Stochastic Differential Equations for Generative Modeling

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We would like to thank Anton Bolychev for contribution in this work

TASK

I. Reproduce results for Score-based Generative Modelling through stochastic differential equations with CIFAR dataset

II. Train GANs as energy based models (EBM-GAN) — train with comparable architectures

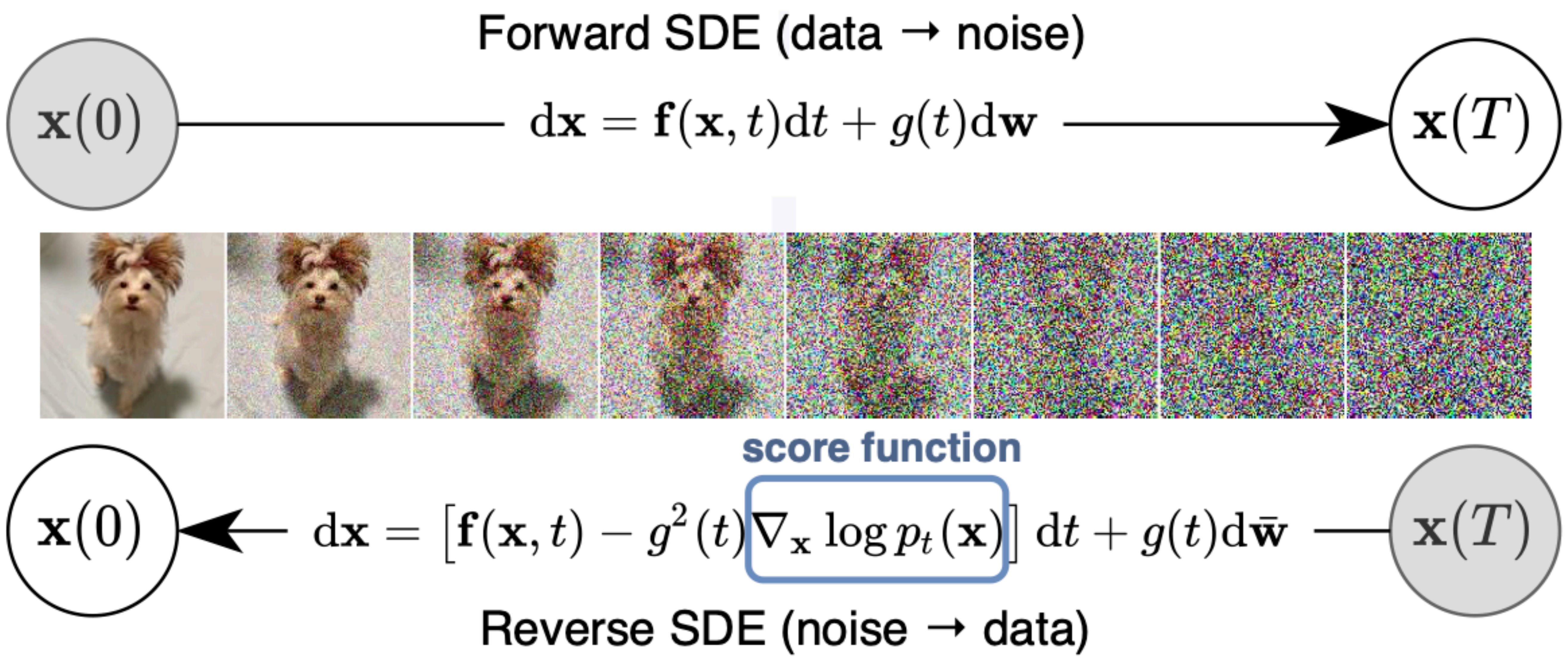
III. Compare DDPM/SMLD experiments with EBM-GAN

PROBLEM TO SOLVE

- **sampling techniques are inefficient**
- **decreased quality of image generation**

Task 1 DDPM/SMLD reproduction

SCORE-BASED GENERATIVE MODELING THROUGH STOCHASTIC DIFFERENTIAL EQUATIONS with CIFAR



01.

Forward SDE

Transforming data to a simple noise distribution with a continuous-time SDE

02.

Reverse SDE

Generating images from the noise based on denoising diffusion probabilistic models (DDPM)

Source: https://openreview.net/pdf?id=PxTIG12RRHS

Background & approaches

1st approach

Denoising score matching with Langevin dynamics (SMLD)

2nd approach

Denoising diffusion probabalistic models

NOISE CONDITIONAL SCORE

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \boxed{\sigma_i^2} \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{p_{\sigma_i}(\tilde{\mathbf{x}}|\mathbf{x})} \big[\| \mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}, \sigma_i) - \nabla_{\tilde{\mathbf{x}}} \log p_{\sigma_i}(\tilde{\mathbf{x}} \mid \mathbf{x}) \|_2^2 \big].$$

