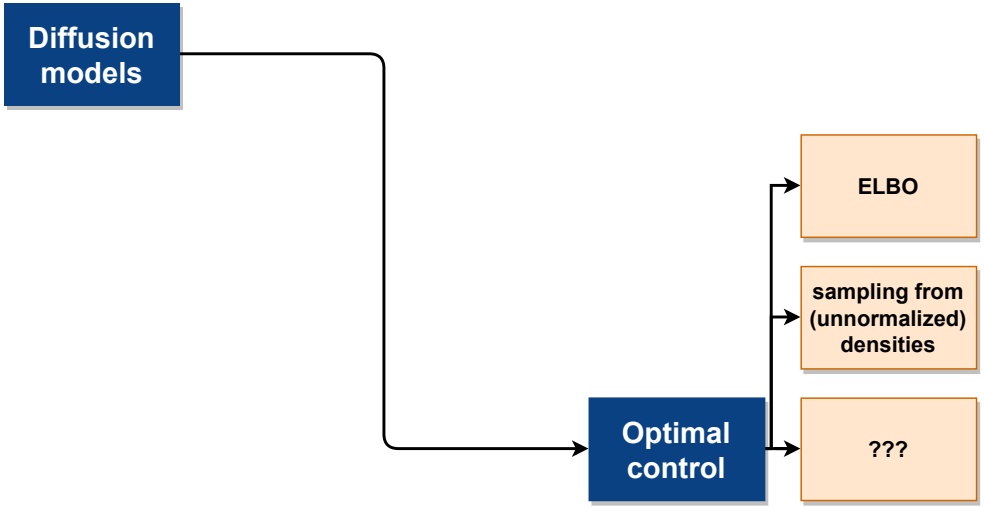
Diffusion models
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ELBO
sampling from (unnormalized) densities
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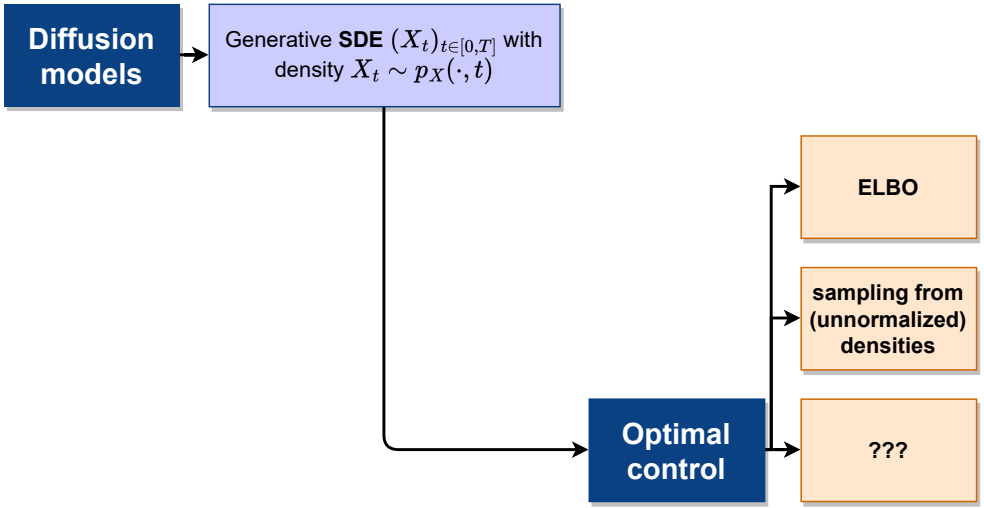
Diffusion models
Generative SDE $(X_t)_{t\in[0,T]}$ with density $X_t \sim p_X(\cdot, t)$
ELBO
sampling from (unnormalized) densities
???
Optimal control

# SDE-based generative modeling

- **Model:** Stochastic differential equation (SDE)

$$\mathrm{d}X_s = \bar{\mu}(X_s, s)\,\mathrm{d}s + \bar{\sigma}(s)\,\mathrm{d}B_s.$$

