Large Scale ML: Generative models

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What this lesson is about

Figure: Images generated by several different prompts using the FLUX model.[1]

[1] `https://huggingface.co/black-forest-labs/FLUX.1-schnell`

The probabilistic point of view

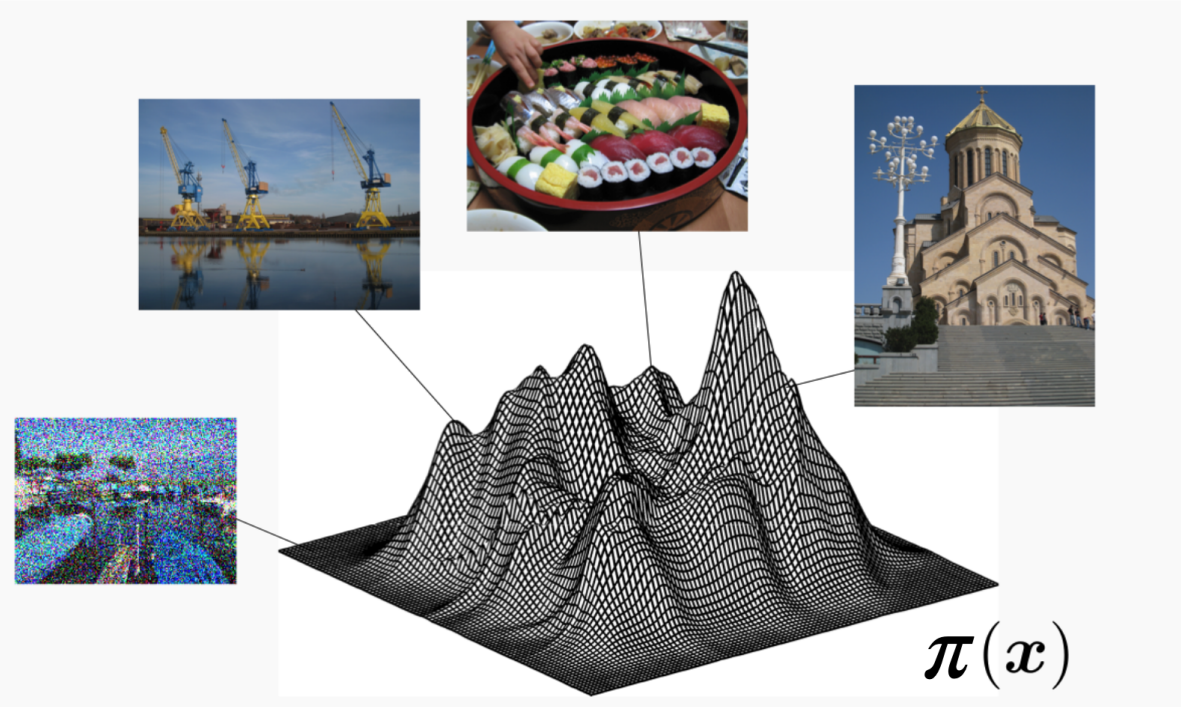

Figure: Landscape of the underlying data distribution [2].

[2] Source: https://www.charles-deledalle.fr/pages/files/ucsd_ece285_mlip/

A bit of context

- π lives in a high-dimensional space $d_x > 10^5$.
- We have access to big datasets $\mathcal{D} = \{X_1, \cdots, X_n\}$, $n > 10^5$, of samples of π.
- We have no parametric model for our data. [3]

Problem: For general π, density estimation in high-dimensions requires an exponential amount of data.

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The original miracle!

Figure: $X_0 \sim \pi$.

Figure: $X_\sigma = X_0 + \sigma Z$. [4]1

- D_{θ_0} untrained CNN,
- $L_\sigma(\theta) = \|D_\theta(X_\sigma) - X_\sigma\|^2$, $L_0(\theta) = \|D_\theta(X_\sigma) - X_0\|^2$,
- $\theta_t = \theta_{t-1} - \nabla L_\sigma(\theta_{t-1})$

What happens to $\{L_\sigma(\theta_t)\}_{t=1}^N$ and $\{L_0(\theta_t)\}_{t=1}^N$?

[1] $Z \sim \mathcal{N}(0, \mathrm{I})$, $X_0 \perp Z$.

