Score-Matching Models

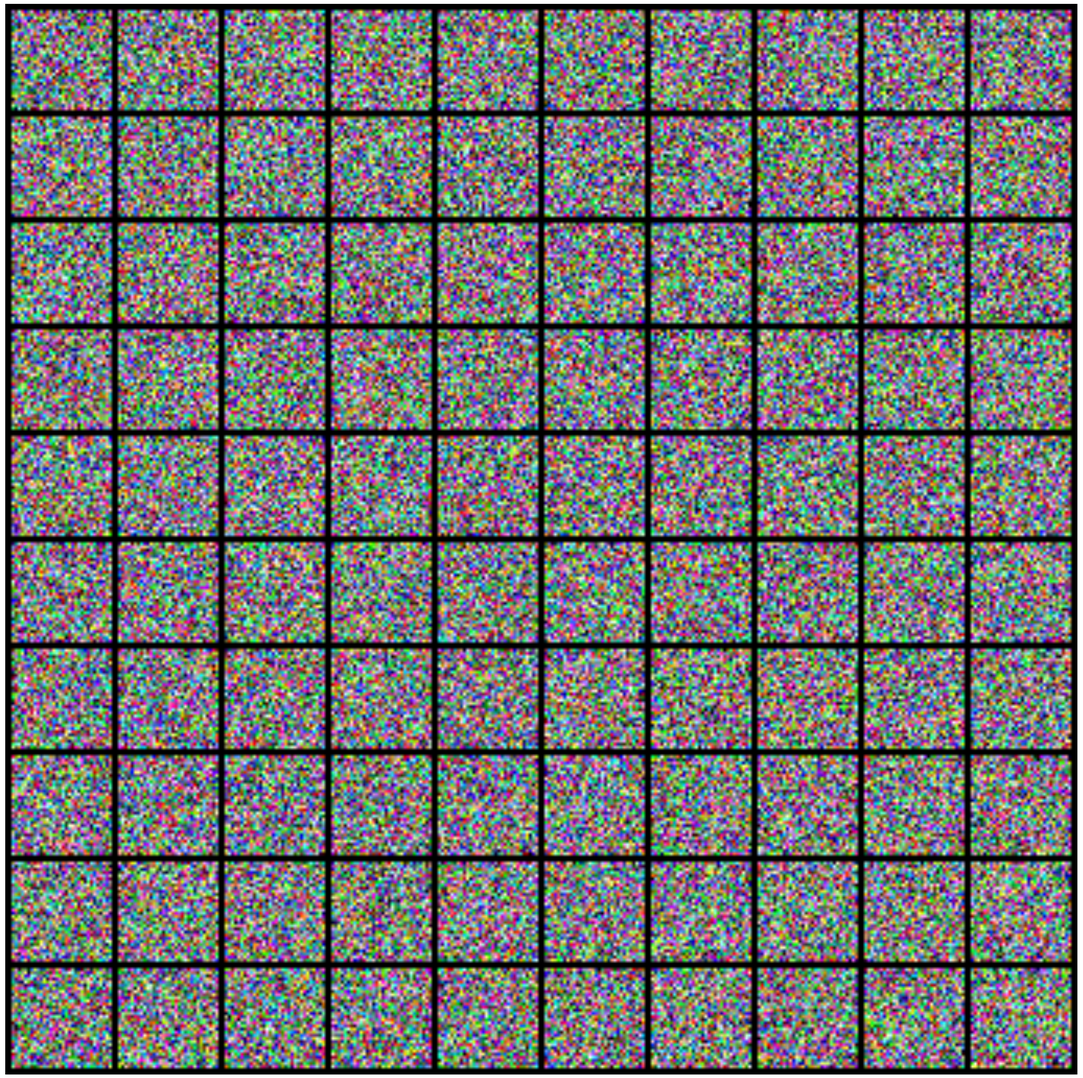
Deep Learning II - uvald2c.github.io

Efstratios Gavves - University of Amsterdam

Overview

Introduction to score-matching
Noise conditional score networks
Score-based generation via SDEs
Diffusion models

https://yang-song.github.io/blog/2021/score/



Tractability v. Flexibility

- In generative modelling there are two opposing forces: tractability and flexibility
- Tractable models are usually analytically computable, thus easy to evaluate and fit
- But they are usually not flexible enough to learn the true data structure
- Flexible models can fit arbitrary structures in data
- But they are usually expensive to evaluate, fit, or sample from

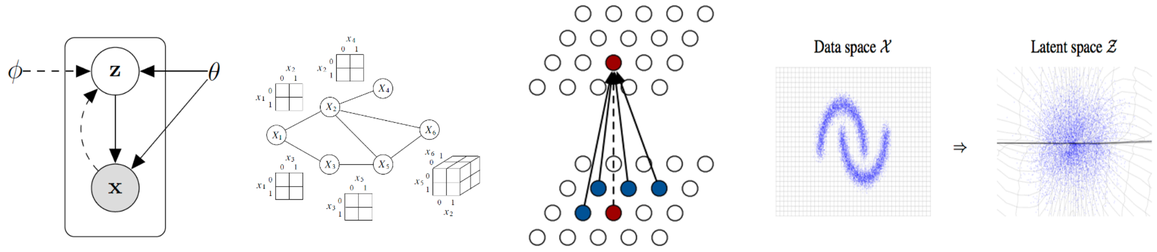
Overview of generative models

Likelihood-based generative models

Implicit generative models

Likelihood-based generative models

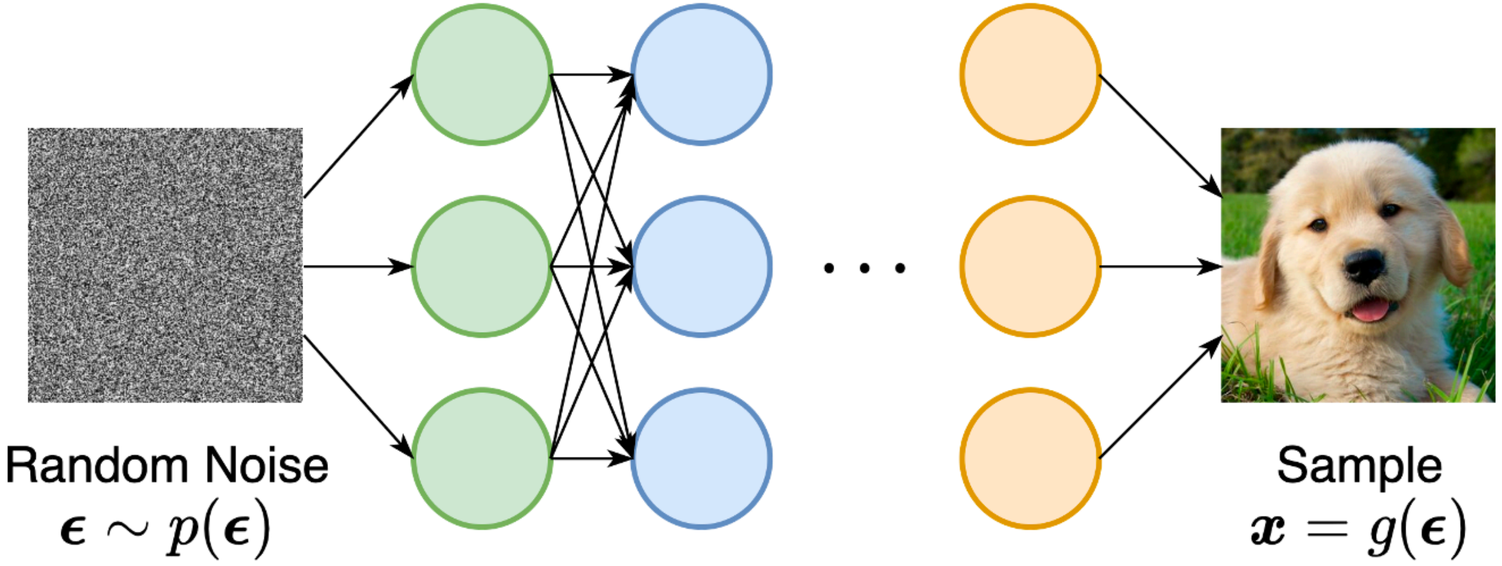
- Typically make strong assumptions to ensure tractability of likelihood
- Specifically of the normalising constant $Z(x)$ in $p(x) = \dfrac{\tilde{p}(x)}{Z(x)}$
- For instance, VAEs assume a tractable variational approximation
- Autoregressive models require causal convolutions
- Normalizing Flows require invertibility in the network architecture



Bayesian networks (e.g., VAEs) | MRF | Autoregressive models | Flow models

Implicit generative models

- Adversarial training for implicit generative models is very unstable
- Adversarial training leads often to mode collapse and reduced sampling variance
- Implicit generative models cannot compute likelihood of a sample, they just sample



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Score-based generative models

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- But they are usually expensive to evaluate, fit, or sample from
- <u>Diffusion/score-matching models are both tractable and flexible</u>