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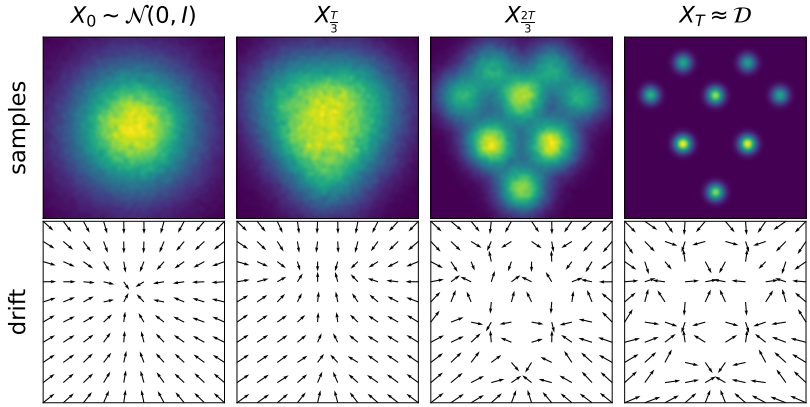
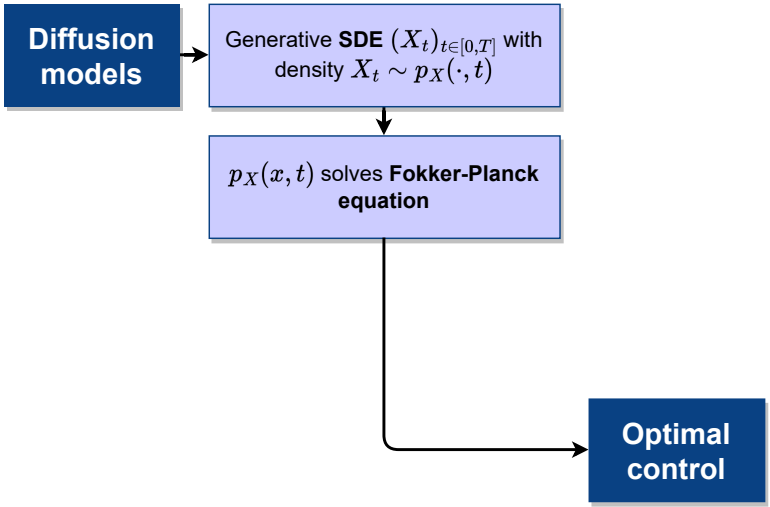


# PDE for the log-density



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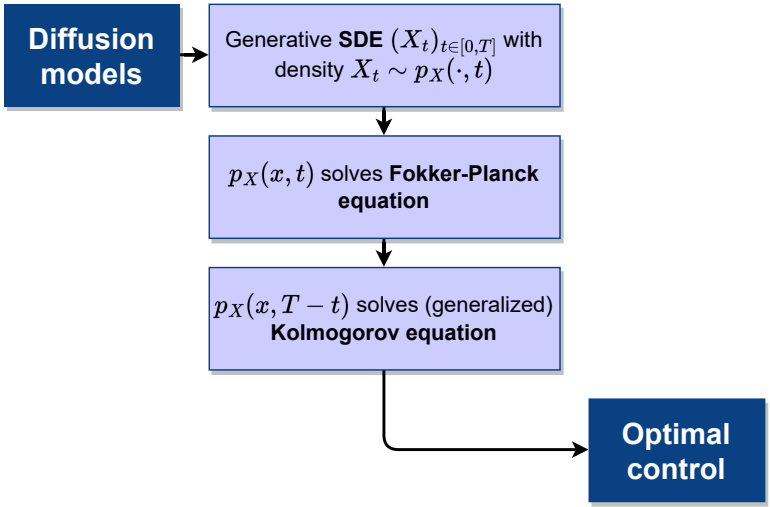

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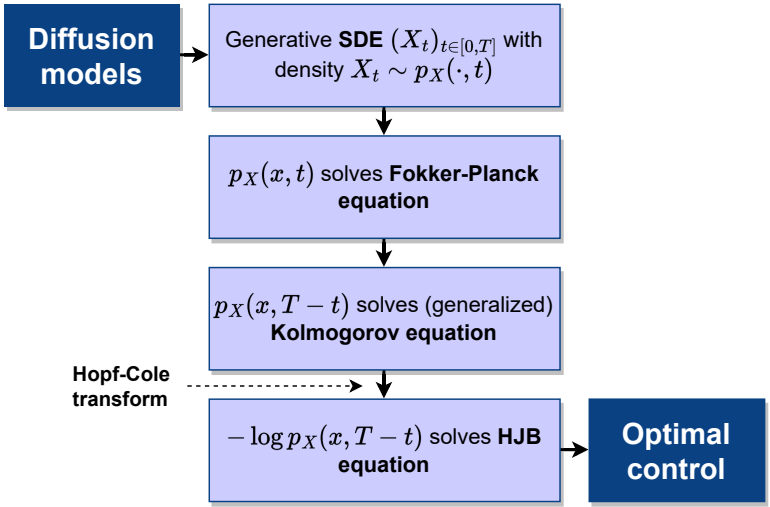


