Normalizing Flows

Intuition about easy to sample

- Goal: design $p(x)$ such that
  - Easy to sample
  - Tractable likelihood (density function)

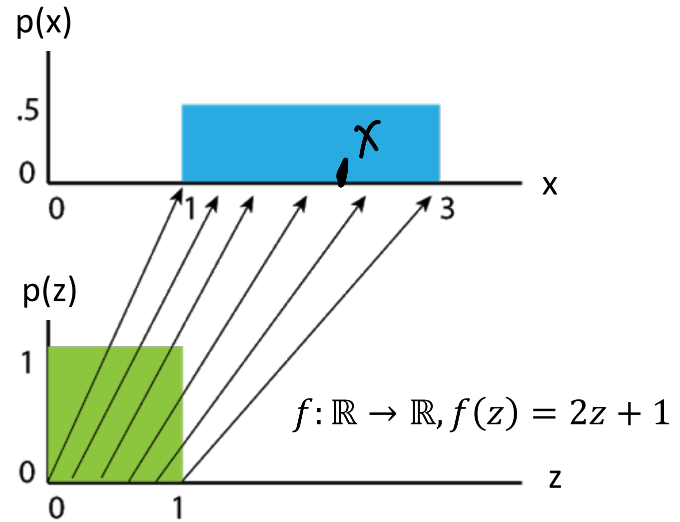
- Easy to sample
  - Assume a continuous variable z
  - e.g., Gaussian $z \sim N(0,1)$, or uniform $z \sim \text{Unif}[0,1]$
  - $x = f(z)$, x is also easy to sample

Intuition about tractable density

- Goal: design $f(z;\theta)$ such that
  - Assume z is from an "easy" distribution
  - $p(x) = p(f(z;\theta))$ has tractable likelihood

- Uniform: $z \sim$ Unif$[0,1]$
  - Density $p(z) = 1$
  - $x = 2z + 1$, then $p(x) = ?$ 0.5

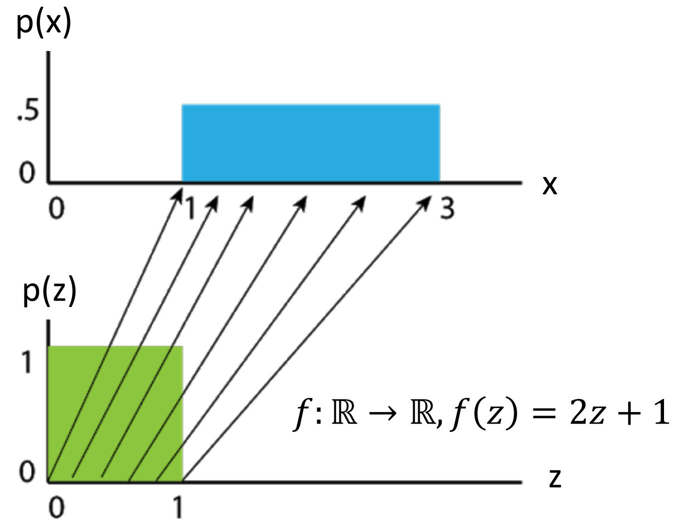
$f(z) = 2z+1$



Intuition about tractable density

- Goal: design $f(z;\theta)$ such that
  - Assume z is from an "easy" distribution
  - $p(x) = p(f(z;\theta))$ has tractable likelihood

- Uniform: $z \sim \text{Unif}[0,1]$
  - Density $p(z) = 1$
  - $x = 2z + 1$, then $p(x) = 1/2$
    - $x = az + b$, then $p(x) = 1/|a|$ (for $a \neq 0$)
  - $x = f(z), p(x) = p(z)\left|\frac{dz}{dx}\right| = |f'(z)|^{-1}p(z)$
    - Assume $f(z)$ is a bijection