Score-matching

Energy-based models: a recap

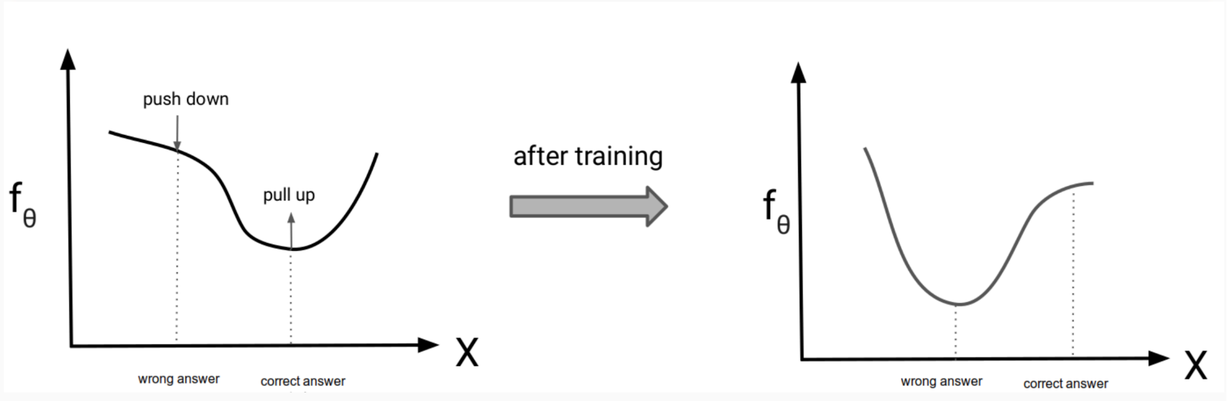
- Energy-based models $f_\theta(x)$ have likelihood

$$p_\theta(\mathbf{x}) = \frac{\exp(-f_\theta(\mathbf{x}))}{Z_\theta}$$

$$Z_\theta = \int \exp(-f_\theta(\mathbf{x}))dx$$

- We cannot ignore Z_θ during training as it also depends on parameters

- For general functions & architectures f_θ intractable to maximise wrt likelihood due to Z_θ



Stefano Ermon and Aditya Grover

Score-based models: impressive results

- Energy-based models with GAN-like quality in generation, while having the advantages of explicit probabilistic models
- Explicit likelihood computation
- Representation learning
- State-of-the-art results in generation, audio synthesis, shape generation, etc

Song et al., Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2021 (outstanding paper award)

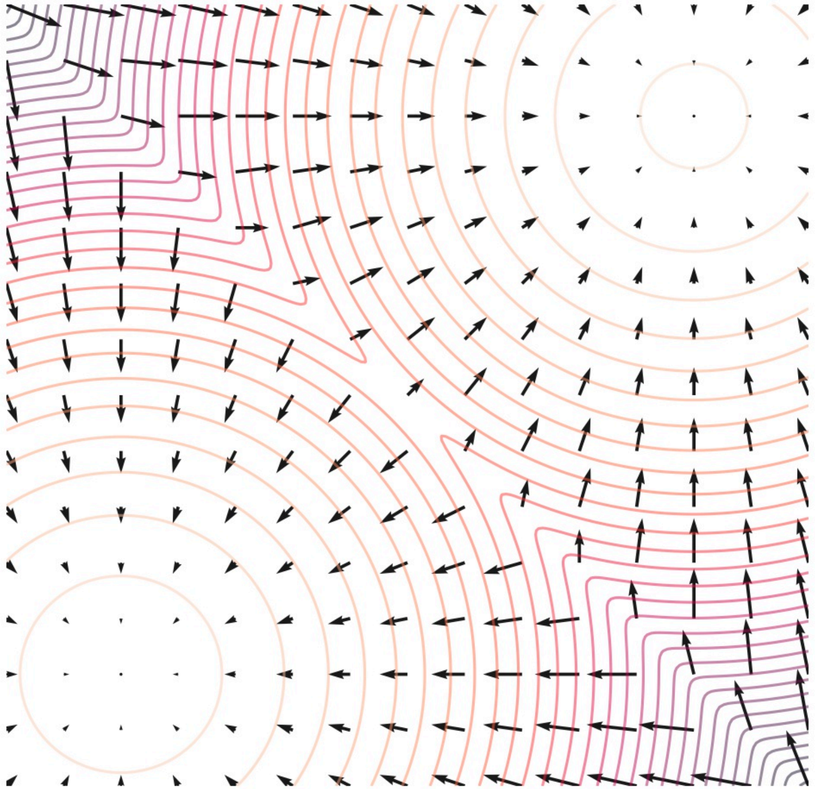
Score function

- The (Stein) score function is the gradient of the log-probability of a distribution w.r.t. to the input

$$\nabla_{\mathbf{x}} \log p(\mathbf{x})$$

- A model $s_\theta(x)$, which models the score function explicitly, is a score-based model

$$s_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p(\mathbf{x})$$



The score function of a mixture of two Gaussians

Score-based generative models

- The score function does not depend on the normalising constant Z_θ

$$s_\theta(\mathbf{x}) = \nabla_{\mathbf{x}} \log p(\mathbf{x}) = -\nabla_{\mathbf{x}} f_\theta(\mathbf{x}) - \underbrace{\nabla_{\mathbf{x}} \log Z_\theta}_{=0} = -\nabla_{\mathbf{x}} f_\theta(\mathbf{x})$$

- Thus we do not care if Z_θ is tractable or not
- What to optimise since score-based model outputs a vector representing gradients?
- Minimise the Fisher divergence ← optimal gradient/ground truth data score

$$\mathbb{E}_{p(\mathbf{x})} \| \nabla_{\mathbf{x}} \log p(\mathbf{x}) - s_\theta(\mathbf{x}) \|_2^2$$

Y. Song, S. Ermon, Generative Modeling by Estimating Gradients of the Data Distribution. NeurIPS 2019

Score-matching

- It can be shown* that optimising $\mathbb{E}_{p(\mathbf{x})}\|\nabla_{\mathbf{x}}\log p(\mathbf{x}) - s_\theta(\mathbf{x})\|_2^2$ is equivalent to

$$\mathbb{E}_{p_{data}(\mathbf{x})}\left[\mathrm{tr}\left(\nabla_{\mathbf{x}} s_\theta(\mathbf{x})\right) + \frac{1}{2}\|s_\theta(\mathbf{x})\|_2^2\right]$$

  up to some regularity conditions
- No dependence on ground truth score gradients
- Still, the trace of the Jacobian is too expensive for large networks and approximations are needed

* Estimation of Non-Normalized Statistical Models by Score Matching, Hyvarinen, 2005
Song et al., Sliced score matching: A scalable approach to density and score estimation, UAI 2019

Denoising score-matching

- Denoising score matching works well for small level of noise

$$\frac{1}{2}\mathbb{E}_{q_\sigma(\tilde{\mathbf{x}}|\mathbf{x})p_{data}(\mathbf{x})}\left[\left\|s_\theta(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}}\log q_\sigma(\tilde{\mathbf{x}}\,|\,\mathbf{x})\right\|_2^2\right]$$

where the data $\mathbf{x}$ is corrupted to $\tilde{\mathbf{x}}$ as $q_\sigma(\tilde{\mathbf{x}}) = \int q_\sigma(\tilde{\mathbf{x}}\,|\,\mathbf{x})p_{data}(\mathbf{x})\mathrm{d}\mathbf{x}$

- First sample a training example from the training set
- Then add noise to it from a pre-specified distribution
- You can repeat the process and average with Monte Carlo simulation (or do it once)

* Vincent, A connection between score matching and denoising auto encoders, Neural Computation, 2011

Sliced score-matching

- Sliced score-matching, which uses random projections to approximate the trace

$$\mathbb{E}_{p(\mathbf{v})}\mathbb{E}_{p_{data}}\left[\mathbf{v}^\top \nabla_{\mathbf{x}} s_\theta(\mathbf{x})\mathbf{v} + \frac{1}{2}\|s_\theta\|_2^2\right]$$

where $p(\mathbf{v})$ is a simple distribution of random vectors like multivariate Gaussian

- First sample a few vectors $\mathbf{v}$ that define the random projections
- Then compute $\mathbf{v}^\top \nabla_{\mathbf{x}} s_\theta(\mathbf{x})\mathbf{v}$ using forward-mode auto-differentiation
- Works on the original, unperturbed data distribution
- But it requires 4x the compute due to the extra auto-differentiation

* Song et al., Sliced score matching: A scalable approach to density and score estimation, UAI 2019

Score-matching: advantages

- We can train with score-matching directly with SGD like maximising log-likelihood
- We have no constraints on the form of $f_\theta(x)$ as we do not require $s_\theta(x)$ to be the score function of a normalised distribution
- We just compare our neural network output with the ground-truth data score
- The only requirement is that $s_\theta(x)$ is a vector valued function with the same input and output dimensionality

Sampling using Langevin dynamics

- During training we do not involve an explicit "sampling" mechanism
- After training the score-based model, we can sample with Langevin dynamics
- Langevin dynamics are an MCMC procedure to sample from distribution $p(x)$ using only the score function $\nabla_x \log p(x)$

