Advanced Machine Learning

SCORE-BASED GENERATIVE MODELING THROUGH STOCHASTIC DIFFERENTIAL EQUATIONS

by Yang Song et al.

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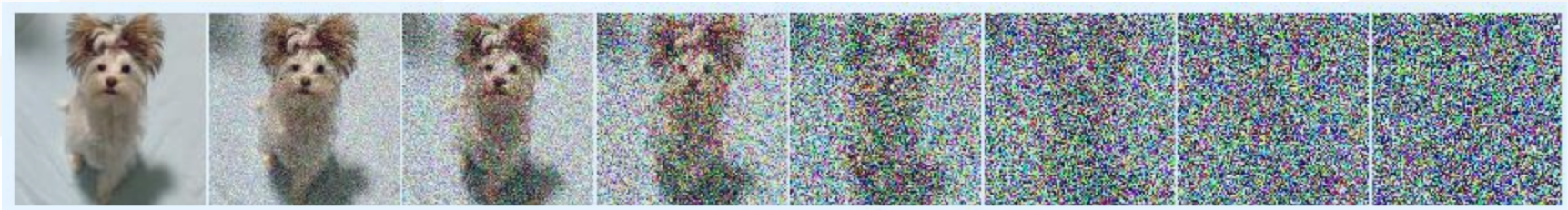
Motivation of generative modeling

- What is it?
- Why do we need it?
- A bit of history (GAN's, VAE's, ...)

Generative Modeling

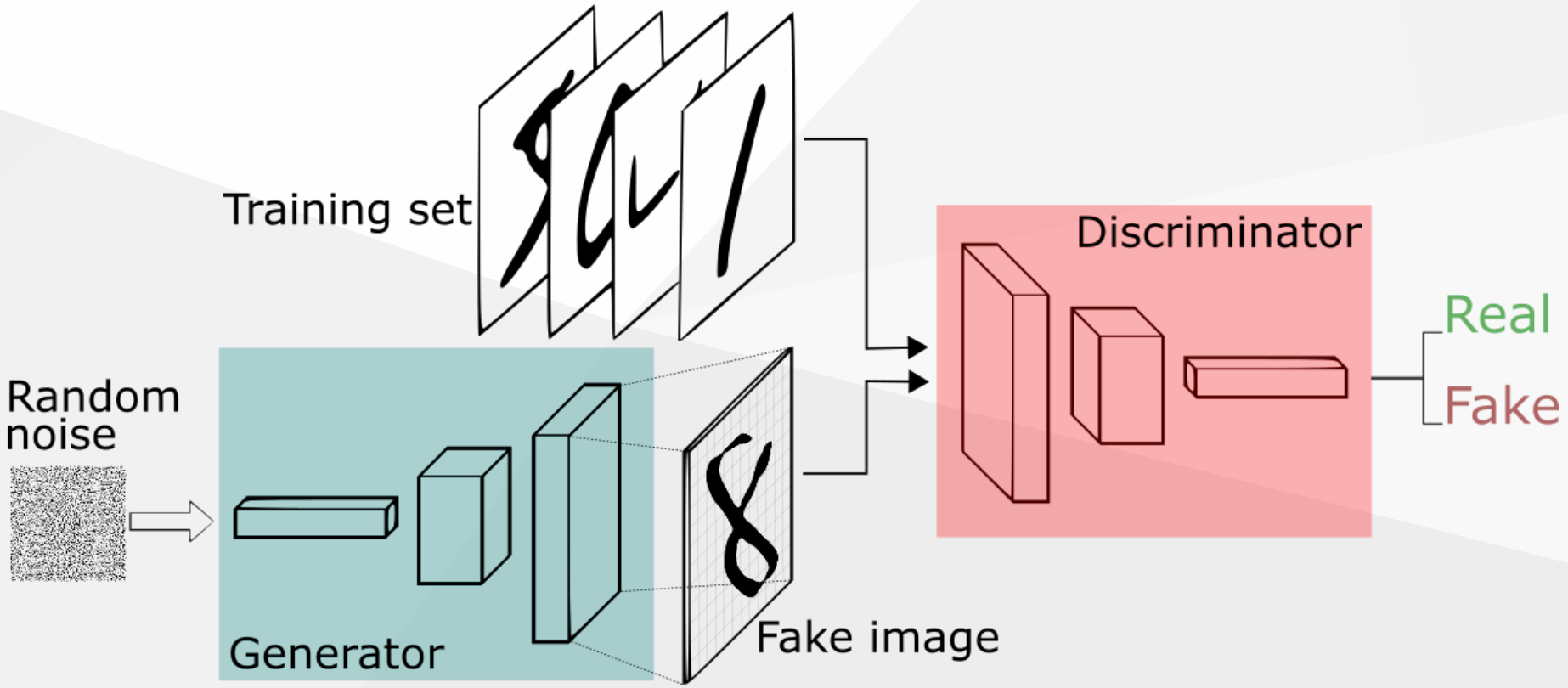


Process of generating data from noise.

- Data augmentation
- Anomaly detection
- Image/Audio synthesis
- Colorization
- ...

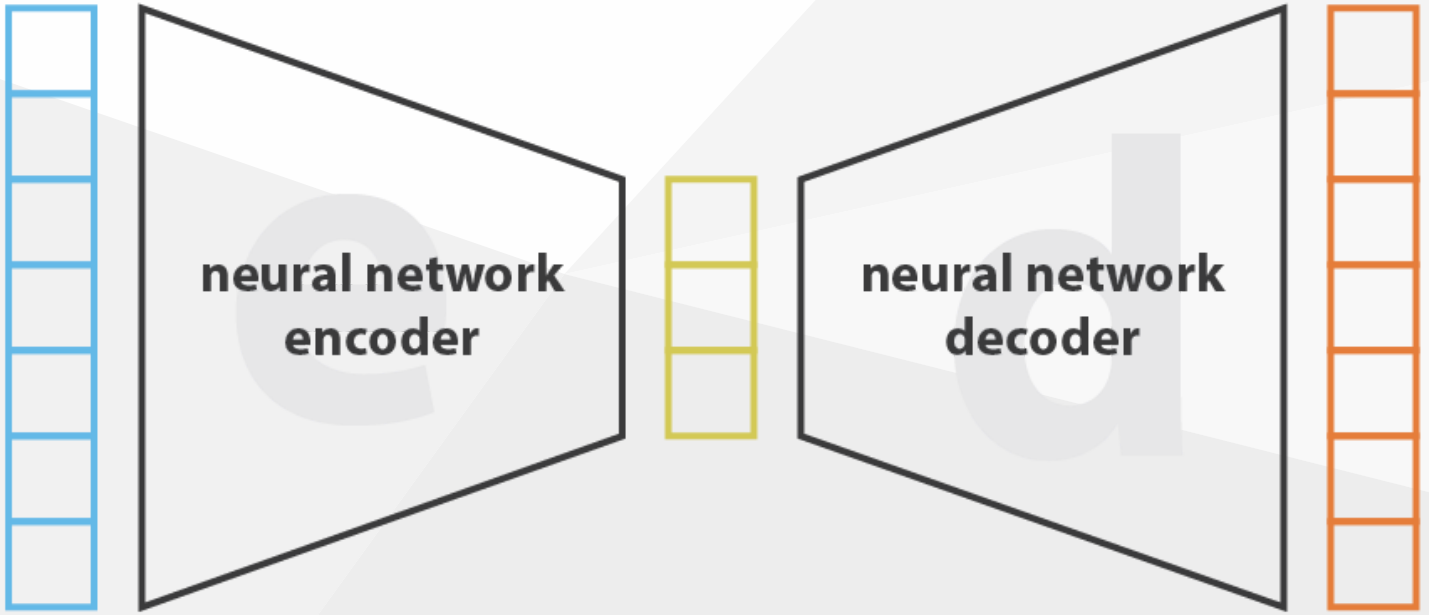
GANs and VAEs

Generative adversial networks (GANs)