Change of variable

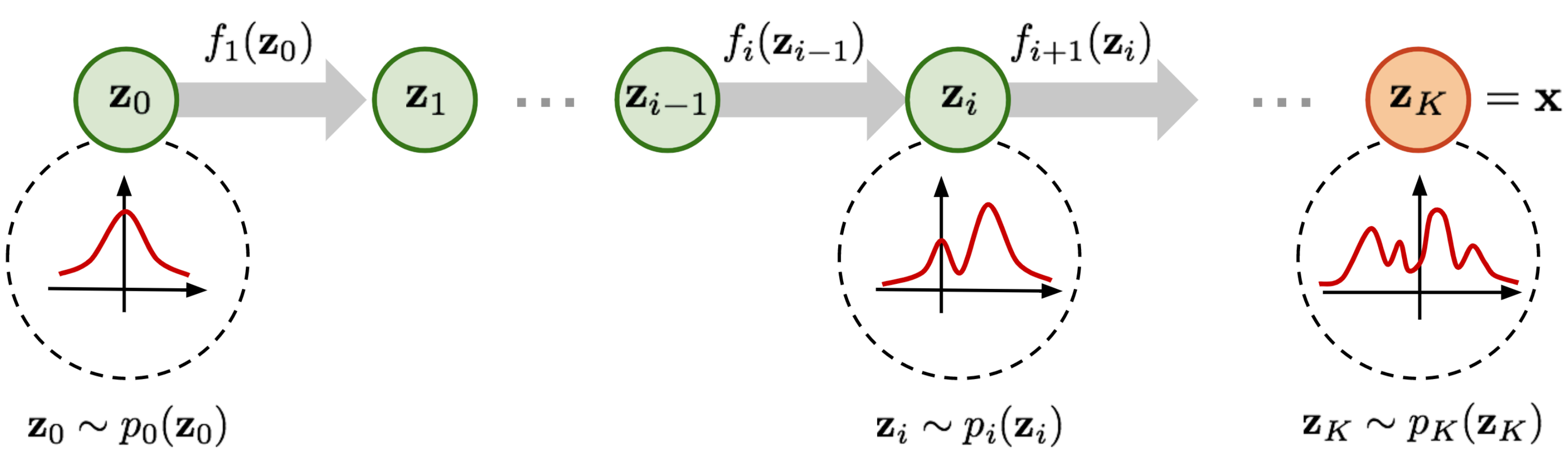
$z \leftarrow f^{-1}(x)$

- Suppose $x = f(z)$ for some general non-linear $f(\cdot)$
  - The linearized change in volume is determined by the Jacobian of $f(\cdot)$:
  - $$\frac{\partial f(z)}{\partial z} = \begin{bmatrix} \frac{\partial f_1(z)}{\partial z_1} & \cdots & \frac{\partial f_1(z)}{\partial z_d} \\ \cdots & \cdots & \cdots \\ \frac{\partial f_d(z)}{\partial z_1} & \cdots & \frac{\partial f_d(z)}{\partial z_d} \end{bmatrix} \in \mathbb{R}^{d \times d}$$

    $z, x \in \mathbb{R}^d$
- Given a bijection $f(z) : \mathbb{R}^d \to \mathbb{R}^d$
  - $z = f^{-1}(x)$
  - $$p(x) = p(\underbrace{f^{-1}(x)}_{z})\left|\det\left(\frac{\partial f^{-1}(x)}{\partial x}\right)\right| = p(z)\left|\det\left(\frac{\partial f^{-1}(x)}{\partial x}\right)\right|$$
  - Since $\frac{\partial f^{-1}}{\partial x} = \left(\frac{\partial f}{\partial x}\right)^{-1}$ (Jacobian of invertible function)
  - $$p(x) = p(z)\left|\det\left(\frac{\partial f^{-1}(x)}{\partial x}\right)\right| = p(z)\left|\det\left(\frac{\partial f(z)}{\partial z}\right)\right|^{-1}$$

Normalizing Flow

- Idea
  - Sample z_0 from an "easy" distribution, e.g., standard Gaussian
  - Apply K bijections $z_i = f_i(z_{i-1})$ $f_1, \dots f_K$
  - The final sample $x = f_K(z_K)$ has tractable desnity
- Normalizing Flow
  - $z_0 \sim N(0,I)$, $z_i = f_i(z_{i-1})$, $x = Z_K$ where $x, z_i \in \mathbb{R}^d$ and f_i is invertible
  - Every revertible function produces a normalized density function
  - $p(z_i) = p(z_{i-1}) \left| \det \left(\dfrac{\partial f_i}{\partial z_{i-1}} \right) \right|^{-1}$ $p(x) = \prod \left| \det(\cdot\cdot) \right|^{-1} \cdot p(z_0)$