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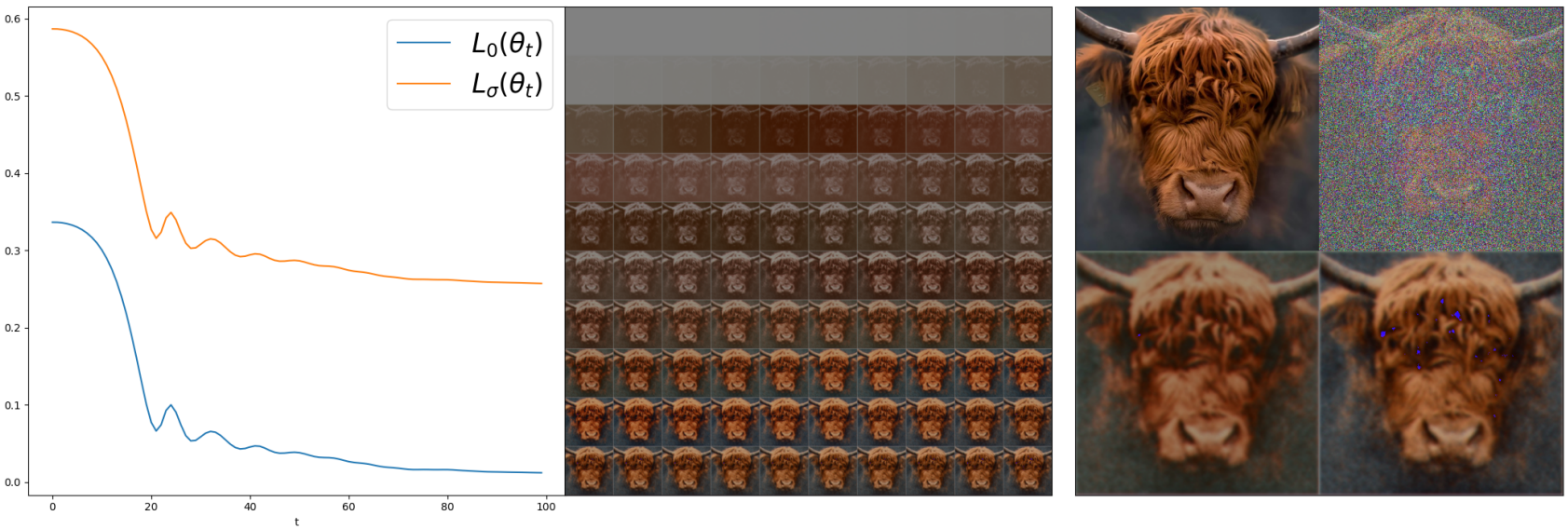
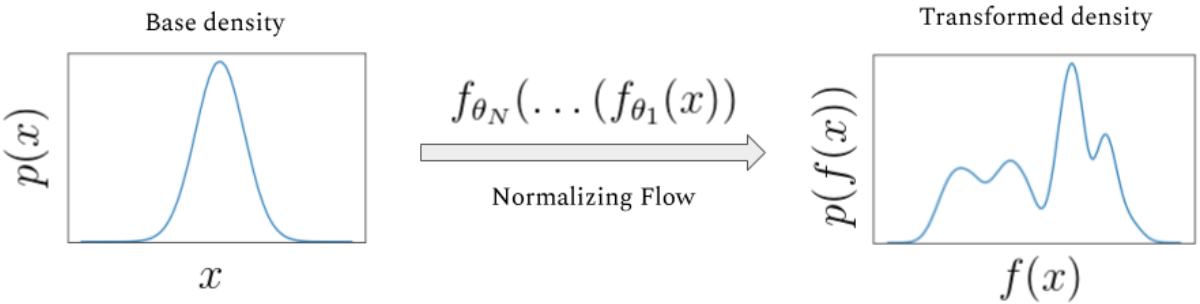


[5] This experiment is inspired by Ulyanov, Vedaldi, and Lempitsky, 2018

Outline

General strategy

1. Define a family of distributions $\mathcal{F} = \{p_\theta \in \mathcal{P}(\mathbb{R}^{d_x}) | \theta \in \Theta\}$. Typically this is done by
   1. Defining a neural network architecture f_θ parameterized by θ
   2. Define a reference distribution λ[6]
   3. $p_\theta := \text{Law}(f_\theta(Z))$ where $Z \sim \lambda$.