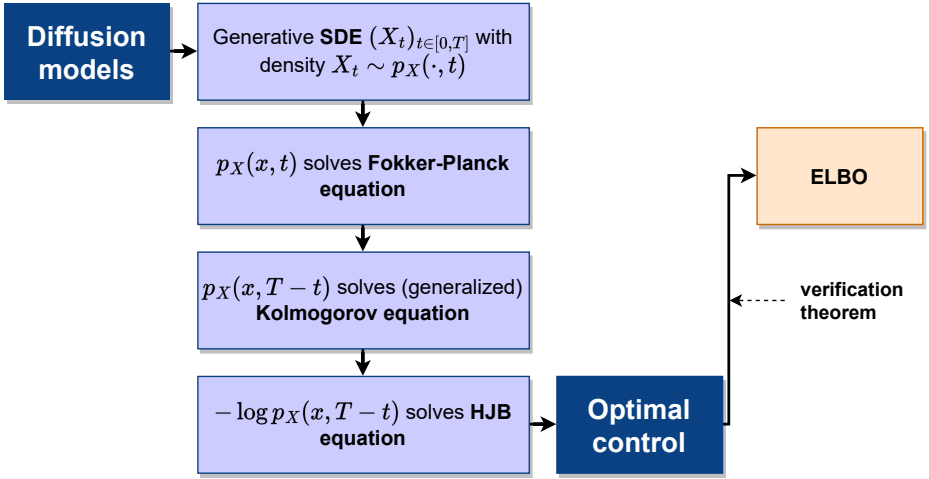
# PDE for the log-density

**Lemma (Hamilton-Jacobi-Bellman equation for log-density)**

*Define* $V(x,t) \coloneqq -\log \overleftarrow{p}_X$, *where* $\overleftarrow{p}_X(x,t) \coloneqq p_X(x, T-t)$ *denotes the time-reversal. Then*

$$\partial_t V = -\frac{1}{2}\operatorname{Tr}\left(\sigma\sigma^\top \nabla^2 V\right) + \mu \cdot \nabla V - \operatorname{div}(\mu) + \frac{1}{2}\left\|\sigma^\top \nabla V\right\|^2.$$

# Applications



# Deriving the ELBO

## Theorem (Verification theorem)

*Let $Y^u$ be defined by*

$$\mathrm{d}Y_s^u = (\sigma u - \mu)(Y_s^u, s)\,\mathrm{d}s + \sigma(s)\,\mathrm{d}B_s.$$

*Then it holds that*

$$V(Y_0^u, 0) = \min_{u \in \mathcal{U}} \mathbb{E}\left[ \underbrace{\int_0^T \left( \operatorname{div}(\mu) + \frac{1}{2}\|u\|^2 \right)(Y_s^u, s)\,\mathrm{d}s}_{\text{running costs}} + \underbrace{V(Y_T^u, T)}_{\text{terminal cost}} \,\middle|\, Y_0^u \right],$$

*where the unique minimum is attained by $u^* := -\sigma^\top \nabla V$.*

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$$-\log p_{X_T}(Y_0^u) = \min_{u \in \mathcal{U}} \mathbb{E}\left[ \int_0^T \left( \operatorname{div}(\mu) + \frac{1}{2}\|u\|^2 \right)(Y_s^u, s)\,\mathrm{d}s - \log p_{X_0}(Y_T^u) \,\middle|\, Y_0^u \right],$$

*where the unique minimum is attained by $u^* := \sigma^\top \nabla \log \overleftarrow{p}_X = \sigma^\top \nabla \log p_{Y^{u^*}}$.*