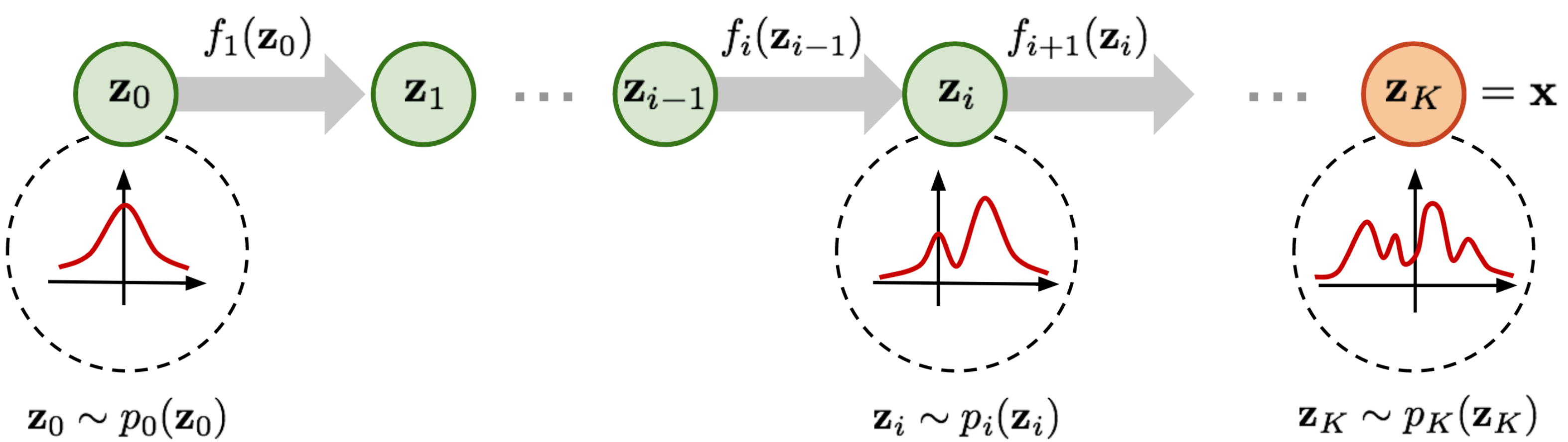


Normalizing Flow

$f_1, f_2 \cdots f_K$

- Generation is trivial
  - Sample z_0 then apply the transformations
- Log-likelihood
  - $\log p(x) = \log p(Z_{k-1}) - \log \left| \det \left(\frac{\partial f_K}{\partial z_{K-1}} \right) \right|$
  - $\log p(x) = \log p(z_0) - \sum_i \log \left| \det \left(\frac{\partial f_i}{\partial z_{i-1}} \right) \right|$

$O(d^3)$!!!



Normalizing Flow

- Naive flow model requires extremely expensive computation
  - Computing determinant of $d \times d$ matrices
- Idea:
  - Design a good bijection $f_i(z)$ such that the determinant is easy to compute

Plannar Flow

$A \in \mathbb{R}^{d \times d}$ $u, v \in \mathbb{R}^{d}$, $uv \in \mathbb{R}^{d \times d}$

$O(d^3)$

- Technical tool: Matrix Determinant Lemma:
  - $\det(A + uv^\top) = (1 + v^\top A^{-1} u) \det A$

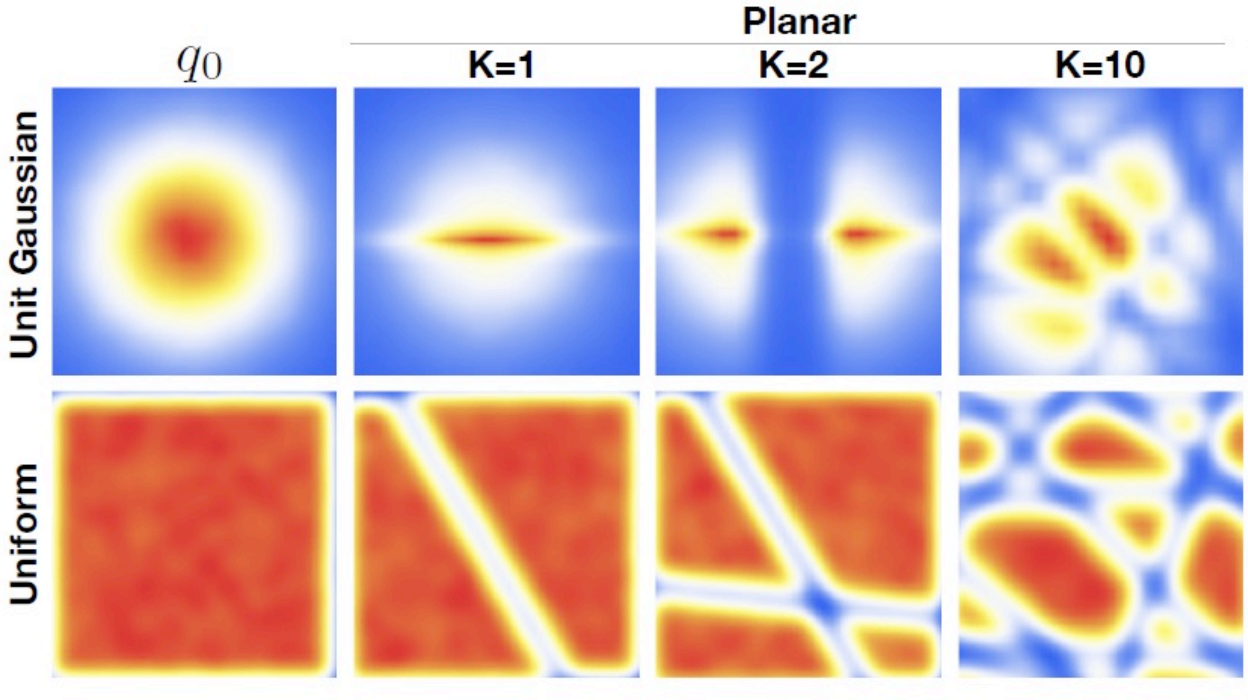
$\odot$: pointwise product

$A = I$

- Model:
  - $f_\theta(z) = z + u \odot h(w^\top z + b)$
  - $h(\cdot)$ chosen to be $\tanh(\cdot)(0 < h'(\cdot) < 1)$
  - $\theta = [u, w, b], \det\left(\frac{\partial f}{\partial z}\right) = \det(I + h'(w^\top z + b)uw^\top) = 1 + h'(w^\top z + b)u^\top w$
  - Computation in $O(d)$ time
  - Remarks:
    - $u^\top w > -1$ to ensure invertibility
    - Require normalization on u and w

Planar Flow (Rezende & Mohamed, '16)

- $f_\theta(z) = z + uh\left(w^\top z + b\right)$
- 10 planar transformations can transform simple distributions into a more complex one



Extensions

- Other flow models uses triangular Jacobian (NICE, Dinh et al. ’14)