2. Choose a divergence[7] over distributions $D : \mathcal{P} \times \mathcal{P} \to \mathbb{R}_*$
3. Solve

$$\theta^* \in \arg\min_{\theta \in \Theta} D(\pi, p_\theta)$$

[6] Typically, a Gaussian or Uniform.
[7] Only property we need is $D(p, q) = 0 \iff p = q$.

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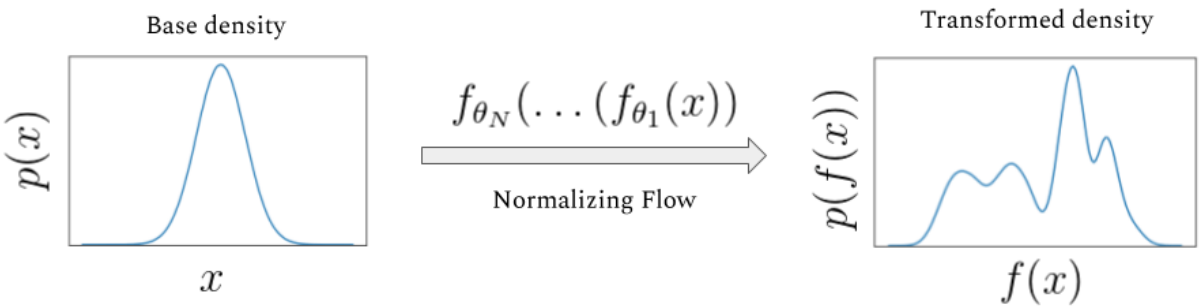

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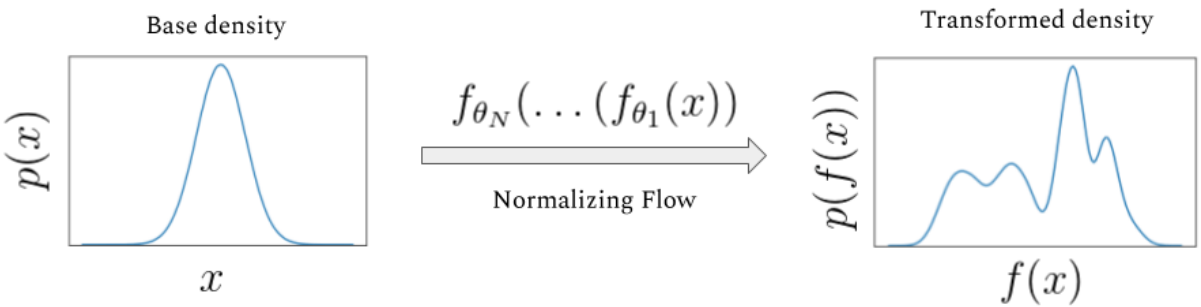

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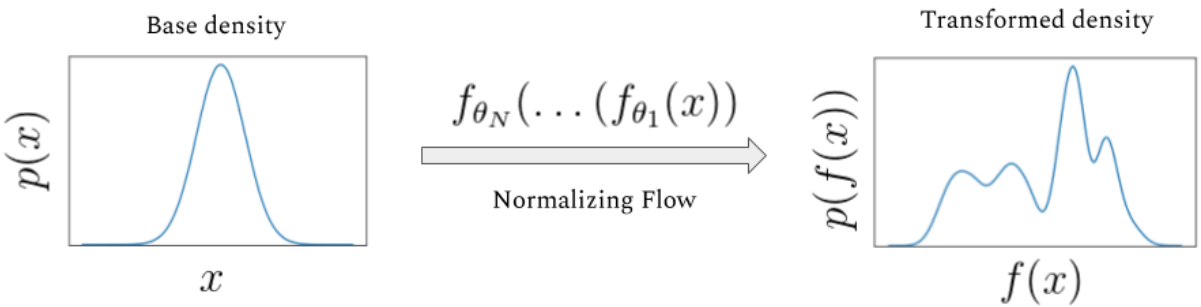