GANs and VAEs

Variational autoencoders (VAEs)



Related work

Related work 1 : Generative Modeling by Estimating Gradients of the Data Distribution (Song et al.)

Contributions : Generate synthetic data through annealed Langevin Dynamics

Related work 1 : Denoising Diffusion Probabilistic Models (Ho et al.)

Contributions : Generate synthetic data through diffusion models

Related work 1

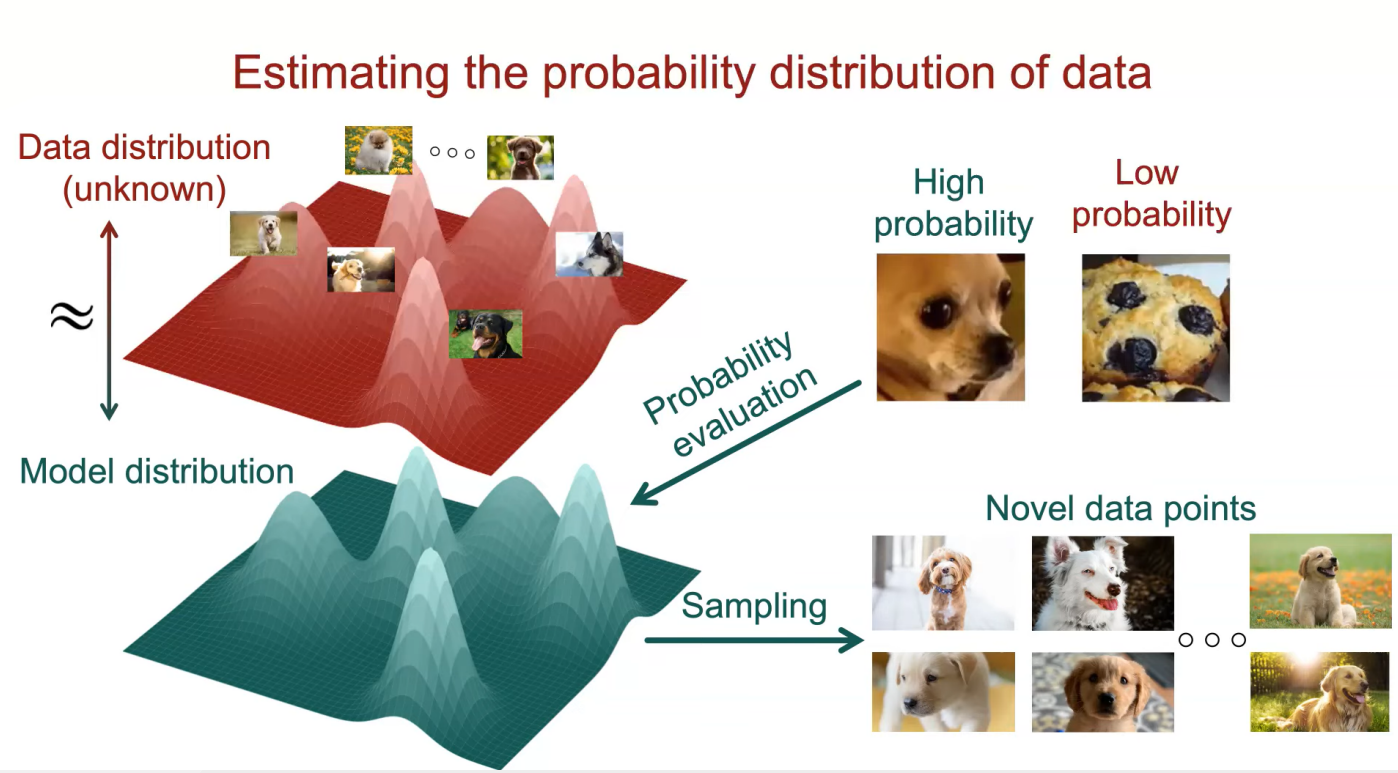
Goal of the paper : Answer the following question

How would you generate new data given a data set of i.i.d samples $\{\mathbf{x}_i \in \mathcal{R}^D\}_{i=1}^N$ drawn from an unknown data distribution $p_{data}(\mathbf{x})$?

Related work 1

PDF modelling

Simple idea : Model the data distribution



PDF modelling

Data distribution is very complex and high dimensional -> Use a deep NN for the density $f_\theta(\mathbf{x})$.
Since NN is not defined positive we model the data distribution by :

$$p_\theta(\mathbf{x}) = \frac{e^{f_\theta(\mathbf{x})}}{Z_\theta}$$

And thus

$$Z_\theta = \int e^{f_\theta(\mathbf{x})} \mathbf{dx}$$

PDF modelling

Problem : this integral is completely ***intractable*** as it integrates over all possible images

Solution : Get rid of the normalization constant by taking the gradient of the log-density

$$\nabla_{\mathbf{x}} log(p_\theta(\mathbf{x})) = \nabla_{\mathbf{x}} f_\theta(\mathbf{x}) - \nabla_{\mathbf{x}} log(Z_\theta) = \nabla_{\mathbf{x}} f_\theta(\mathbf{x})$$

The normalization constant is gone and we no longer have a direct access to the distribution but we now have the score

Langevin Dynamics

Sampling from high-density regions can be done by following the score.

Idea : Start from a random position in the sample space and follow the score until you arrive at a high-density region, sort of a gradient ascent in the image space.

Langevin dynamics :

$$x_{t+1} = x_t + \frac{\epsilon_t}{2} \nabla_x \log p(x_t) + \sqrt{\epsilon_t}\, z_t$$

We simply need a good score approximator to generate samples!