- Invertible 1x1 convolutions (Kingma et al. ’18)

- Auto-regressive flow:
  - WaveNet (Deepmind ’16)
  - PixelCNN (Deepmind ‘16)

Summary

- Pros:
  - Easy to sample by transforming from a simple distribution
  - Easy to evaluate the probability
  - Easy training (MLE)

- Con
  - Most restricted neural network structure
  - Trade expressiveness for tractability

Score-Based Models and Diffusion Models

Recap: Boltzmann Machine Training

- Objective: maximum likelihood learning (assume T =1):
  - Probability of one sample:

$$P(y) = \frac{\exp(\frac{1}{2}y^\top W y)}{\underbrace{\sum_{y'} \exp(y'^\top W y')}_{Z}}$$

  - Maximum log-likelihood:

$$L(W) = \frac{1}{N}\sum_{y \in D} \frac{1}{2} y^\top W y - \log \sum_{y'} \exp(\frac{1}{2} y'^\top W y')$$

Can we avoid calculating the gradient of normalizing constant ($\nabla_x Z_\theta$)?

Score Matching

$$P(X) = \frac{e^{f_\theta(Y)}}{\sum_{X'} e^{f_\theta(X')}}$$

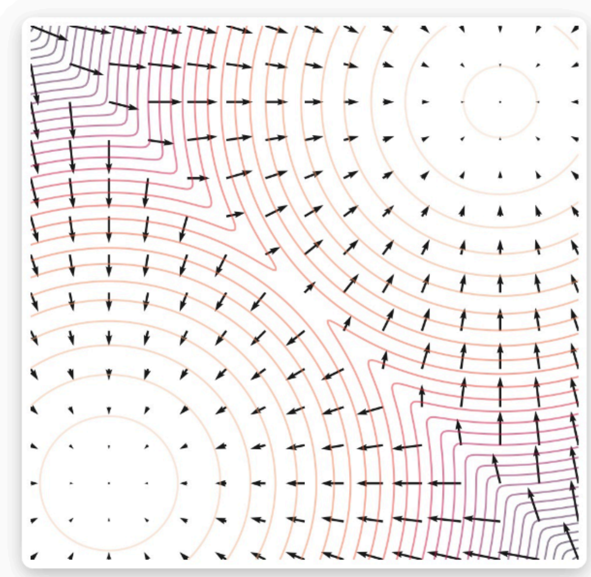
$$\nabla_X \log P(X) = \nabla f_\theta(X) \cancel{- \log\left(\sum_{X'} e^{f_\theta(X)}\right)}$$

- Score Function
  - Definition:

$$\nabla_x \log p_{data}(x) : \mathbb{R}^d \to \mathbb{R}^d$$

- Idea: directly fitting the score function:
  - $\min_\theta \mathbb{E}_{p_{data}} \|\nabla_x \log p_\theta(x) - \nabla_x \log p_{data}(x)\|^2$
  - No need to compute $\nabla_x Z_\theta$!
- Problem:
  - How to compute $\nabla_x \log p_{data}(x)$?

$\{X_1, \ldots, X_N\}$



Score function (the vector field) and density function (contours) of a mixture of two Gaussians.

Score Matching

$$\mathbb{E}_{p_{data}} \| \nabla_x \log p_\theta(x) - \nabla_x \log p_{data}(x) \|^2$$

$$= \mathbb{E}_{p_{data}} \| \nabla_x \log p_\theta(x) \|^2 + \mathbb{E}_{p_{data}} \| \nabla_x \log p_{data}(x) \|_2^2$$

$$- 2\, \mathbb{E}_{p_{data}} \langle \nabla_x \log p_\theta(x), \nabla_x \log p_{data}(x) \rangle$$

(Integration by parts

$$\mathbb{E}_p \langle f(x), \nabla_x \log p(x) \rangle = -\mathbb{E}_p [\mathrm{div} f(x)]$$

where $\mathrm{div} f(x) = \sum_i \frac{\partial f_i(x)}{\partial x_i}$)

$$\Rightarrow \mathbb{E}_{p_{data}} \langle \nabla_x \log p_\theta(x), \nabla_x \log p_{data}(x) \rangle$$

$$= -\mathbb{E}[\mathrm{Tr}(\nabla_x^2 \log p_\theta(x))]$$

$$\text{loss} \Longleftrightarrow \mathbb{E}_{p_{data}} \| \nabla_x \log p_\theta(x) \|_2^2 - 2\, \mathbb{E}_{p_{data}} [\mathrm{Tr}(\nabla_x^2 \log p_\theta(x))]$$

Score Matching

$\nabla_x \log p_\theta(x) : \mathbb{R}^d \to \mathbb{R}^d$

Use NN to parametrize $s_\theta(x)$

$\{x_1, \ldots, x_N\}$

loss : $\frac{1}{N} \sum_{i=1}^{N} \underbrace{\| s_\theta(x_i) \|_2^2}_{O(d)} - 2 \left[\mathrm{Tr} \left(\underbrace{\nabla s_\theta(x_i)}_{O(d^2)} \right) \right]$