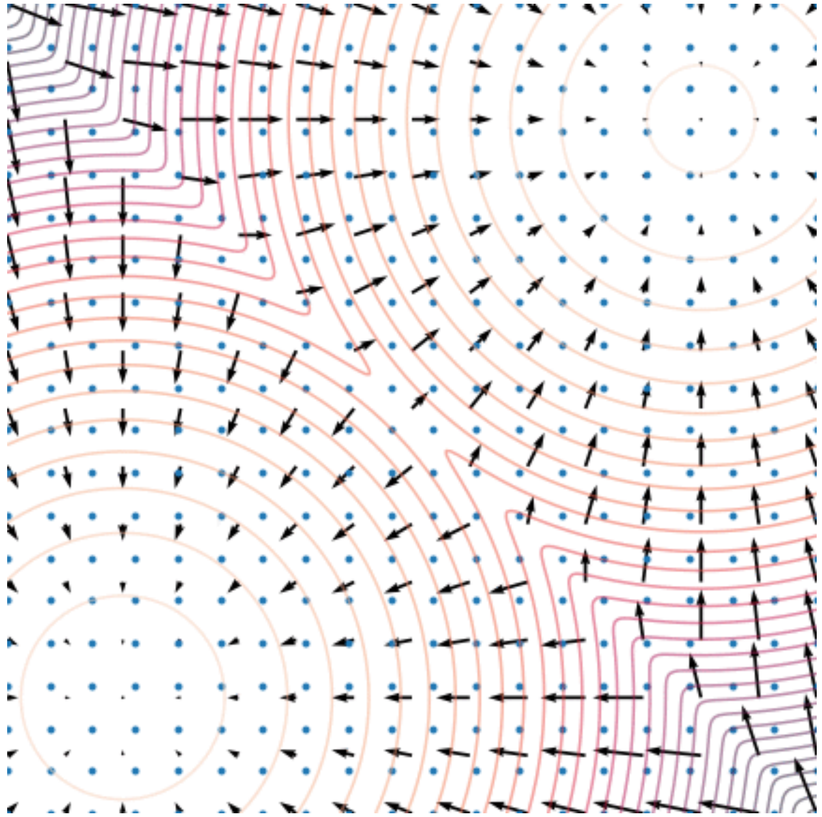
$$\mathbf{x}_{t+1} \leftarrow \mathbf{x}_t + \epsilon \nabla_{\mathbf{x}} \log p(\mathbf{x}_t) + \sqrt{2\epsilon}\mathbf{z}_t, \;\; t = 0, \ldots, K, \;\; \mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

- At $t = 0$ we sample from an arbitrary prior distribution $\mathbf{x}_0 \sim \pi(\mathbf{x})$

Sampling using Langevin dynamics

$$\mathbf{x}_{t+1} \leftarrow \mathbf{x}_t + \epsilon \nabla_{\mathbf{x}} \log p(\mathbf{x}_t) + \sqrt{2\epsilon}\mathbf{z}_t, t = 0, \ldots, K$$

- For $\epsilon \to 0$ and $K \to \infty$ we sample from $p(\mathbf{x})$
- Iterative sampling process relying only on score function
- Sample $\mathbf{x}_{t+1}$ iteratively via $s_\theta(x) \approx \nabla_x \log p(x)$



Langevin Dynamics

$$\mathbf{x}_{t+1} \leftarrow \mathbf{x}_t + \epsilon \nabla_{\mathbf{x}} \log p(\mathbf{x}_t) + \sqrt{2\epsilon}\mathbf{z}_t, \;\; t = 0, \ldots, K, \;\; \mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

- Originally developed to model molecular dynamics
- Similar to noised-up SGD, but not for optimising parameters
- Given current $\mathbf{x}_t$ move towards more likely densities ($\nabla_{\mathbf{x}}$) of $\log p(\mathbf{x}_t)$, yet corrupted with noise $\mathbf{z}_t$ for randomness, and scaled by annealed ϵ (like 'learning rate')
- A very nice work making the connection to Bayesian Learning*

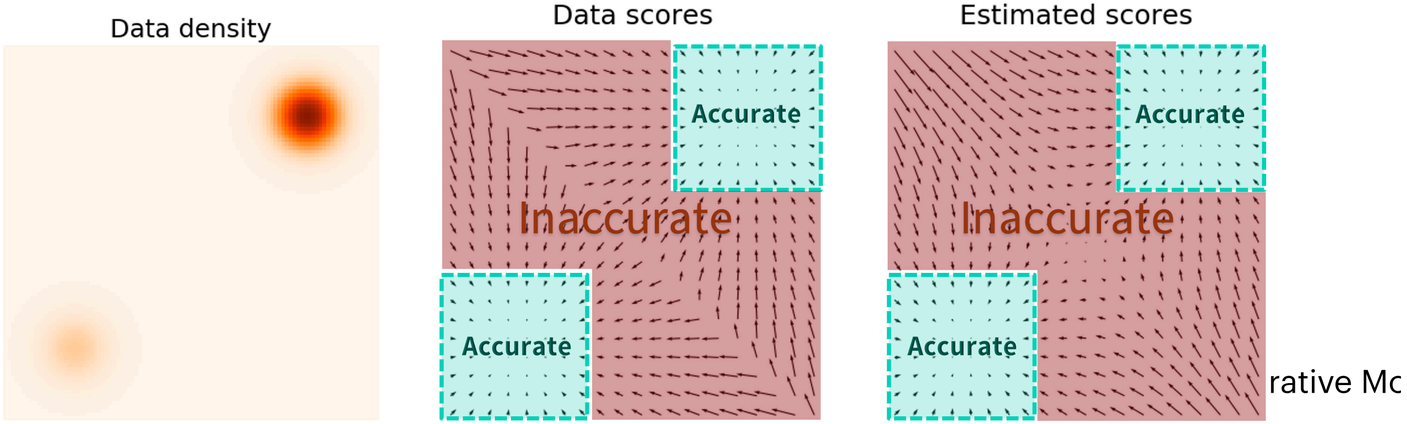
'Bayesian Learning via Stochastic Gradient Langevin Dynamics', M. Welling, Y. W. Teh

Low data density regions

- Minimising Fisher divergence → emphasising high $p(\mathbf{x})$ regions as they matter most

$$\mathbb{E}_{p(\mathbf{x})}\left[\|\nabla_x \log p(\mathbf{x}) - s_\theta(\mathbf{x})\|_2^2\right] = \int p(\mathbf{x})\|\nabla_{\mathbf{x}} \log p(\mathbf{x}) - s_\theta(\mathbf{x})\|_2^2 \mathrm{d}\mathbf{x}$$

- In high-dimensions harder as space is mostly empty
- Monte Carlo estimates will not be accurate enough



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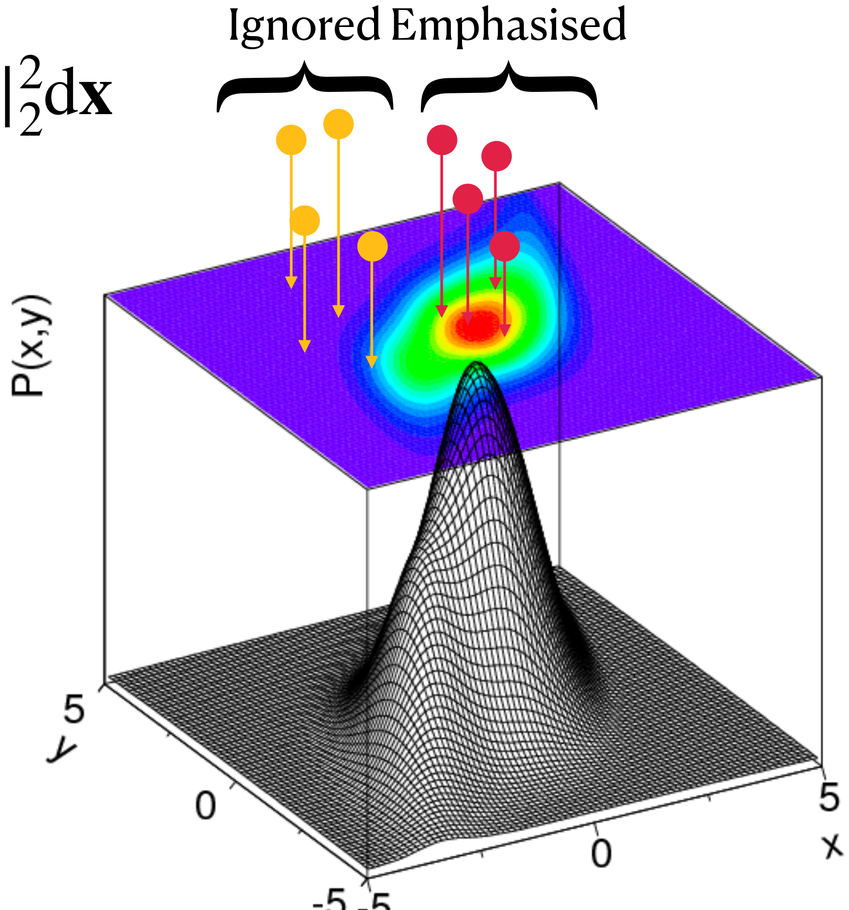


Slow mixing of Langevin dynamics

$$\mathbf{x}_{t+1} \leftarrow \mathbf{x}_t + \epsilon \nabla_{\mathbf{x}} \log p(\mathbf{x}_t) + \sqrt{2\epsilon}\mathbf{z}_t, \quad t = 0, \ldots, K, \quad \mathbf{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