Score estimation

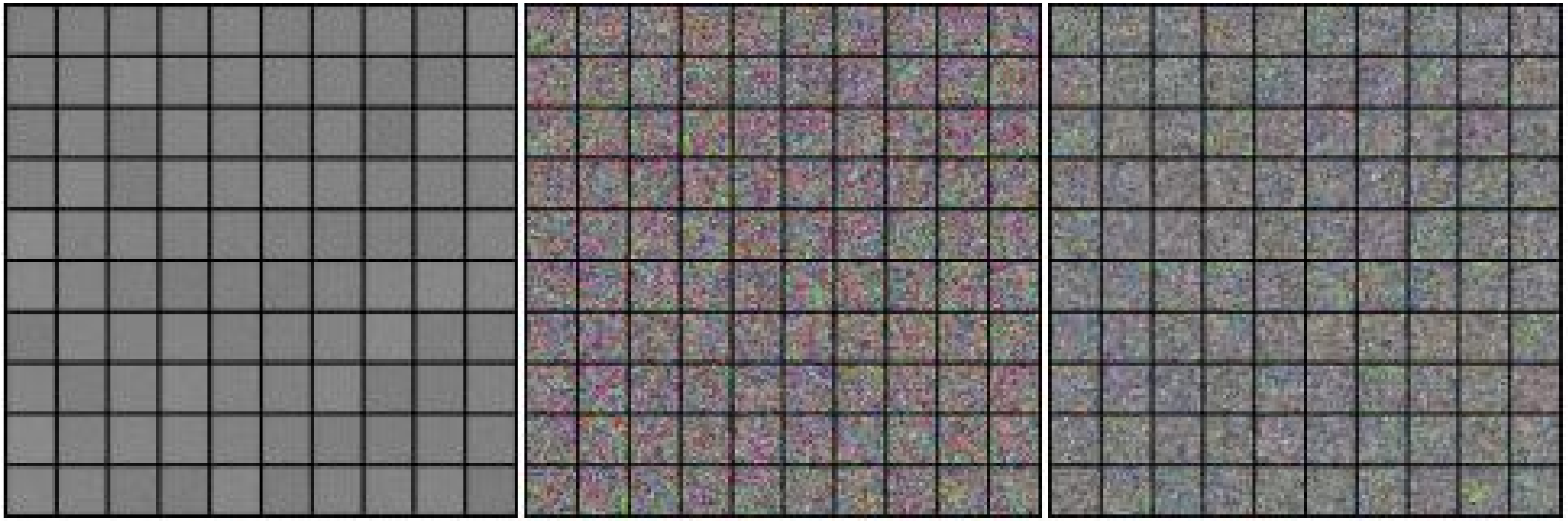
Let $s_\theta(\mathbf{x}) \approx \nabla_\mathbf{x} log(p_\theta(\mathbf{x}))$ be a NN where $s_\theta(\mathbf{x}) : \mathcal{R}^D \rightarrow \mathcal{R}^D$
We minimize the $\mathcal{L}_2$ norm of the vector difference, so-called "Fisher divergence"

$$\theta^* = \underset{\theta}{argmin} E_{p_{data(x)}}[\|\nabla_\mathbf{x} log(p_\theta(\mathbf{x})) - s_\theta(\mathbf{x})\|_2^2]$$

We do not know the true $\nabla_\mathbf{x} log(p_\theta(\mathbf{x}))$ but Hyvärinen showed this objective is equivalent to

$$\theta^* = \underset{\theta}{argmin} E_{p_{data(x)}}[tr(\nabla_\mathbf{x} s_\theta(\mathbf{x})) + \|\frac{1}{2} s_\theta(\mathbf{x})\|_2^2]$$

Results

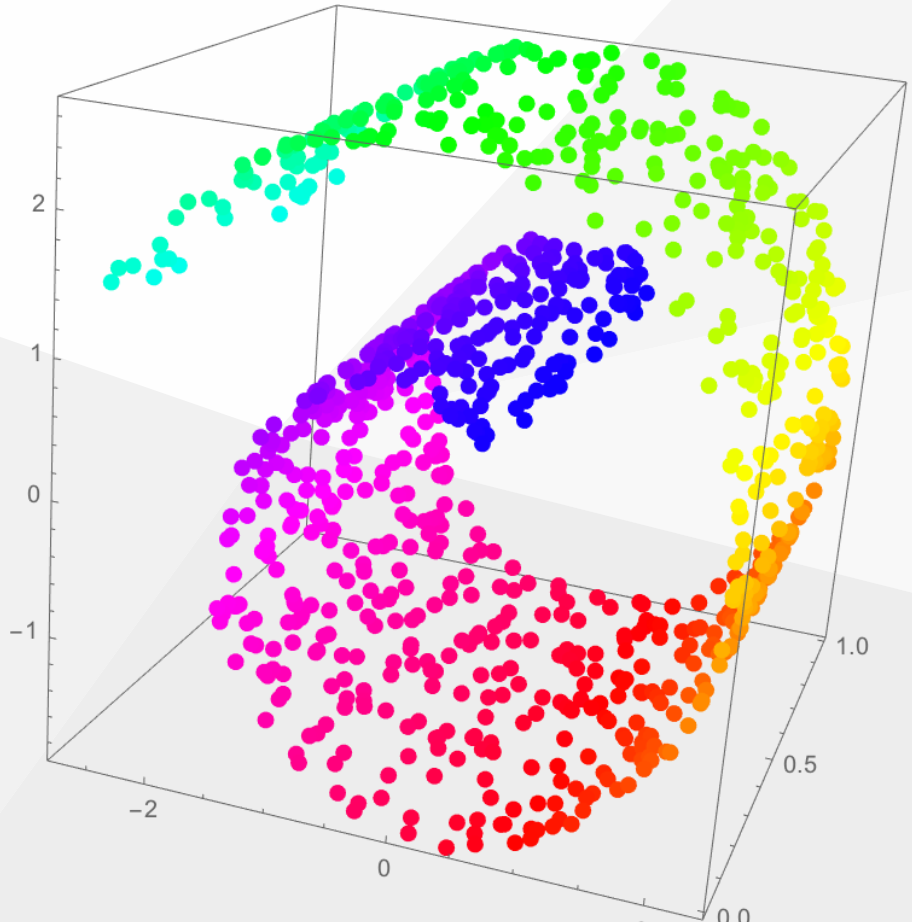


(a) MNIST (b) CelebA (c) CIFAR-10

Figure 7: Uncurated samples on MNIST, CelebA, and CIFAR-10 datasets from the baseline model.

Pitfalls

Manifold hypothesis : high-dimensional data lie on low-dimensional manifolds within the high-dimensional space.