Sliced Score Matching

$$L(\theta) = \frac{1}{N}\sum_{x\in D} \|s_\theta(x)\|^2 - 2\left[Tr(Ds_\theta(x))\right]$$

Random projection

Let $M \in \mathbb{R}^{d\times d}$, v random, $\mathbb{E}[vv^T] = I$

$$\mathbb{E}_v[v^T M v] = \mathbb{E}[Tr(M vv^T)] = Tr(M \cdot \mathbb{E}[vv^T]) = Tr(M)$$

Sample $v_1, \ldots v_K$, for large K

$$\frac{1}{K}\sum_{i=1}^{K} v_i^T M v_i \longrightarrow Tr(M)$$

Score Matching: Langevin Dynamics

x_0 arbitrary $\qquad \epsilon \ll 1$

$$x_{t+1} \leftarrow x_t + \epsilon \nabla_x \log p(x) + \sqrt{2\epsilon} z_t, z_t \sim N(0, I)$$

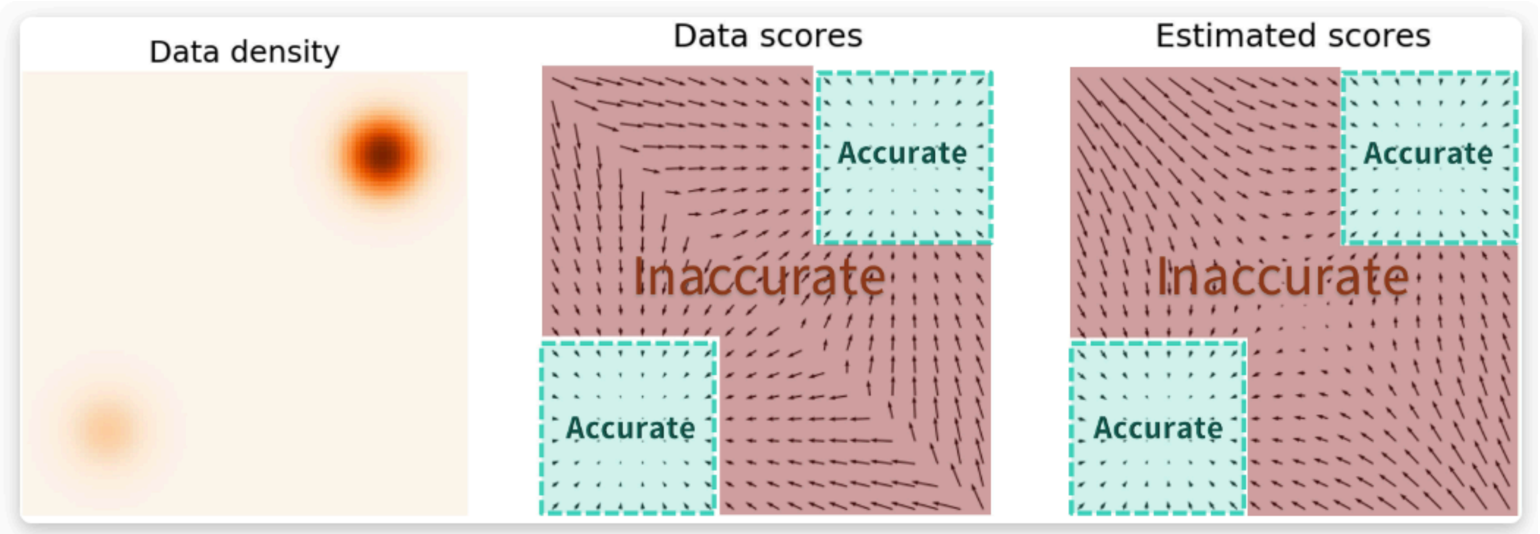
Stationary (equilibrium distribution): p(x)

$\{x_1, \ldots, x_\infty\} \rightarrow p(x)$

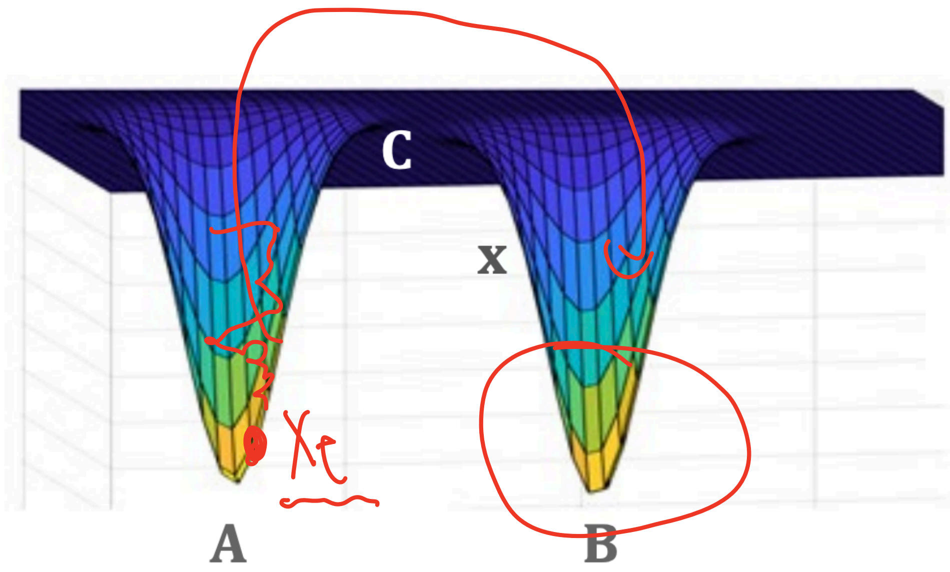
Practical Issues

$\nabla_x \log p(x)$

- Score function estimation is inaccurate in low density regions (few data available).