- When the true density has two (or multiple) modes separated by a low-density region, it is hard for Langevin dynamics to visit them in a reasonable time
- That makes sense: the 'jumps' local around current location of score function and the added noise is unlikely to be large enough to push far enough

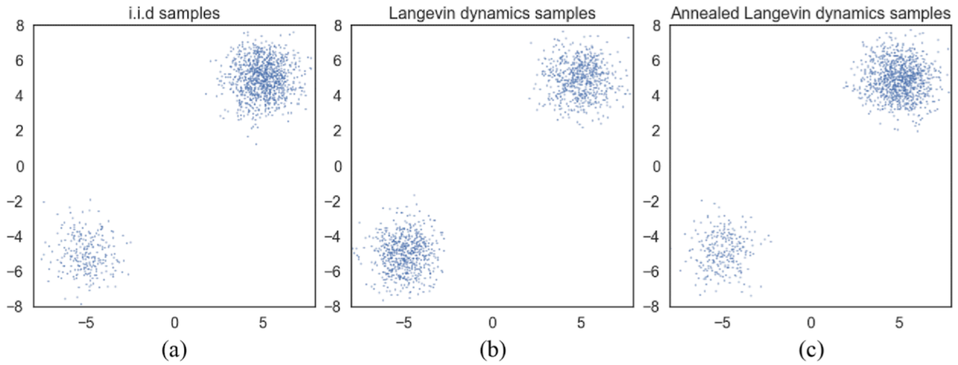
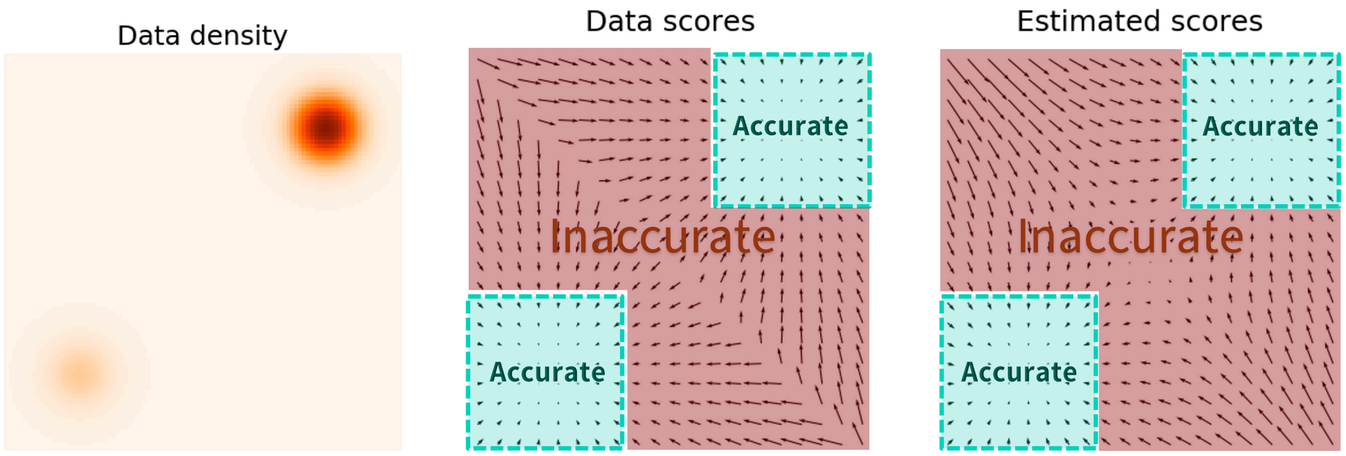


Figure 3: Samples from a mixture of Gaussian with different methods. (a) Exact sampling. (b) Sampling using Langevin dynamics with the exact scores. (c) Sampling using annealed Langevin dynamics with the exact scores. Clearly Langevin dynamics estimate the relative weights between the two modes incorrectly, while annealed Langevin dynamics recover the relative weights faithfully.

From 'Generative Modelling by Estimating Gradients of the Data Distribution', by Song and Ermon

Naive score-based ignores low-density regions

- Naive score-based training leads to inaccurate score function estimation
- And we have slow mixing of Langevin dynamics
- As a result, the Langevin chain will start from a low density region and get stuck

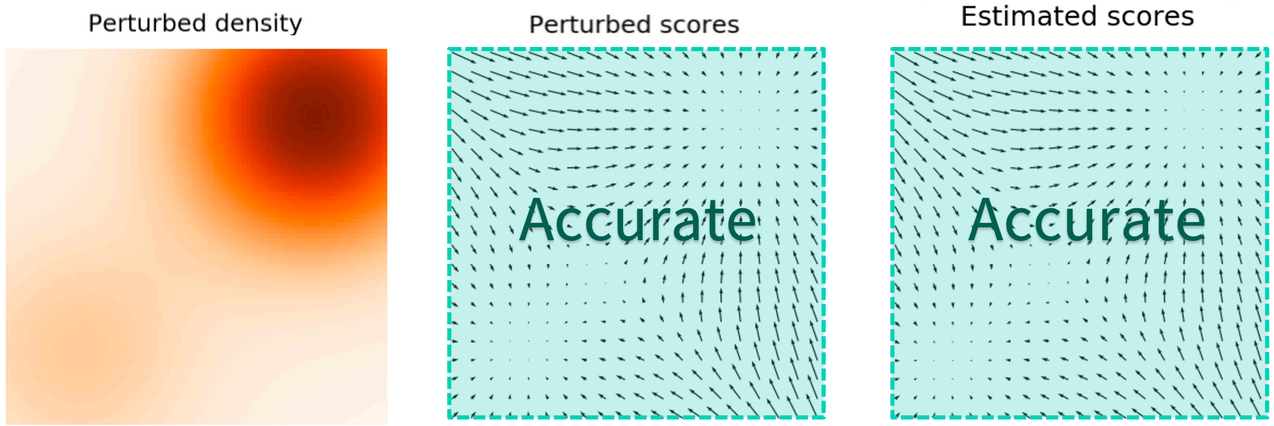


Solution: Perturb with noise (and denoise)

- For noised-up score matching perturb data with noise

$$q_{\sigma_t}(\tilde{\mathbf{x}}) = \int p(\mathbf{x}) q(\tilde{\mathbf{x}} \,|\, \mathbf{x}) \mathrm{d}\mathbf{x} = \int p(\mathbf{x}) \mathcal{N}(\tilde{\mathbf{x}} \,|\, \mathbf{x}, \sigma_t^2 \mathbf{I}) \mathrm{d}\mathbf{x}$$

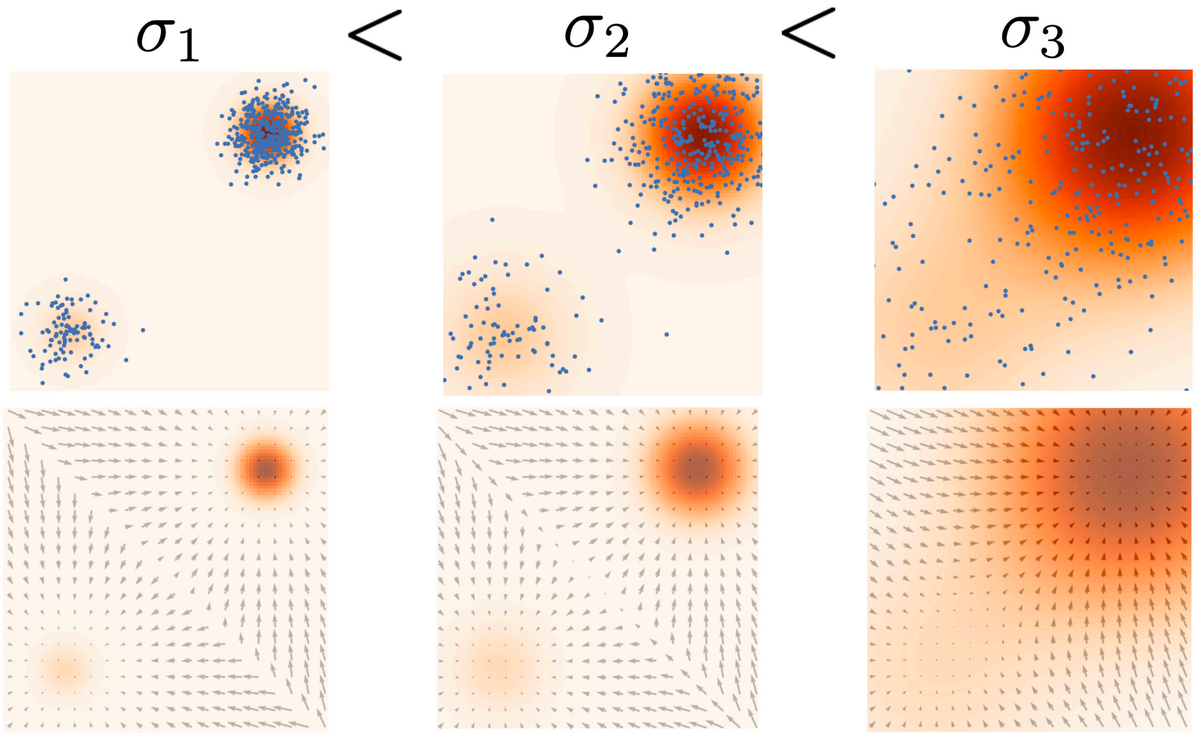
- Noised up data fill up the “empty” space
- Be careful: if too much noise data will be over-corrupted (strong distribution shift)



Noise-conditional Score-based Models

- Learn the score-matching function on the perturbed data points

Multiple scales of Gaussian noise to perturb data (above) so that to learn the respective score-matching function (below).