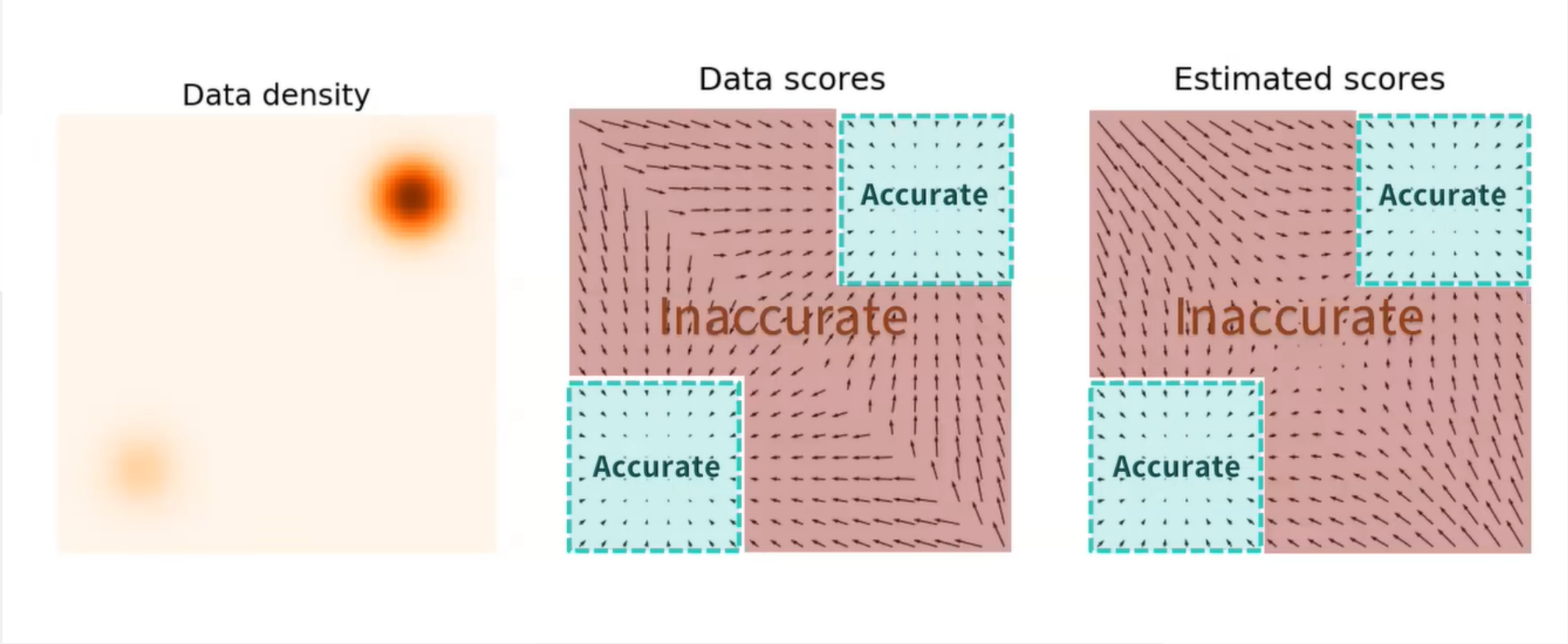


Pitfalls

Our data set samples occupy an absurdly small fraction of the space thus our score is a good approximation almost nowhere.
Why ?

- The noisy samples that occupy the space are not part of the Monte-Carlo expectation approximation
- Inaccurately approximating the score in their neighbourhood is thus not a big deal

Pitfalls


Data density
Data scores
Accurate
Inaccurate
Accurate
Estimated scores
Accurate
Inaccurate
Accurate

Solution

ADDING SEVERAL LEVELS OF NOISE to enlarge the support of the distribution

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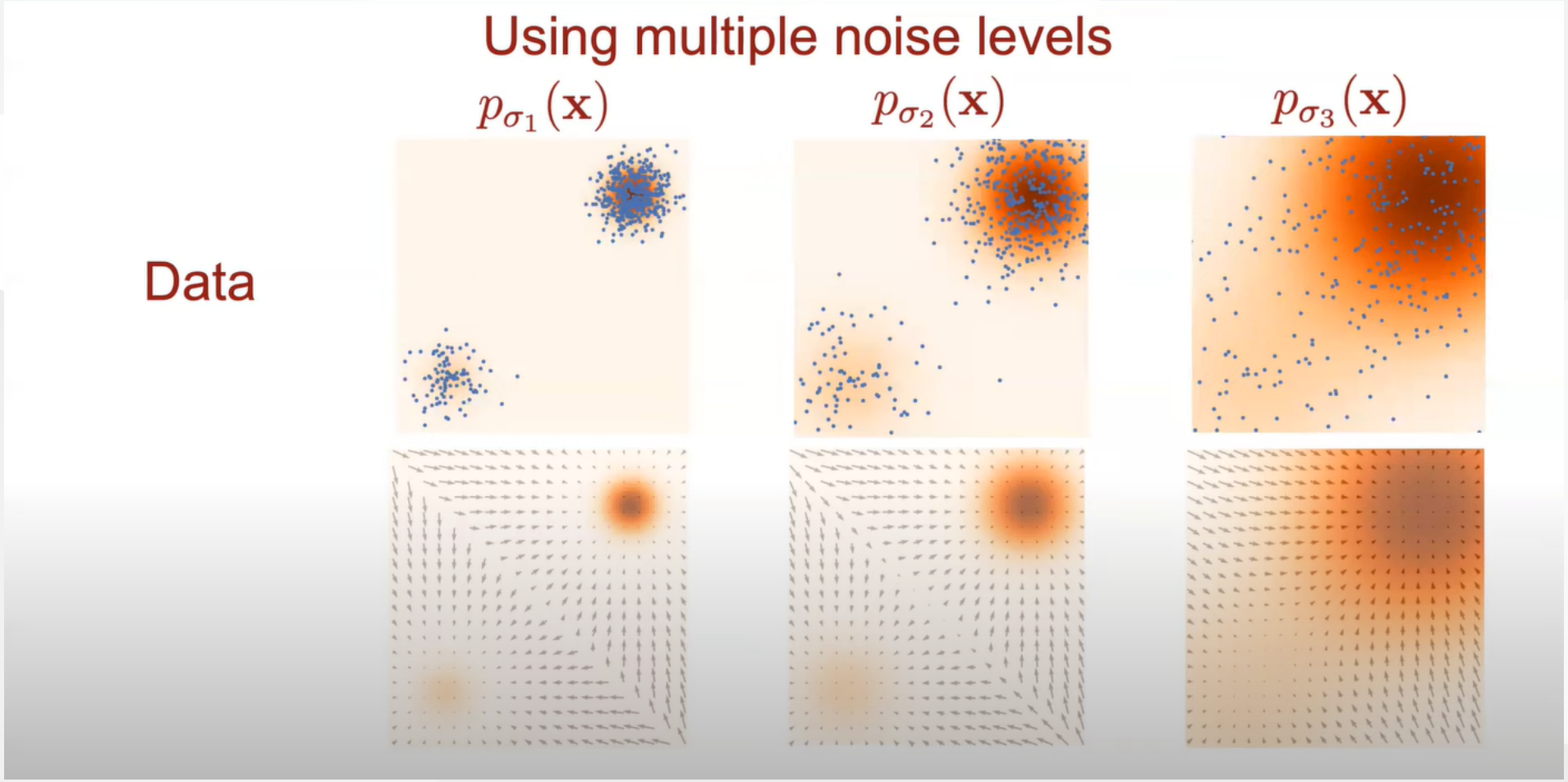
Annealed Langevin Dynamics



Results

(a) MNIST (b) CelebA (c) CIFAR-10

Figure 5: Uncurated samples on MNIST, CelebA, and CIFAR-10 datasets.