# Score-based generative modeling

- **Reparametrization:** $\mu := \sigma u - f$ yields the SDEs

$$\mathrm{d}Y_s = f(Y_s, s)\,\mathrm{d}s + \sigma(s)\,\mathrm{d}B_s, \quad Y_0 \sim \mathcal{D}, \qquad \mathrm{d}X_s^u = \left(\overleftarrow{\sigma}\overleftarrow{u} - \overleftarrow{f}\right)(X_s^u, s)\,\mathrm{d}s + \overleftarrow{\sigma}(s)\,\mathrm{d}B_s.$$

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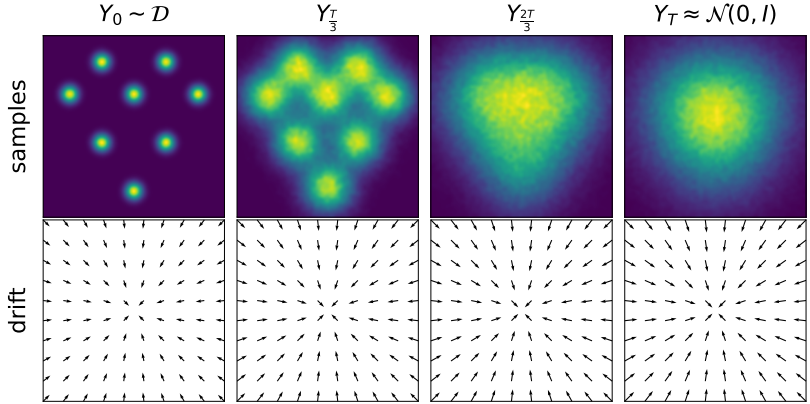

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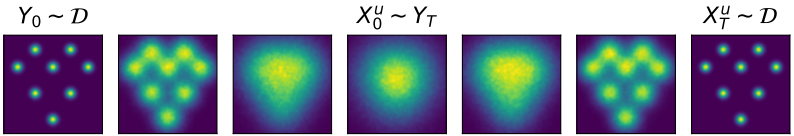
- **Time-reversal:** If $u = u^* = \sigma^\top \nabla \log p_Y$, one can achieve $X_T^u \sim \mathcal{D}$ by setting $X_0^u \sim Y_T$.



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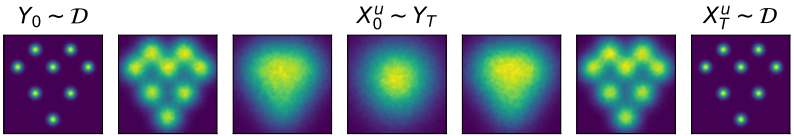
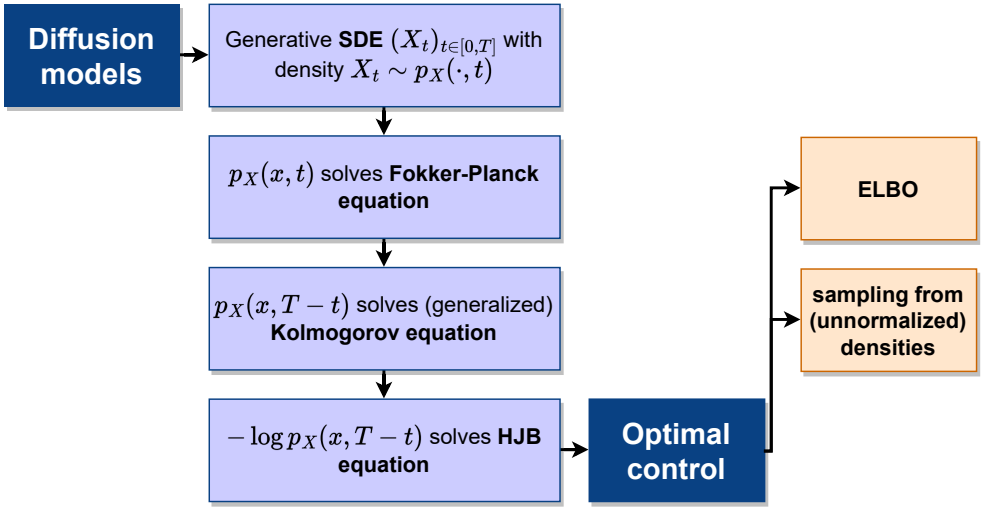



- **Denoising score matching objective:** The verification theorem implies

$$-\log p_{X_T^u}(Y_0) \leq \frac{T}{2}\,\mathbb{E}\left[\left\|u(Y_\tau, \tau) - \sigma^\top(\tau)\nabla \log p_{Y_\tau|Y_0}(Y_\tau|Y_0)\right\|^2\right] + \text{const.},$$

# Applications



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- **Application:** Data distribution $\mathcal{D}$ admits the density $\frac{\rho}{\mathcal{Z}}$ where $\rho$ is known. We cannot use denoising score matching since we do not have access to samples.