Noise-Conditional Score-based Models

- For a single noise scale and denoising a Gaussian noise auxiliary noise

$$\mathcal{N}(\tilde{\mathbf{x}}; \mathbf{x}, \sigma^2\mathbf{I}) \Rightarrow \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}} \,|\, \mathbf{x}) = -(\tilde{\mathbf{x}} - \mathbf{x})/\sigma^2$$

The loss becomes

$$\frac{1}{2}\mathbb{E}_{p_{data}(\mathbf{x})}\mathbb{E}_{\tilde{\mathbf{x}}\mathcal{N}(\mathbf{x},\sigma^2\mathbf{I})}\left[\left\|\mathbf{s}_\theta(\tilde{\mathbf{x}}, \sigma) + \frac{\tilde{\mathbf{x}} - \mathbf{x}}{\sigma^2}\right\|_2^2\right]$$

- And for multiple scales

$$\sum_t \lambda(t)\mathbb{E}_{p_{\sigma_t}(\mathbf{x})}\left[\|\nabla_{\mathbf{x}} \log p_{\sigma_t}(\mathbf{x}) - s_\theta(\mathbf{x}, t])\|\right]$$

where $\lambda(t)$ is a weighting function, typical choice $\lambda(t) = \sigma_t^2$

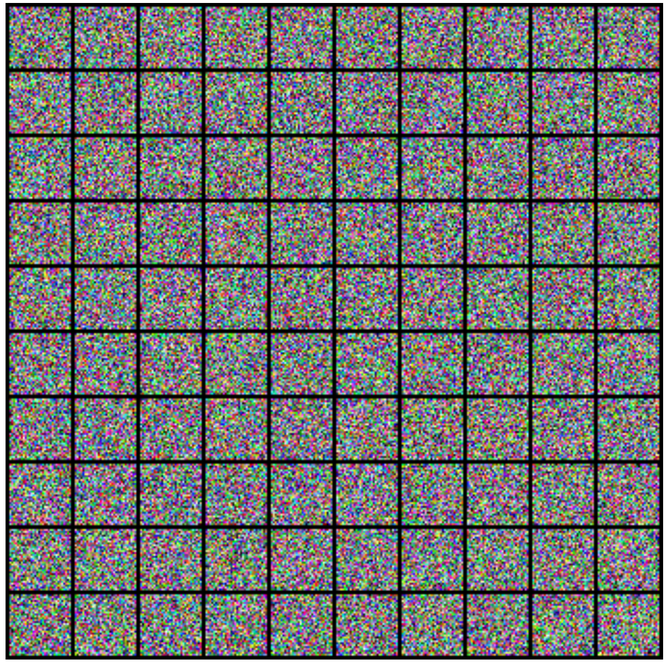
Annealed Langevin Dynamics

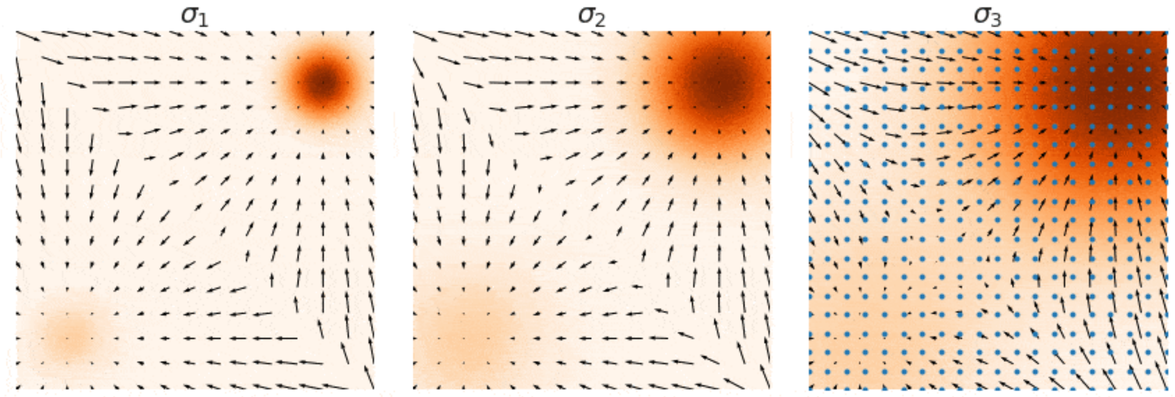
- Like before, but we start sampling from larger noise, which we gradually decrease

Algorithm 1 Annealed Langevin dynamics.

Require: $\{\sigma_i\}_{i=1}^{L}, \epsilon, T$.

Initialize $\tilde{\mathbf{x}}_0$
for $i \leftarrow 1$ to L **do**
  $\alpha_i \leftarrow \epsilon \cdot \sigma_i^2 / \sigma_L^2$ ▷ α_i is the step size.
  for $t \leftarrow 1$ to T **do**
    Draw $\mathbf{z}_t \sim \mathcal{N}(0, I)$
    $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \frac{\alpha_i}{2} \mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i}\, \mathbf{z}_t$
  end for
  $\tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$
end for
return $\tilde{\mathbf{x}}_T$



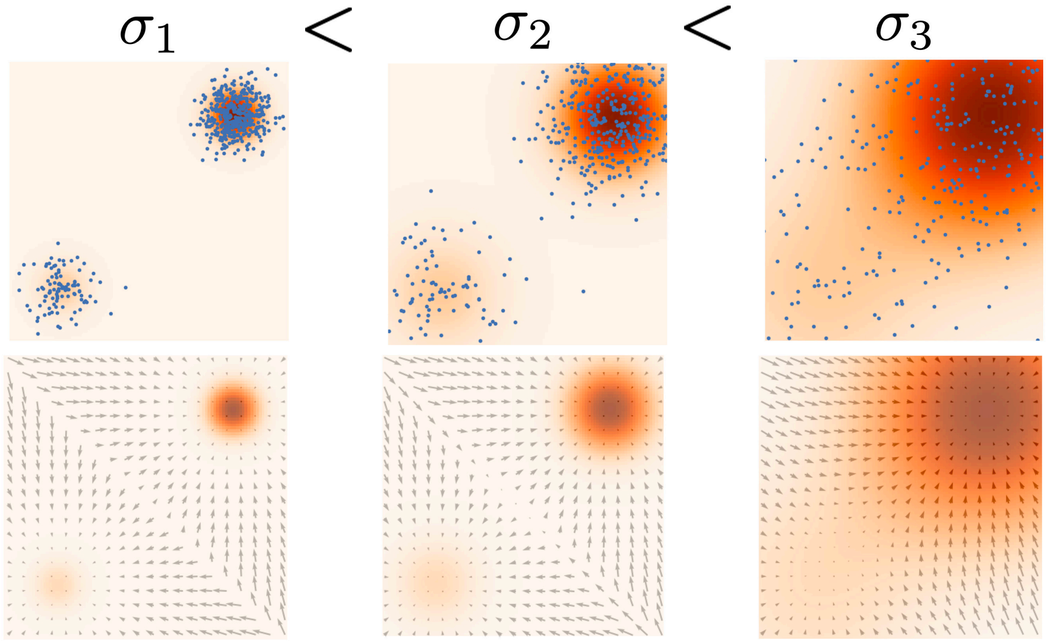


Practical tips

- Pick σ_t in geometric progression $\frac{\sigma_1}{\sigma_2} = \frac{\sigma_2}{\sigma_3} = \dots.$
- σ_L should be comparable to max distance between samples in the training set
- L is usually a few hundreds or thousands
- Parameterise the score-based model with a U-Net with skip connections
- At test time use exponential moving averages on the weights

Diffusion models & Stochastic Differential Equations

Score-based models with SDEs



- Adding noise fills up low-density regions
- But why "hardcode" to $\sigma_1, \sigma_2, \ldots$?
- With infinite noise scales, we can have
  - Higher quality samples
  - Exact log-likelihood computation
  - Controllable generation with inverse problem solving
- A stochastic process defines a process of generating infinite noise scales

Y. Song, J. Sohl-Dickstein, D. Kingma, A. Kumar, S. Ermon, B. Poole, Score-Based Generative Modeling through Stochastic Differential Equations, ICLR 2019