Far better than before

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Related work 2

Goal of the paper : Answer the following question

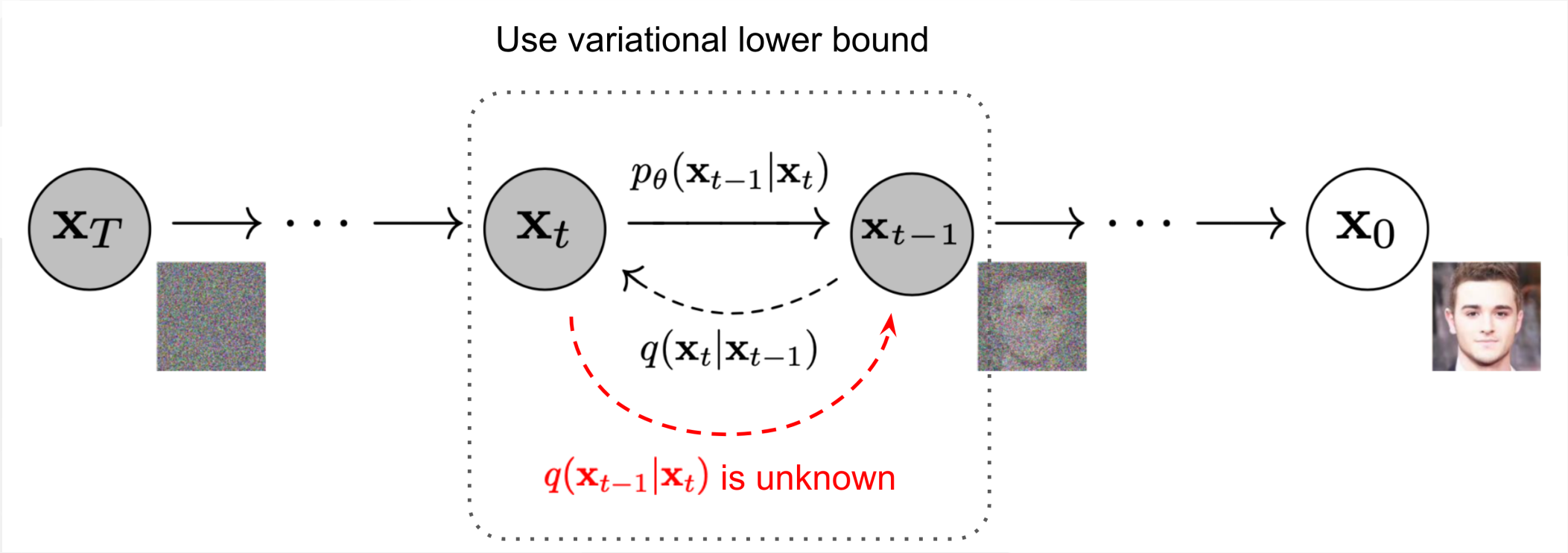
How would you generate new data given a data set of i.i.d samples $\{\mathbf{x}_i \in \mathcal{R}^D\}_{i=1}^N$ drawn from an unknown data distribution $p_{data}(\mathbf{x})$?

Big picture

Diffusion models aim at learning the reverse of the noise generation procedure :

- Forward process : Add noise to the original sample x_0 such that converges to x_T gaussian
- Backward process : Recover the original sample from the noise

Big picture



source : "https://lilianweng.github.io/posts/2021-07-11-diffusion-models/"

How it works

We consider a sequence of positive increasing noise scales and for each data point we construct a discrete markov chain $\{x_0, x_1, x_2, \ldots, x_T\}$ such that x_T can be considered fully gaussian for large T.

The backward process defines a variational Markov chain in the reverse direction that constructs $\{x_T, x_{T-1}, \ldots, x_1, x_0\}$ such that they are sampled from $p_\theta(x_{t-1}|x_t)$

Markov chains definition

The forward process is defined by :
$q(x_t|x_{t-1}) = N(x_t; \mu_t = (1-\beta_t)x_{t-1}, \Sigma_t = \beta_t I)$

The backward process is defined by :
$p_\theta(x_{t-1}|x_t) = N(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$

Ideally we would like our model $p_\theta(x_{t-1}|x_t)$to learn the distribution $q(x_{t-1}|x_t)$.

Note : by Bayes $q(x_{t-1}|x_t)$ is intractable.

Training

What loss to use between distributions ? KL divergence

Loss : $E_q[D_{KL}(q(x_{t-1}|x_t, x_0)||p_\theta(x_{t-1}|x_t))]$

Or equivalently

$$E_{x_0,\epsilon,t}[||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\epsilon, t)||^2]$$

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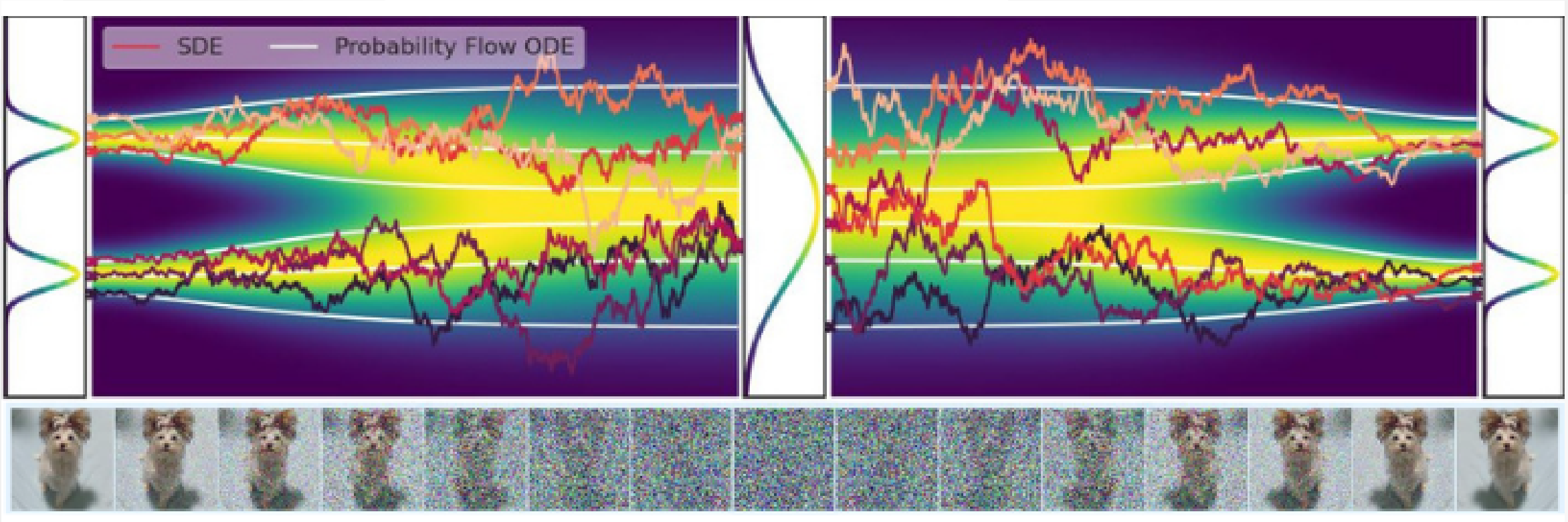
Back to our paper