- Sampling is Slow



Annealing: Denoising Score Matching

- Fit several "smoothed" versions of p_{data}:
  - Choose temperatures: $\sigma_1, \sigma_2, \ldots, \sigma_T$
  - $p_{\sigma_i,data}(x) = p_{data}(x) * N(0,\sigma_i) = \int_\delta p_{data}(x-\delta)N(x;\delta,\sigma_i)d\delta$
  - Implementation:
    - Take a sample x, draw a sample $z \sim N(0,\sigma_i)$, output $x' = x + z$.

$$\sigma_1 > \sigma_2 > \cdots > \sigma_{L-1} > \sigma_L$$

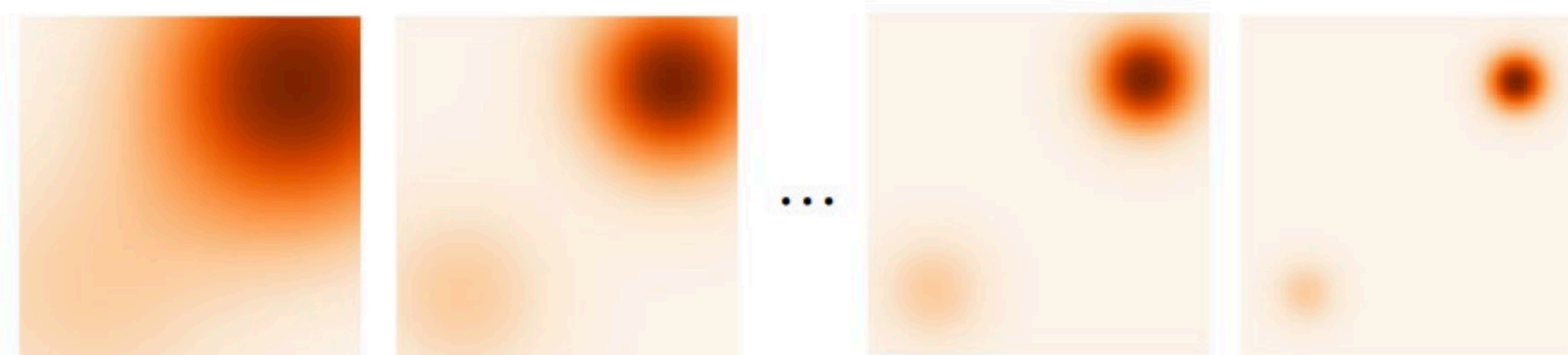


Figure by Stefano Ermon.

Annealing: Denoising Score Matching

$$\arg\min_{\theta} \sum_i \lambda(\sigma_i) \mathbb{E}_{x \sim p_{\sigma_i,data}} \| s_\theta(x, i) - \nabla_x \log p_{\sigma_i,data}(x) \|^2$$