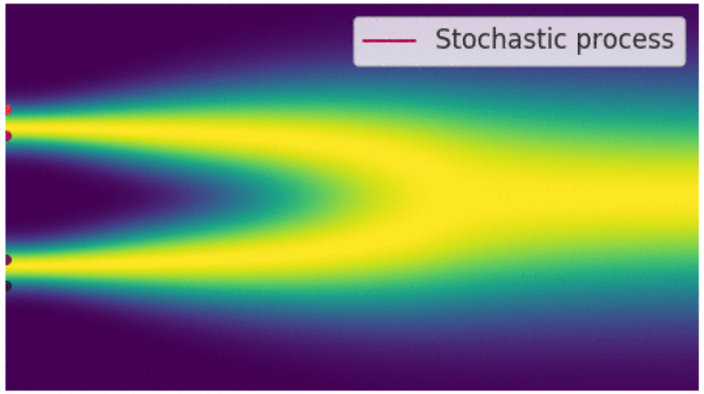
Stochastic processes via SDEs

- Stochastic processes as solutions of stochastic differential equations

$$\mathrm{d}\mathbf{x} = f(\mathbf{x}, t)\mathrm{d}t + g(t)\mathrm{d}\mathbf{w}, \quad f(\,\cdot\,, t) : \mathbb{R}^d \to \mathbb{R}^d, g \in \mathbb{R}$$

- Change in our RV governed by a function of RV and time (drift) plus noise whose scale is a function of time (diffusion)

- $\mathbf{w}$ is Brownian motion, $\mathrm{d}\mathbf{w}$ is infinitesimal white noise (Gaussian distribution)



Solutions to SDEs

- SDEs usually solved with numerical methods ($\mathbf{x}_{t+1} = \mathbf{x}_t + \dots$) over small time steps
- Solutions of SDEs are stochastic RVs $\{\mathbf{x}(t)\}_{t\in[0,T]} \rightarrow$ trajectories over time
- The pdf of $\mathbf{x}(t)$ is $p_t(\mathbf{x})$ (like $p_{\sigma_i}(\mathbf{x})$ for the discrete case)
- $p_0(\mathbf{x})$ means the distribution in the data space, i.e., $p_0(\mathbf{x}) = p(\mathbf{x})$
- $p_T(\mathbf{x})$ is the distribution after all the noising up for period T until we end up to our prior distribution for our data generation process, i.e., $p_T(\mathbf{x}) = \pi(\mathbf{x})$

Perturbing data with noise from SDEs

- In score-matching the SDE is the generalisation of the finite scaling $\sigma_0, \ldots, \sigma_L$
- In the discrete case perturb with a handpicked (geometric) progression of scales
- Now, noise scale controlled by SDE, where we (manually) select the governing SDE
- If $\mathrm{d}\mathbf{x} = e^t \mathrm{d}\mathbf{w}$, our Gaussian noise $\mathrm{d}\mathbf{w}$ grows exponentially with time

What SDE?

- Noise-conditional score-matching (the discrete case)

$$\mathbf{x}_i = \mathbf{x}_{i-1} + \sqrt{\sigma_i^2 - \sigma_{i-1}^2}\mathbf{z}_{i-1} \Rightarrow \mathrm{d}\mathbf{x} = \sqrt{\frac{\mathrm{d}\sigma^{\mathbf{2}}(\mathbf{t})}{\mathrm{d}t}}\mathrm{d}\mathbf{w}$$

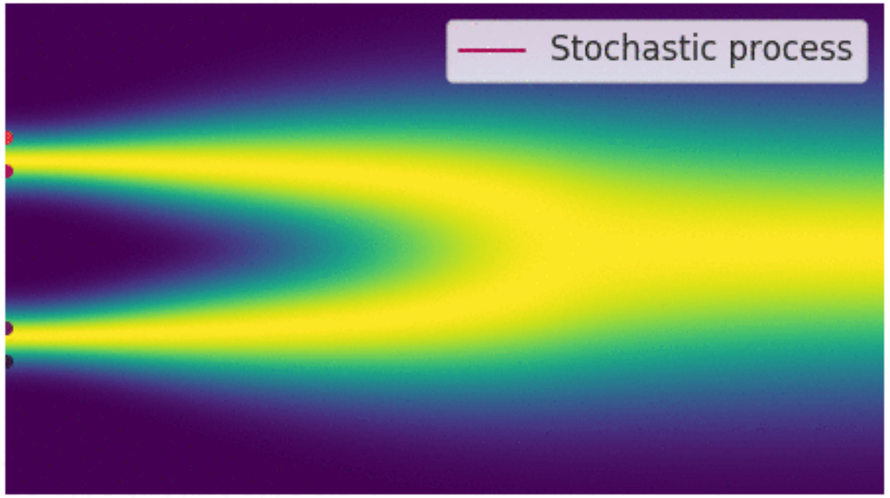
- Another SDE that worked pretty well

$$\mathrm{d}\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}\ \mathrm{d}t + \sqrt{\beta(t)\left(1 - \exp(-2\int_0^t \beta(s)\mathrm{d}s)\right)}\mathrm{d}\mathbf{w}$$

- Might look scary but we merely need to pass it to our numerical solver

From data to SDE noise

- We pick a sample $\mathbf{x}$ from $p_{data}(x)$, e.g., an image from our training set
- We add again and again noise until data looks like a standard Gaussian $\pi(\mathbf{x})$
- We can always make noise from data
- Million dollar question: can we make data from noise (reverse process)?

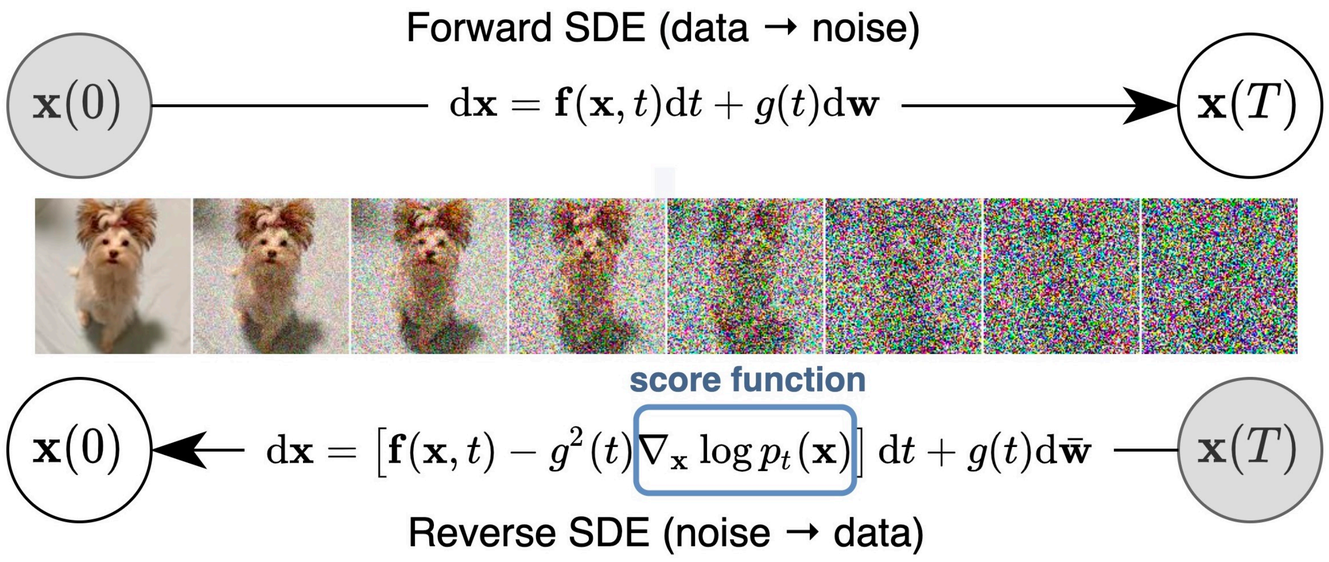


From reverse SDE noise to data

- For any SDE there is a reverse SDE with the reverse trajectories

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

- For the reverse SDE we need precisely the score function of $p_t(\mathbf{x})$



Learning the reverse SDE

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

- A neural network approximates the score function
- Take an initial sample from the prior distribution $\mathbf{x}(T) \sim \pi(\mathbf{x})$
- Solve reverse SDE to get $\mathbf{x}(t),\ \ \forall t \in (T,0]$ till model matches data distribution $p_\theta \approx p_0$
- With $\lambda(t) = g^2(t)$ we have

$$\mathrm{KL}(p_0(\mathbf{x}) \| p_\theta(\mathbf{x}))) \leq \mathbb{E}_{t\sim\mathcal{U}(0,T)}\mathbb{E}_{x\sim p_t(x)}\left[\left\|\nabla_{\mathbf{x}} \log p_t(\mathbf{x}) - s_\theta(\mathbf{x})\right\|_2^2\right] + \mathrm{KL}(p_T(\mathbf{x}) \| \pi(\mathbf{x})))$$

- With perfect score-matching, matching the prior implies approximating data distribution

Time-dependent score-matching

- Train a neural network for score-matching that depends on time

$$\mathbb{E}_{t\in\mathcal{U}(0,T)}\mathbb{E}_{p_t(x)}\left[\lambda(t)\left\|\nabla_{\mathbf{x}}\log p_t(\mathbf{x}\,|\,\mathbf{x}_0) - s_\theta(\mathbf{x},t)\right\|_2^2\right]$$

where typically $\lambda(t) \propto 1/\mathbb{E}\left[\|\nabla_{\mathbf{x}(t)}\log p(\mathbf{x}(t)\,|\,x(0))\|_2^2\right]$

- Randomly sample time steps
- Then sample data from training set
- Then optimise your score matching approximation