Stochastic Differential Equations

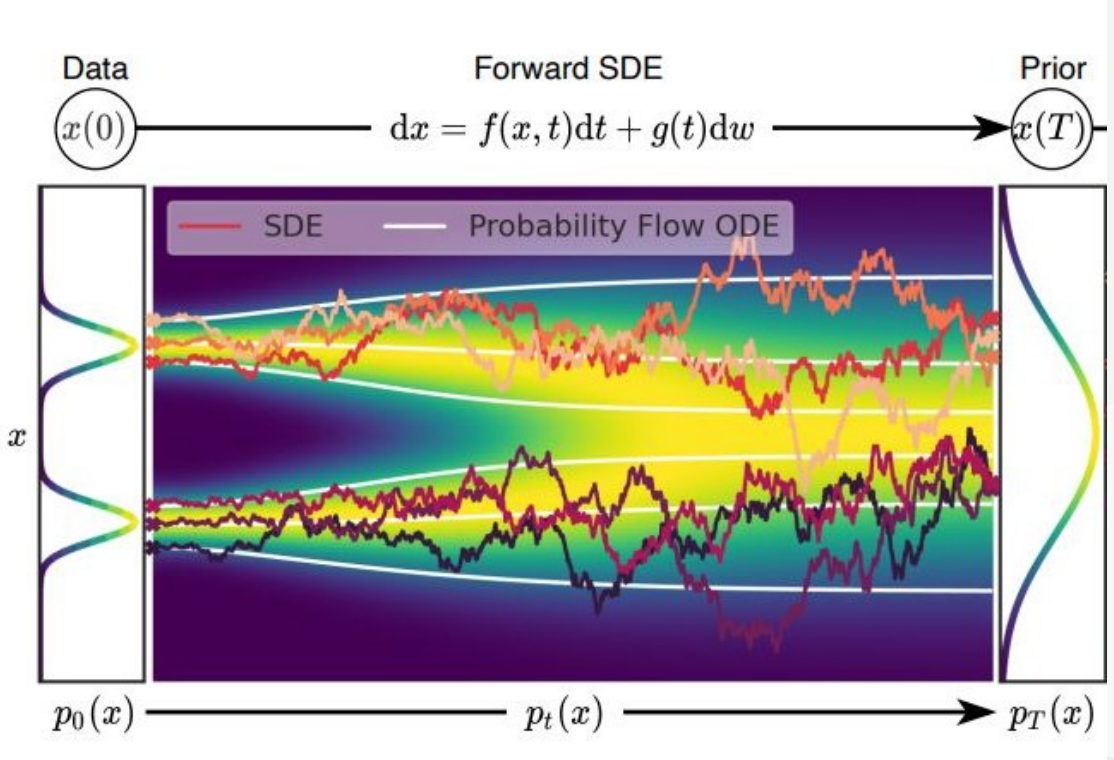
Diffusion Process

$$\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t) + g(t)\mathrm{d}\mathbf{w}$$

with :

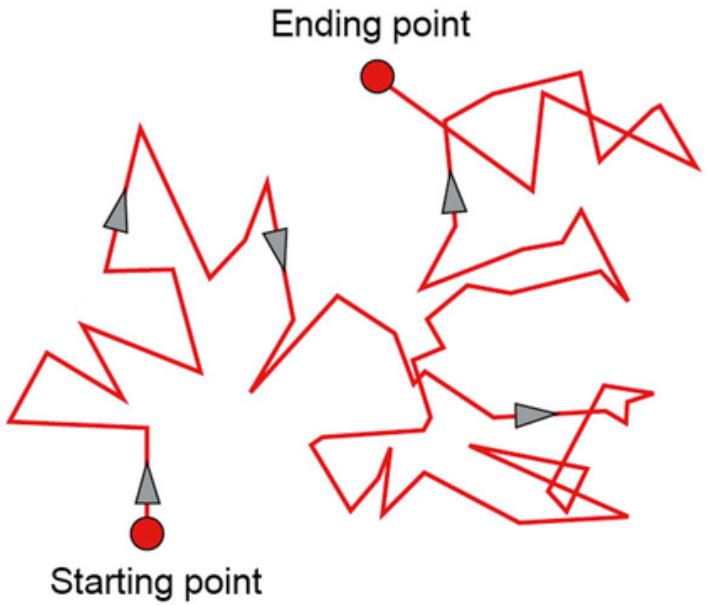
- $\mathbf{w}$ the standard Weiner process (Brownian motion),
- $\mathbf{f}(\,.\,, t) : \mathbb{R}^d \to \mathbb{R}^d$ the drift coeffitient of $x(t)$
- $g(\,.\,) : \mathbb{R} \to \mathbb{R}$ diffusion coefficient