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## Corollary (Sampling from densities)

*The verification theorem implies*

$$-\log \mathcal{Z} = \min_{\bar{u}\in\mathcal{U}} \mathbb{E}\left[\int_0^T \left(\operatorname{div}(\overleftarrow{f}) + \frac{1}{2}\|\bar{u}\|^2\right)(X_s^u, s)\,\mathrm{d}s + \log p_{Y_T}(X_0^u) - \log \rho(X_T^u)\middle| Y_0\right],$$

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*where the minimum is attained by* $u^* = \sigma^\top \nabla \log p_Y$.

- **Related work:** Path Integral Sampler by Zhang and Chen (2021). Our diffusion-based approach is more flexible (SDE type, initial distribution, probability flow ODE) and stable.

# Numerical example

- Successful application to tasks in molecular dynamics, e.g.,

$$\rho(x) \coloneqq \exp\left(-\sum_{i=1}^{5}(x_i^2-2)^2 - \frac{1}{2}\sum_{i=6}^{50} x_i^2\right)$$

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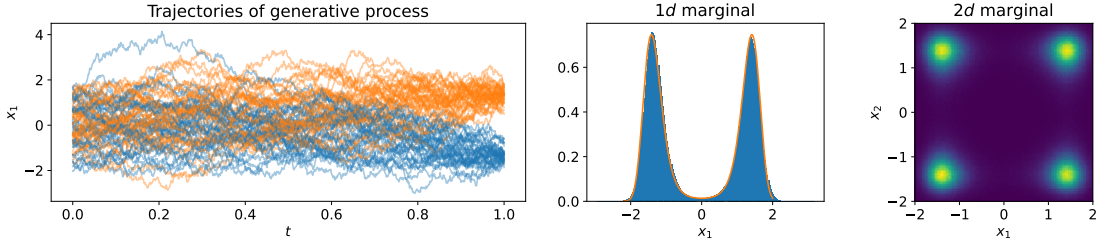

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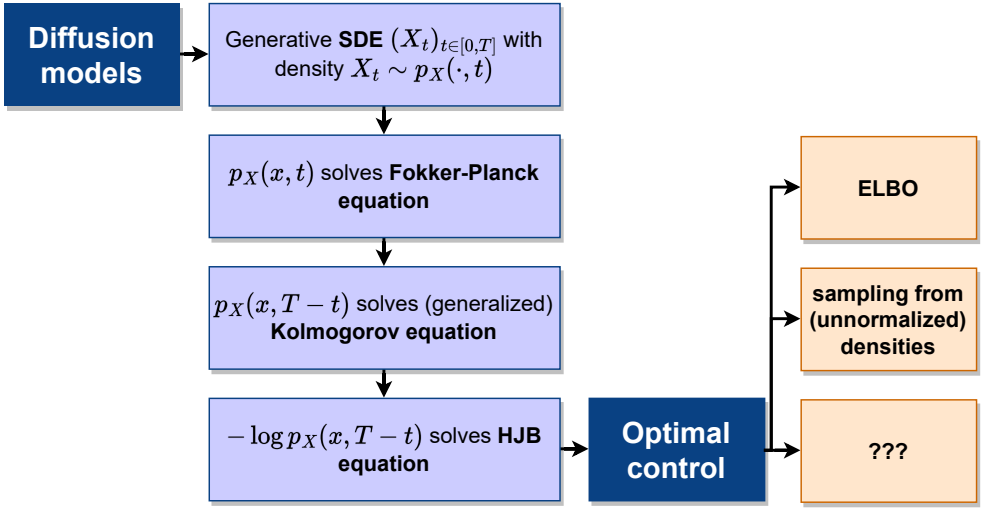

# Thank you for your attention!

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