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{N} \boxed{(1-\alpha_i)} \mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{p_{\alpha_i}(\tilde{\mathbf{x}}|\mathbf{x})} [\| \mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}, i) - \nabla_{\tilde{\mathbf{x}}} \log p_{\alpha_i}(\tilde{\mathbf{x}} \mid \mathbf{x}) \|_2^2].$$

SAMPLES GENERATION

$$\mathbf{x}_i^m = \mathbf{x}_i^{m-1} + \epsilon_i \mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_i^{m-1}, \sigma_i) + \sqrt{2\epsilon_i}\mathbf{z}_i^m, \quad m = 1, 2, \cdots, M,$$

$$\mathbf{x}_{i-1} = \frac{1}{\sqrt{1-\beta_i}}(\mathbf{x}_i + \beta_i \mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_i, i)) + \sqrt{\beta_i}\mathbf{z}_i, \quad i = N, N-1, \cdots, 1.$$

$$\mathbf{x}_N \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

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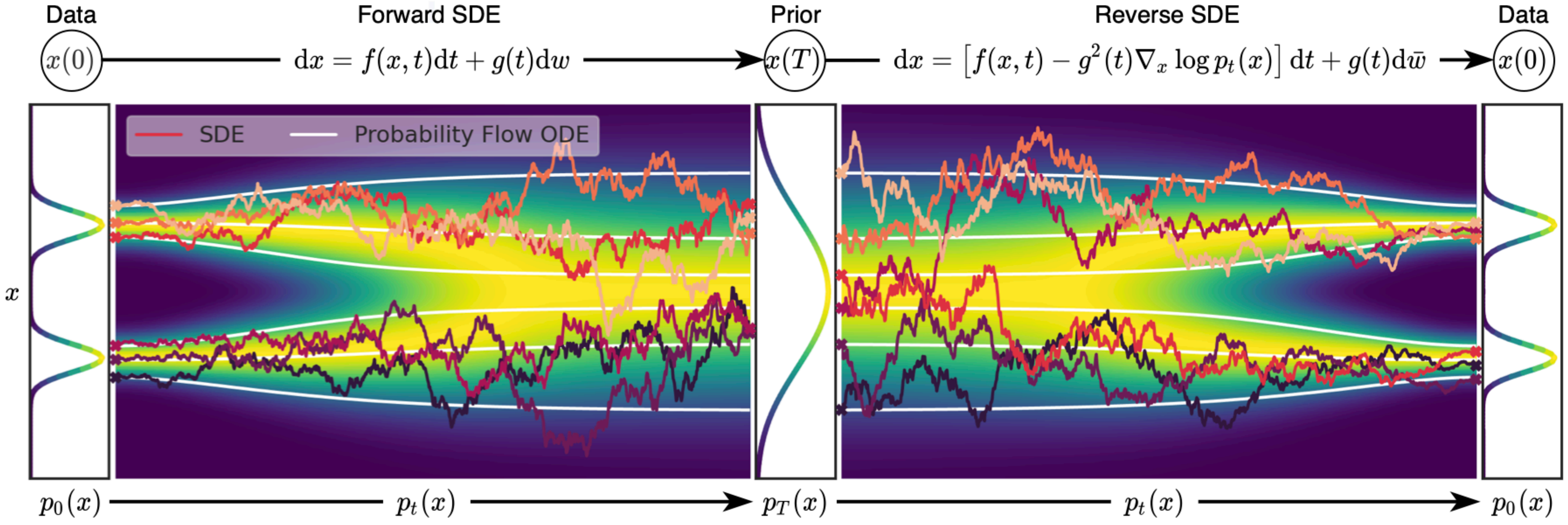
DDPM / SMLD reproduction solution

01. Noise distribution

data mapping with SDE

02. Generative modelling

back reverse SDE



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Combination of approaches

The noise perturbations used in SMLD and DDPM can be regarded as discretizations of two different

1st approach

$$\mathrm{d}\mathbf{x} = \sqrt{\frac{\mathrm{d}\left[\sigma^2(t)\right]}{\mathrm{d}t}}\mathrm{d}\mathbf{w}.$$

2nd approach

$$\mathrm{d}\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}\,\mathrm{d}t + \sqrt{\beta(t)}\,\mathrm{d}\mathbf{w}. \qquad N \to \infty,$$

$$\mathrm{d}\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}\,\mathrm{d}t + \sqrt{\beta(t)(1 - e^{-2\int_0^t \beta(s)\mathrm{d}s})}\mathrm{d}\mathbf{w}.$$

perform particularly well on likelihoods

Source: https://openreview.net/pdf?id=PxTIG12RRHS

Research Task

GANs as energy based models (EBM-GAN)

Task

Implement Lagevin dynamics for generation from latent noise space

Goals:

- Implement Langevin dynamics
- Evaluate it using Fréchet Inception Distance

Solution

Implemented computation of energy for pre-trained DCGAN

Source: https://arxiv.org/pdf/2003.06060.pdf

Research Task Conducted experiments (EBM-GAN)