Diffusion process



- p_0 is data distribution
- p_t is the prior distribution

Brownian Motion



A particule that is particle changing directions randomly after every collision

Anderson Backward process

Forward SDE : maps $p_{data}(x)$ -> $p_{prior}(x)$

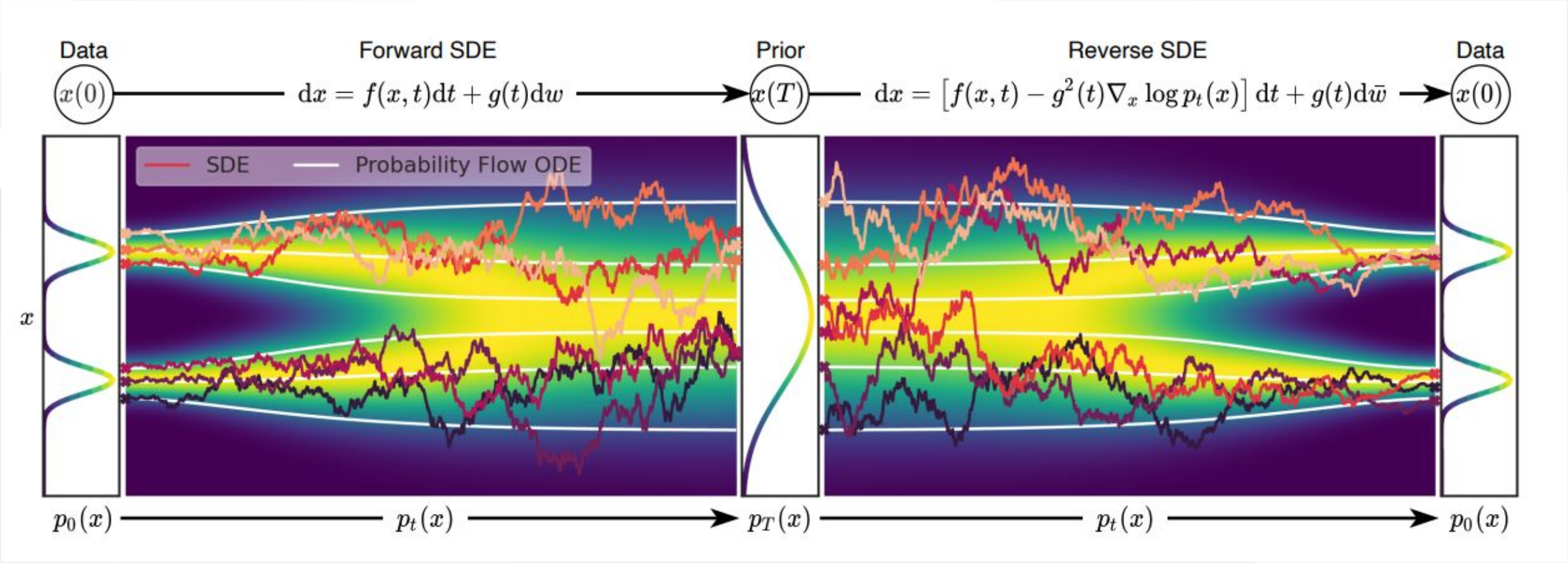
$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t)dt + g(t)d\mathbf{w}$$

Anderson showed there exists a corresponding SDE that goes in the opposite direction.

Reverse-time SDE : maps $p_{prior}(x)$ -> $p_{data}(x)$

$$d\mathbf{x} = [\mathbf{f}(\mathbf{x}, t) - g(t)^2 \nabla_{\mathbf{x}} log(p_t)]dt + g(t)d\bar{\mathbf{w}}$$

2 SDE's



WARNING : THE SDE'S MAP DISTRIBUTION NOT SAMPLES

Estimating the score

Generating samples requires knowing the score of each marginal distribution but once again we don't have it. We thus resort to estimation.

Problem : The marginal $p_t(x_t)$ is once again intractable but the conditional $p_t(x_t|x_0)$ is fully tractable, why ? It vastly reduces the set of trajectories to consider and we have a closed form for the conditionnal.

Estimating the score

Theorem : Any SDE with affine drift function f(x,t) has a gaussian transition kernel $p_{t+1}(x_{t+1}|x_t)$.[Section 5.5 in Särkkä & Solin (2019)]

Consequence : $p_t(x_t|x_0)$ is gaussian as well by a property of gaussians.

Estimating the score

Considering a score network $\mathbf{s}_\theta(x, t)$:

$$\theta^* = \arg\min E_t E_{x_0} E_{x_t|x_0}[\lambda(t)||\mathbf{s}_\theta(x,t) - \nabla_{x_t} log p_t(x_t|x_0)||^2$$

Training is a 4-step procedure :

- Sample a timestep in [0,T] and an image x_0
- Diffuse it either by simulating the SDE or by the underling gaussian kernel
- Compute the loss
- Backpropagate

Conditionnal and marginal score

Even though we approximate the conditional score, at optimality $s_\theta(x,t) = \nabla_x log(p_t(x))$, i.e, we approximated the marginal score.

Why ? For 2 reasons :

- We average over all x_0 of the data set
- The network is given a noisy sample x_t which could come from several x_0's, the network averages over these.

NB: $\lambda(t)$ thus has large importance

Unifying framework

How does this paper relate to the two papers reviewed in the related work section ?
In the first paper, the noise perturbation kernel $p_\sigma(x_i|x_{i-1})$ followed :

$$x_i = x_{i-1} + \sqrt{\sigma_i^2 - \sigma_{i-1}^2} z_{i-1}$$

Which can be written as the following SDE

$$dx = \sqrt{\frac{d\sigma^2(t)}{dt}} dw$$

Unifying framework

In the second paper, the noise perturbation kernel was given by the forward process $p_\beta(x_i|x_{i-1})$ followed :

$$x_i = \sqrt{1-\beta_i}x_{i-1} + \sqrt{\beta_i}z_{i-1}$$

Which can be written as the following SDE

$$dx = -\frac{1}{2}\beta(t)xdt + \sqrt{\beta(t)}dw$$

And sampling can be done for both by reversing the SDE and estimating the score.

Unifying framework

An interesting result in this framework : consider the training loss

$$E_t E_{x_0} E_{x_t|x_0} [\lambda(t) || \mathbf{s}_\theta(x,t) - \nabla_{x_t} log p_t(x_t|x_0)||^2$$

Reparametrization trick : $x_t = \gamma_t x_0 + \sigma_t \epsilon$

Score function :

$$\nabla_{x_t} log p_t(x_t|x_0) = -\nabla_{x_t} \frac{(x_t - \gamma_t x_0)^2}{\sigma_t^2} = -\frac{x_t - \gamma_t x_0}{\sigma_t^2} = -\frac{\gamma_t x_0 + \sigma_t \epsilon - \gamma_t x_0}{\sigma_t^2} = -\frac{\epsilon}{\sigma_t}$$

Under this SDE, the network is simply tasked to learn the added noise, as in DDPM.

Numerical solvers

Sampling can now be done by:

- Predictor method simply simulating the reverse-time SDE, equivalently, solving the SDE under a Euler-Maruyama scheme or even use a more advanced solver such as RK45.
- Predictor-Corrector method : the corrector refines the prediction of the predictor by taking advantage of known information

Numerical solvers

Specifically, the PC method takes advantage of the known score $\nabla_{x_t} log p_t(x_t)$.
The procedure is as follows :

1. Take a backward step according to the reverse-time SDE (temporally)
2. Take a few steps in the gradient direction to move towards high-density regions (geographically)