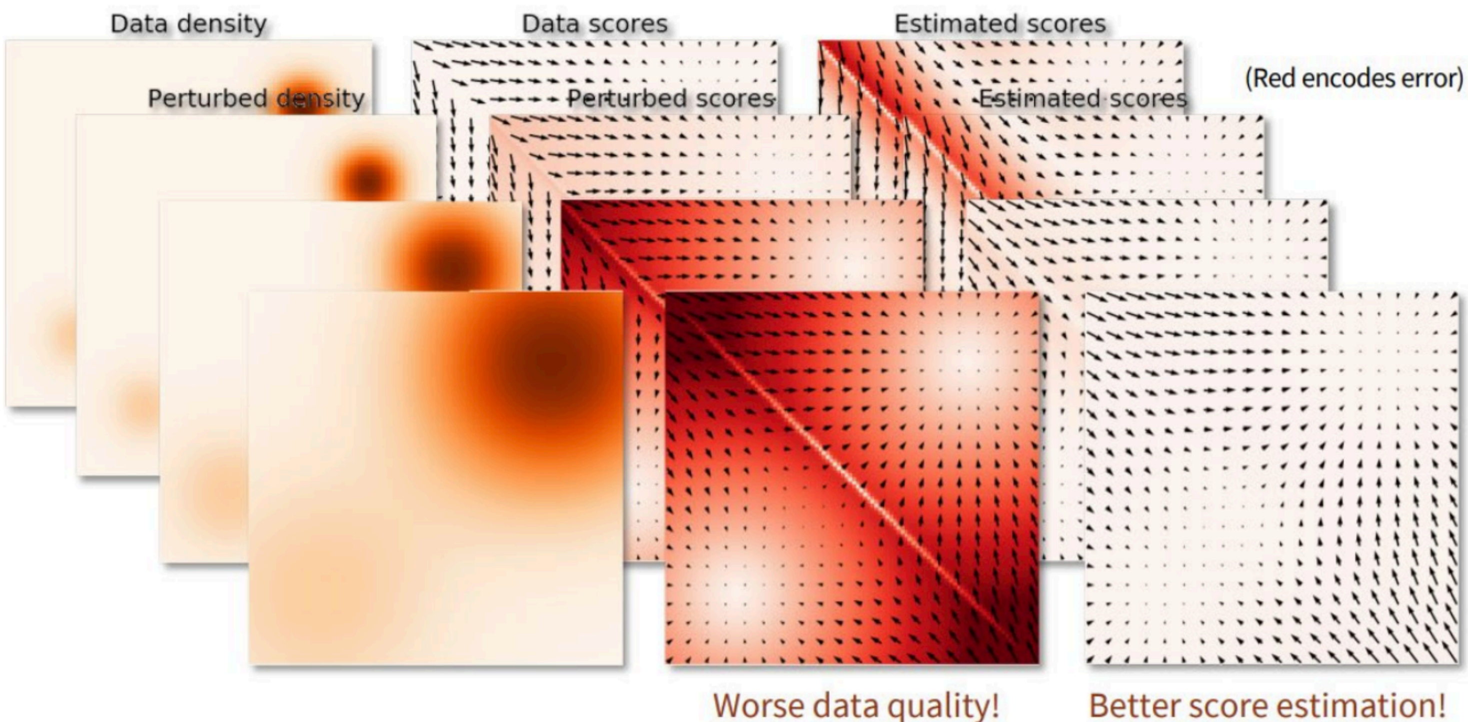


Figure by Stefano Ermon.

Annealed Langevin Dynamics

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 $\mathbf{z}_t \sim \mathcal{N}(0, I)$

    $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \frac{\alpha_i}{2} \mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i}\, \mathbf{z}_t$

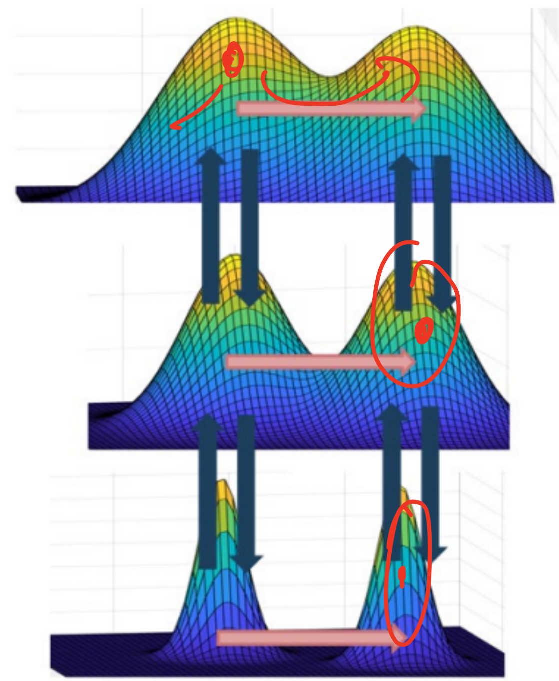
  end for

  $\tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$

end for

return $\tilde{\mathbf{x}}_T$

Figure from Song-Ermon '19



Diffusion Models

An image generated by Stable Diffusion based on the text prompt "a photograph of an astronaut riding a horse"