Solving the reverse SDE

- Once we have trained the score-matching function, we can solve the reverse SDE from the prior π all the way to our data distribution p_0 to generate new data
- Solving means running numerical solver to compute the trajectory (like a decoder)

$$\Delta \mathbf{x} \leftarrow \left[f(\mathbf{x}, t) - g^2(t) s_\theta(\mathbf{x}, t) \right] \Delta t + g(t) \sqrt{|\Delta t|}\, \mathbf{z}_t, \;\; \mathbf{z}_t \sim \mathcal{N}(0, I)$$

$$\mathbf{x} \leftarrow \mathbf{x} + \Delta \mathbf{x}$$

$$t \leftarrow t + \Delta t$$

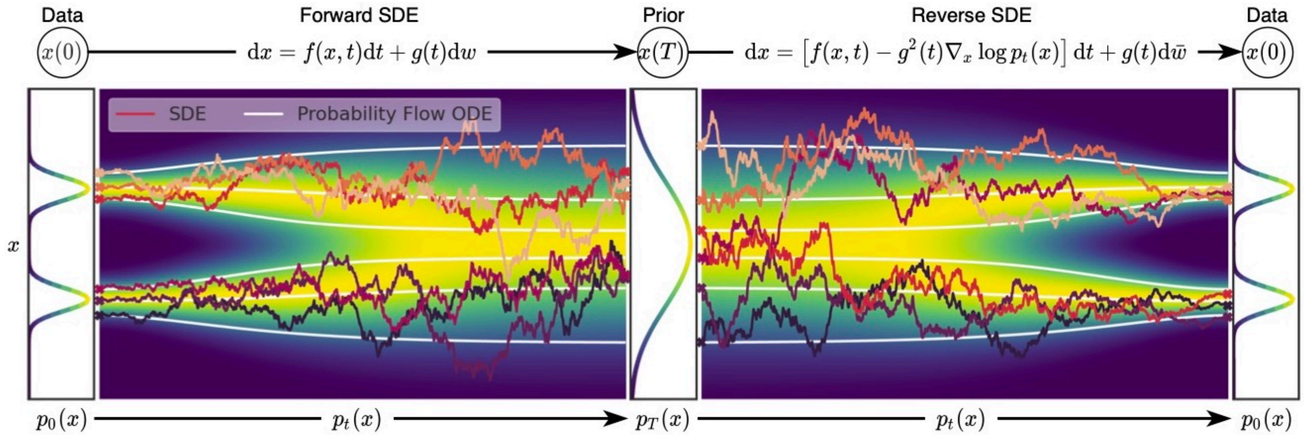
- We solve the SDE (getting the trajectory) for each new sample
- With better sampling procedures and architectures → SoTA generation

Probability flow ODE

- With Langevin MCMC samplers and SDE solvers we can't get exact log-likelihoods
- We can convert the SDE to a corresponding "probability flow" ODE without changing the marginal distributions $\{p_t(\mathbf{x})\}_{t\in[0,T]}$

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

- Solving the ODE, we get the exact log-likelihood



Qualitative examples

Diffusion models

Diffusion Probabilistic Models

- Concurrently, a similar to score-matching class of models: diffusion models
- Diffusion models also define a forward and reverse diffusion process, where $t = 0$ corresponds to the data distribution, and $t = T$ a unit-Gaussian distribution

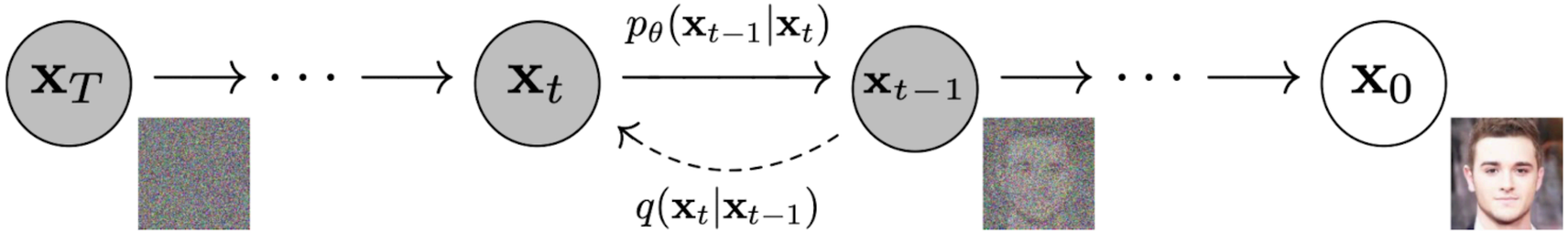


Figure 2: The directed graphical model considered in this work.

Diffusion probabilistic models, Sohl-Dickstein et al., 2015
Denoising diffusion probabilistic models, Ho et al., 2020
Diffusion models beat GANs on image synthesis, 2021
https://lilianweng.github.io/posts/2021-07-11-diffusion-models/

Forward diffusion process

- In forward diffusion we add small Gaussian noise to our data till it looks like isotropic Gaussian

$$q(\mathbf{x}_t \,|\, \mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x}_t; \sqrt{1-\beta_t}\mathbf{x}_{t-1}, \beta_t \mathbf{I}), \;\; q(\mathbf{x}_{1:T} \,|\, \mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t \,|\, \mathbf{x}_{t-1})$$

- We can define the conditional distribution at any time step t w.r.t. step $t = 0$

$$\begin{aligned}
\mathbf{x}_t &= \sqrt{a_t}\mathbf{x}_{t-1} + \sqrt{1-a_t}\mathbf{z}_{t-1} && \text{, where } \mathbf{z}_{t-1}, \mathbf{z}_{t-2}, \ldots \sim \mathcal{N}(0,1) \\
&= \sqrt{a_t a_{t-1}}\mathbf{x}_{t-2} + \sqrt{1-a_t a_{t-1}}\bar{\mathbf{z}}_{t-2} && \text{, where } \bar{\mathbf{z}}_{t-2} \text{ merges two Guassians} \\
&= \ldots \\
&= \sqrt{\bar{a}_t}\mathbf{x}_0 + \sqrt{1-\bar{a}_t}\bar{\mathbf{z}} \\
q(\mathbf{x}_t \,|\, \mathbf{x}_0) &= \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{a}_t}\mathbf{x}_0, \sqrt{1-\bar{a}_t}\mathbf{I})
\end{aligned}$$

- For this we use that <u>when merging two Gaussians</u>, we get another Gaussian with variance $\sigma_1^2 + \sigma_2^2$

Reverse diffusion process

- Efficiently parameterising reverse diffusion we can combine with variational inference

$$L_{VLB} = L_T + L_{T-1} + \ldots + L_0$$

$$\text{where } L_T = D_{KL}\big(q(\mathbf{x}_T \,|\, \mathbf{x}_0) \| p_\theta(\mathbf{x}_T)\big)$$

$$L_t = D_{KL}\big(q(\mathbf{x}_t \,|\, \mathbf{x}_{t+1}, \mathbf{x}_0) \| p_\theta(\mathbf{x}_t \,|\, \mathbf{x}_{t+1})\big) \text{ for } 1 \leq t \leq T-1$$

$$L_0 = -\log p_\theta(\mathbf{x}_0 \,|\, \mathbf{x}_1)$$

- Since we have Gaussian distributions the KL terms can be computed in closed form
- L_T does not depend any parameters and it can be dropped
- L_0 depends on the final decoder output

Parameterising L_t

- By smart parameterisation of the Gaussians, learning boils down to minimising

$$L_t^{\text{simple}} = \mathbb{E}_{\mathbf{x}_0, \boldsymbol{\epsilon}_t}\left[\left\|\boldsymbol{\epsilon}_t - \boldsymbol{\epsilon}_\theta\left(\sqrt{\bar{a}_t}\mathbf{x}_0 + \sqrt{1-\bar{a}_t}\boldsymbol{\epsilon}_t, t\right)\right\|_2^2\right]$$

- The model learns to predict the noise added to the transformed signal!!!!

Algorithm 1 Training

1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \ldots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on
$$\nabla_\theta \left\|\boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t)\right\|^2$$
6: **until** converged

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \ldots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