NB : Make the plane analogy

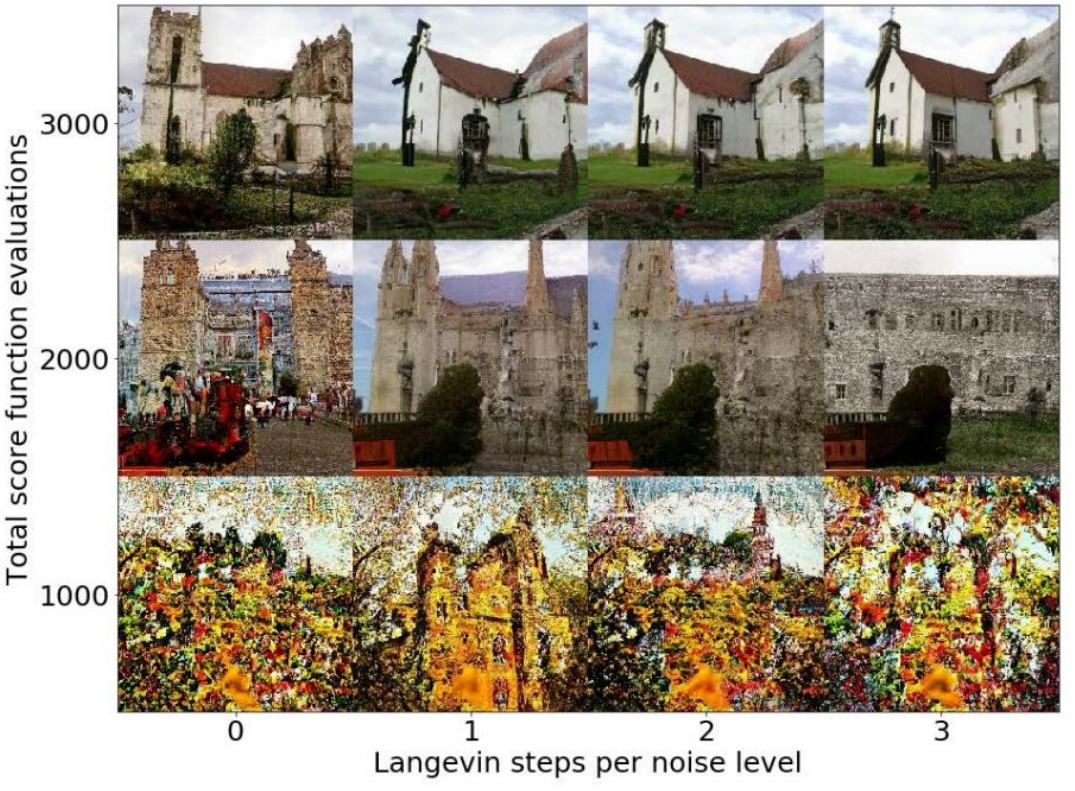
Numerical solvers

Quantitatively, in terms of FID score, the PC samplers outperfom the P samplers by a large margin

	Variance Exploding SDE (SMLD)				Variance Preserving SDE (DDPM)			
FID↓ Sampler / Predictor	P1000	P2000	C2000	PC1000	P1000	P2000	C2000	PC1000
ancestral sampling	4.98 ± .06	4.88 ± .06		**3.62 ± .03**	3.24 ± .02	3.24 ± .02		**3.21 ± .02**
reverse diffusion	4.79 ± .07	4.74 ± .08	20.43 ± .07	**3.60 ± .02**	3.21 ± .02	3.19 ± .02	19.06 ± .06	**3.18 ± .01**
probability flow	15.41 ± .15	10.54 ± .08		**3.51 ± .04**	3.59 ± .04	3.23 ± .03		**3.06 ± .03**

Numerical solvers

Qualitatively, the PC samplers outperform the P samplers



Numerical solvers

Predictor methods might be of poor quality and computationally suboptimal

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Probability flow ODE

Sare same marginal probability densities $\{p_t(\mathbf{x})\}_{t=0}^{T}$ as the SDE

$$\mathrm{d}\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2} g(t)^2 \nabla_{\mathbf{x}} \log p_t(\mathbf{x})\right] \mathrm{d}t,$$

$$\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) \longrightarrow \text{ score function of } p_t(\mathbf{x})$$

Approximation with score based model

$$\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) \approx \mathbf{s}_\theta(\mathbf{x}, t)$$

Probability flow ODE

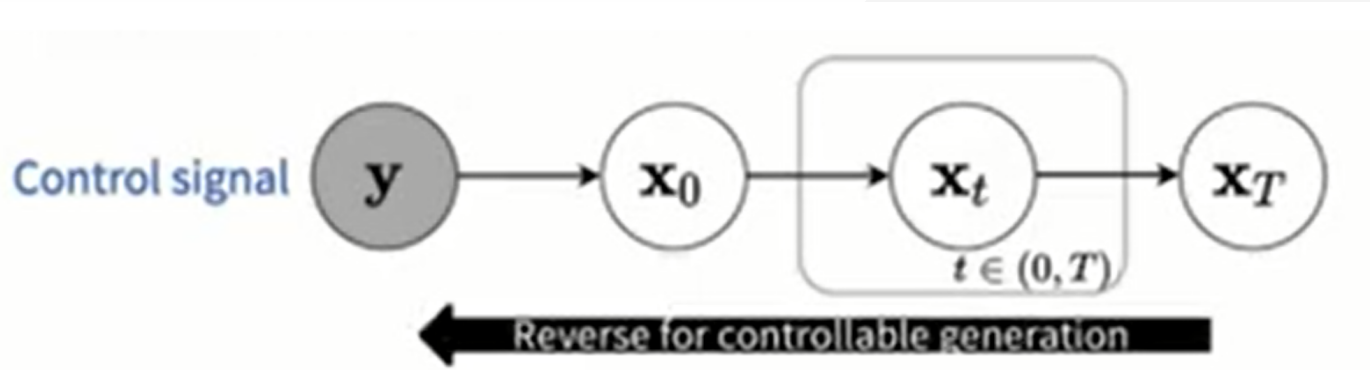
Approximation with score based model

$$\mathrm{d}\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - \frac{1}{2} g(t)^2 \mathbf{s}_\theta(\mathbf{x}, t)\right] \mathrm{d}t,$$

- Exact likelihood computation
- Manipulating latent representations
- Uniquely identifiable encoding
- Efficient sampling

Controllable generation

$\mathbf{y}$ is the controll signal



$$\mathrm{d}\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - g(t)^2 \nabla_{\mathbf{x}} \log p_t(\mathbf{x} \mid \mathbf{y})\right] \mathrm{d}t + g(t) \mathrm{d}\overline{\mathbf{w}}$$

- Unknown

Controllable generation

$$\mathrm{d}\mathbf{x} = \left\{\mathbf{f}(\mathbf{x}, t) - g(t)^2 \left[\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) + \nabla_{\mathbf{x}} \log p_t(\mathbf{y} \mid \mathbf{x})\right]\right\}\mathrm{d}t + g(t)\mathrm{d}\overline{\mathbf{w}}$$

- Unconditional score, same as before
- Trained separately or specified with domain knowledge

Controllable generation

$\mathbf{y}$ is the class label
$p_t(\mathbf{y} \mid \mathbf{x})$ is a time dependant classifier

Class conditional samples on 32x32 CIFAR10, automobiles on the left and horses on the right.

Controllable generation

$\mathbf{y}$ is the masked image
$p_t(\mathbf{y} \mid \mathbf{x})$ can be approximated without training

Impainting on 256x256 LSUN, first column is orginal image, second is masked image, remaining are sample image completions.

Controllable generation

$\mathbf{y}$ is the grey scale image
$p_t(\mathbf{y} \mid \mathbf{x})$ can be approximated without training

Colorization on 256x256 LSUN, first column is orginal image, second is grey scale image, remaining are sample image colorizations.

Critics

- A useful framework but many papers ignore it
- A well designed numerical solver
- Hardly computable likelihood without rough approximation