Perturbing Data with an SDE

$\{\sigma_t\}$

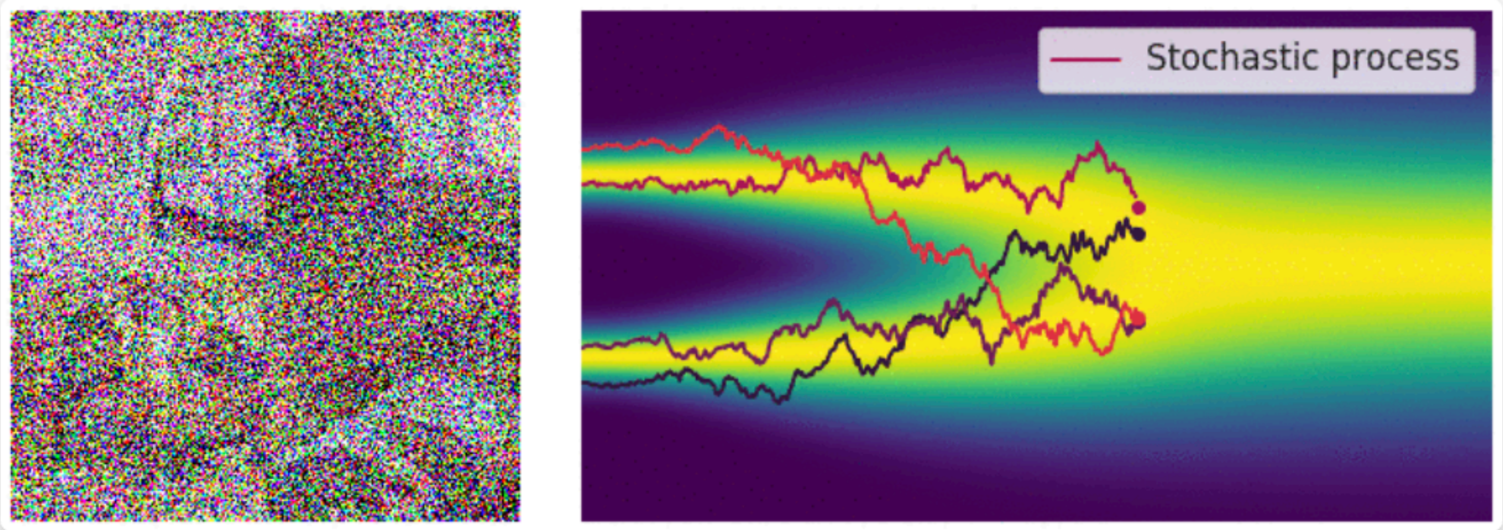
$\sigma_1, \sigma_2, \ldots \sigma_T$

- Let the number of noise scales approaches infinity!

$z \to f(z)$

$x_t = x_{t-1} + N(0, \sigma_t)$

$T \to \infty \Rightarrow$ Gaussian noise



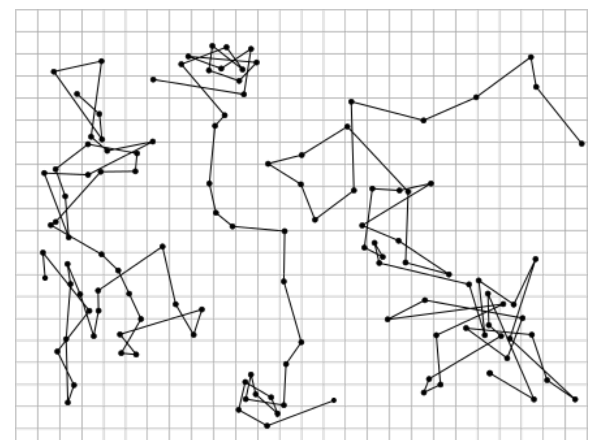
Perturbing data to noise with a continuous-time stochastic process.

Stochastic Differential Equations

$$dx = f(x,t)dt + g(t)dw$$

dw

- x(0): real image, x(T): Gaussian noise.
- f(x,t): drift terms. g(t): diffusion coefficient.
- dw: Brownian motion
  - $w(t+u) - w(t) \sim N(0,u)$
- f(x,t) and g(t) are parts of the model.
  - Variance Exploding SDE: $dx = \sqrt{\frac{d[\sigma^2(t)]}{dt}}dw.$
  - Variance Preserving SDE: $dx = -\frac{1}{2}\beta(t)xdt + \sqrt{\beta(t)}dw.$
  - $\sigma(t), \beta(t)$ are hyper-parameters.



Reversing the SDE

- Reversing the SDE: finding some stochastic process that goes from noise to data.
  - Use to generate data!

- Theorem (Anderson '82): there exists a reversing SDE, and it has a nice form:

$$\boxed{dx = [f(x,t) - g^2(t)\nabla_x \log p_t(x)]dt + g(t)dw}$$

X(0)

- Strategy: learn the score function, then solve this reverse SDE.

Reversing the SDE

- Learning the score function: use score matching!

$$\arg\min_\theta \sum_i \lambda(\sigma_i)\mathbb{E}_{x\sim p_{\sigma_i,data}}\|s_\theta(x,i) - \nabla_x \log p_{\sigma_i,data}(x)\|^2$$

$$\Rightarrow \arg\min_\theta \mathbb{E}_{t\sim unif[0,T]}\mathbb{E}_{p_t(x)}\left[\lambda(t)\|s_\theta(x,t) - \nabla_x \log p_t(x)\|^2\right]$$

- Use existing techniques: sliced score matching
- No need to tune temperature schedule
  - Still need to choose a forward SDE, $\lambda(\sigma_i)$, etc
  - Typically choose $\lambda(t) \propto 1/\mathbb{E}\left[\|\nabla_{x(t)}\log p(x(t)\mid x(0))\|^2\right]$

Sampling by Solving the Reverse SDE

$$dx = [f(x,t) - g^2(t)\nabla_x \log p_t(x)]dt + g(t)dw$$

- Euler-Maruyama discretization:
  - $\Delta x \leftarrow [f(x,t) - g^2(t)s_\theta(x,t)]\Delta t + g(t)\sqrt{\Delta t}z_t$
  - $x \leftarrow x + \Delta x$
  - $t \leftarrow t + \Delta t$
- Other solvers:
  - Runge-Kutta
  - Predictor-corrector (Song et al. '21)

Evaluating Probability by Converting to ODE

- De-randomizing SDE

$$dx = [f(x,t) - g^2(t)\nabla_x \log p_t(x)]dt + g(t)dw$$

Gaussian

$$dx = [f(x,t) - g^2(t)\nabla_x \log p_t(x)]dt, x(T) \sim p_T$$

- Given an initial distribution and an ODE, we can evaluate probability at any time
  - Say given $x(T) \sim p_T$ and $dx = f(x,t)dt$

$$\log p_0(x(0)) = \log p_T(X(T)) + \int_0^T Tr(Df_\theta(x,t))dt$$

  - Solve via ODE.