Example trajectories

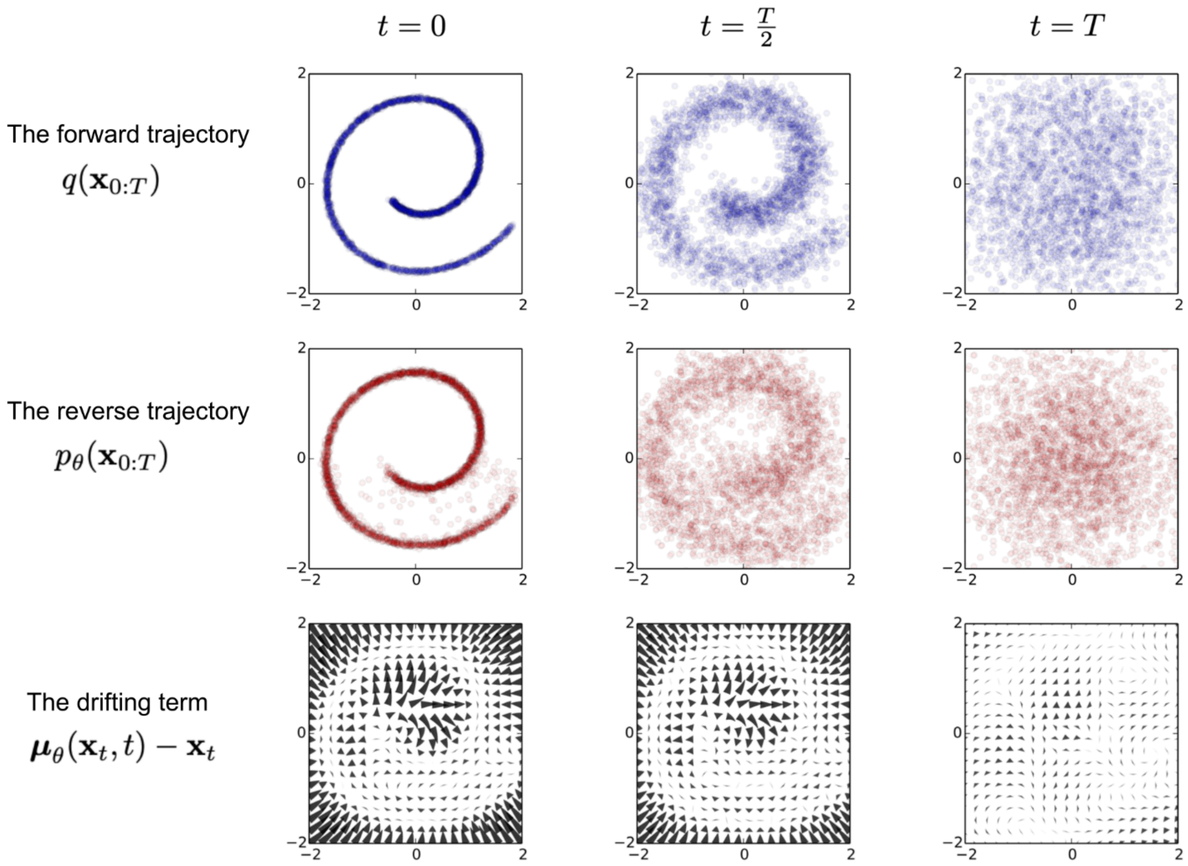
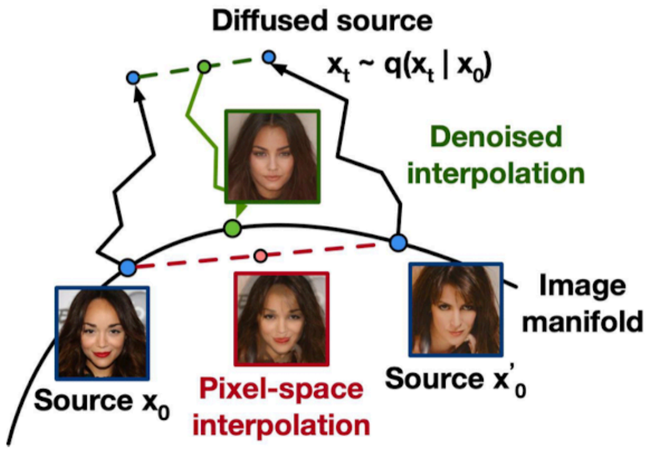


Fig. 3. An example of training a diffusion model for modeling a 2D swiss roll data. (Image source: Sohl-Dickstein et al., 2015)

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

Qualitative results



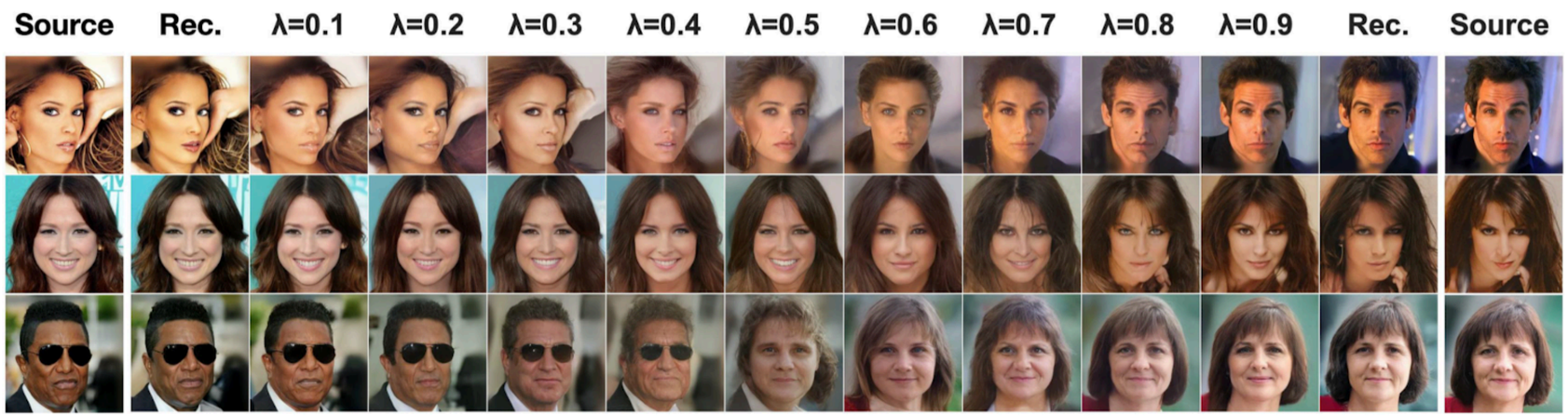
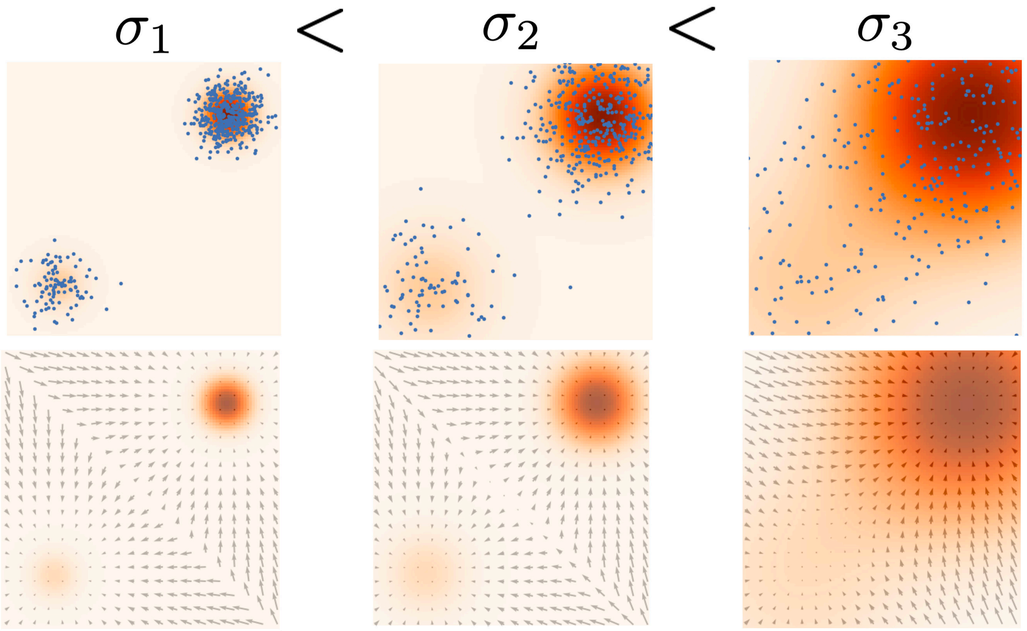
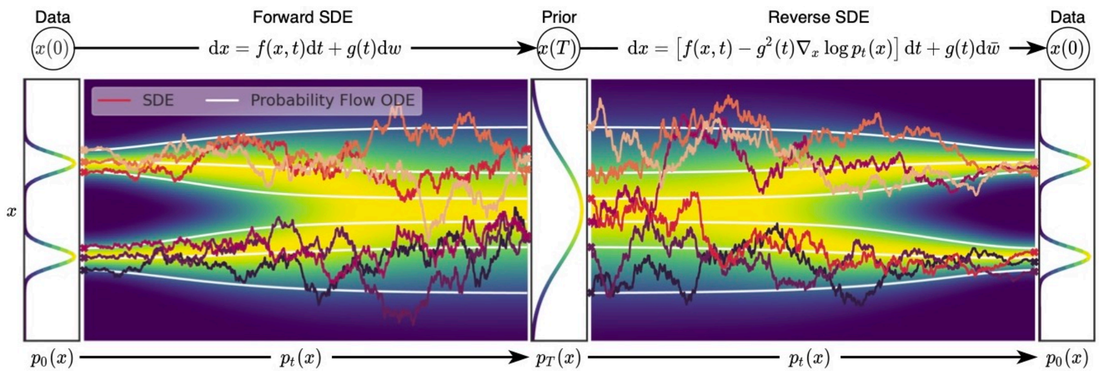


Figure 8: Interpolations of CelebA-HQ 256x256 images with 500 timesteps of diffusion.

Denoising diffusion probabilistic models, Ho et al., 2020

Summary

Diffusion/score-matching models are both tractable and flexible
However, they are still quite slow to sample from compared to GANs
The reason is that they require very long chains of time steps up to $T = 1{,}000$
Great opportunities for learning the data structure effectively and efficiently enough
Promising results in modelling inverse problems