Steps

- **Langevin dynamics** is implemented into the pre-trained GAN

$$E(z) = -\log p_0(z) - d(G(z))$$

$$x_{i+1} = x_i - \frac{\epsilon}{2}\nabla_x E(x) + \sqrt{\epsilon}n, n \sim N(0, I)$$

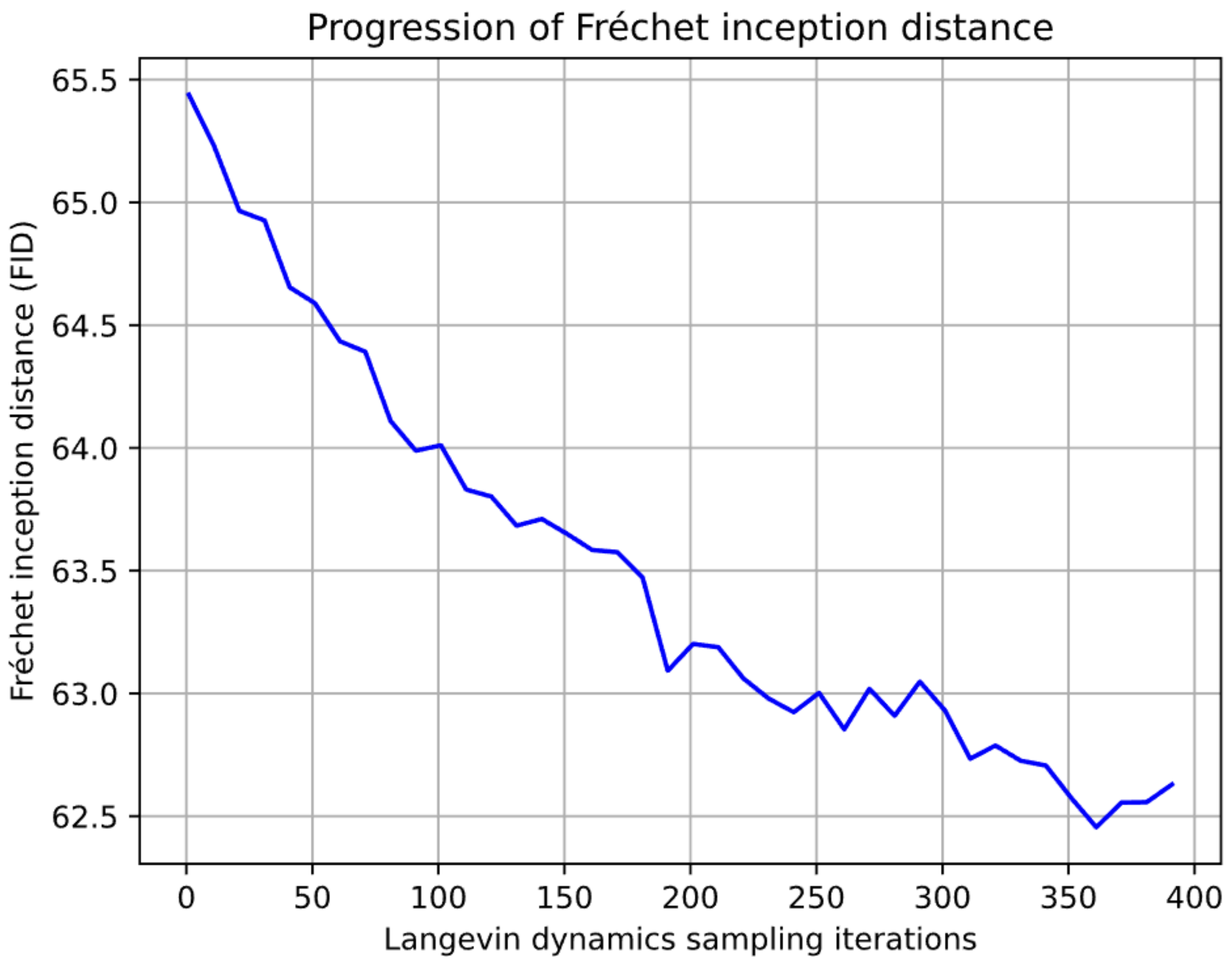
- Obtained results were tasted with Fréchet inception distance

$$d_F(\mathcal{N}(\mu, \Sigma), \mathcal{N}(\mu', \Sigma'))^2 = \|\mu - \mu'\|_2^2 + \operatorname{tr}\left(\Sigma + \Sigma' - 2\left(\Sigma^{\frac{1}{2}} \cdot \Sigma' \cdot \Sigma^{\frac{1}{2}}\right)^{\frac{1}{2}}\right)$$

Results

- Langevin dynamics was implemented
- Expected behaviour of FID curve was observed

Github repo with code and experiments



Source: https://arxiv.org/pdf/2003.06060.pdf

Replication Task

Langevin dynamics for score-based models

Task

Replicate and compare results for predictor and predictor-corrector sampling approaches using different SDE solvers

Solution

Build a pipeline for ancestral sampling and reverse diffusion probability flow

Source: https://arxiv.org/pdf/2003.06060.pdf

Thank you for you attention!

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