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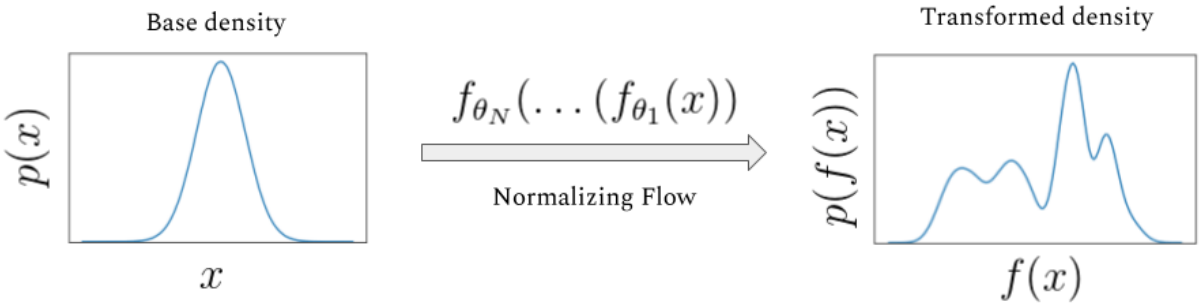

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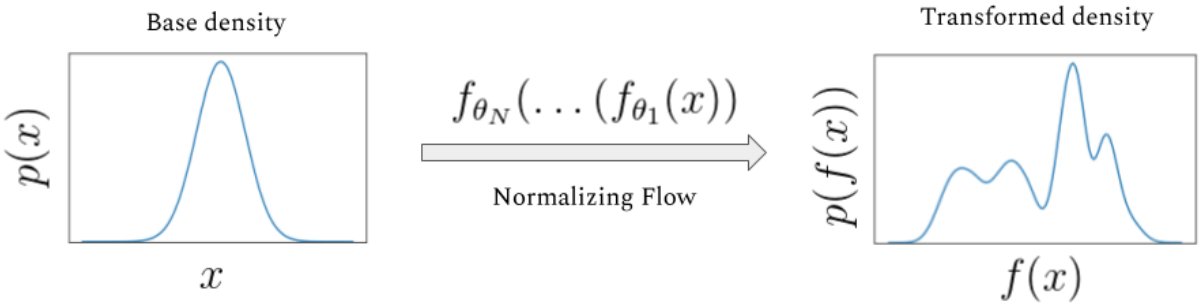

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Kullback Leibler

Let $(p, q) \in \mathcal{P}^2$ such that $p \ll q$

$$\mathrm{D_{KL}}\left(p||q\right) := \mathbb{E}_p\left[\log \frac{\partial p(X)}{\partial q(X)}\right] . \tag{1}$$

If they both admit a density with respect to a given measure μ then

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Some properties

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Minimizing KL $\iff$ doing Maximum likelihood.

So, maybe we can train our generative model by a Monte Carlo approximation of $\mathbb{E}_p\left[\log p_\theta(X)\right]$:

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Can you calculate $\log p_\theta$?

Outline

Change of variable formula

Suppose $f_\theta : \mathbb{R}^{d_x} \to \mathbb{R}^{d_x}$ is invertible. Then,

$$p_\theta(x) = \lambda(f_\theta^{-1}(x))|\mathrm{J}_{f_\theta}(f_\theta^{-1}(x))|^{-1} . \tag{6}$$

Normalizing flow (Rezende and Mohamed, 2015)

A Normalizing flow is a Neural net

$$f_\theta(x) = \mathcal{T}_{\theta_k} \circ \cdots \circ \mathcal{T}_{\theta_0} , \tag{7}$$

where for all $\ell = 0, \cdots, k$, $\mathcal{T}_{\theta_\ell}$ is invertible and has an easy to calculate $|\mathrm{J}_{\mathcal{T}_{\theta_\ell}}|$!

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procedure LOGLIK
Input: x, θ.
Output: $p_\theta(x)$.
    $L = 0$, $z = x$.
    for $\ell = k, \cdots, 0$ **do**
        $z = \mathcal{T}_{\theta_\ell}^{-1}(z)$.
        $L = L - \log |\mathcal{T}_{\theta_\ell}(z)|$.
    end for
    $L = L + \log \lambda(z)$.
    Return: L
end procedure

It is possible to

$$\arg\max_{\theta \in \Theta} n^{-1} \sum_{i=1}^{n} \log p_\theta (X_i) \tag{8}$$

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Illustration

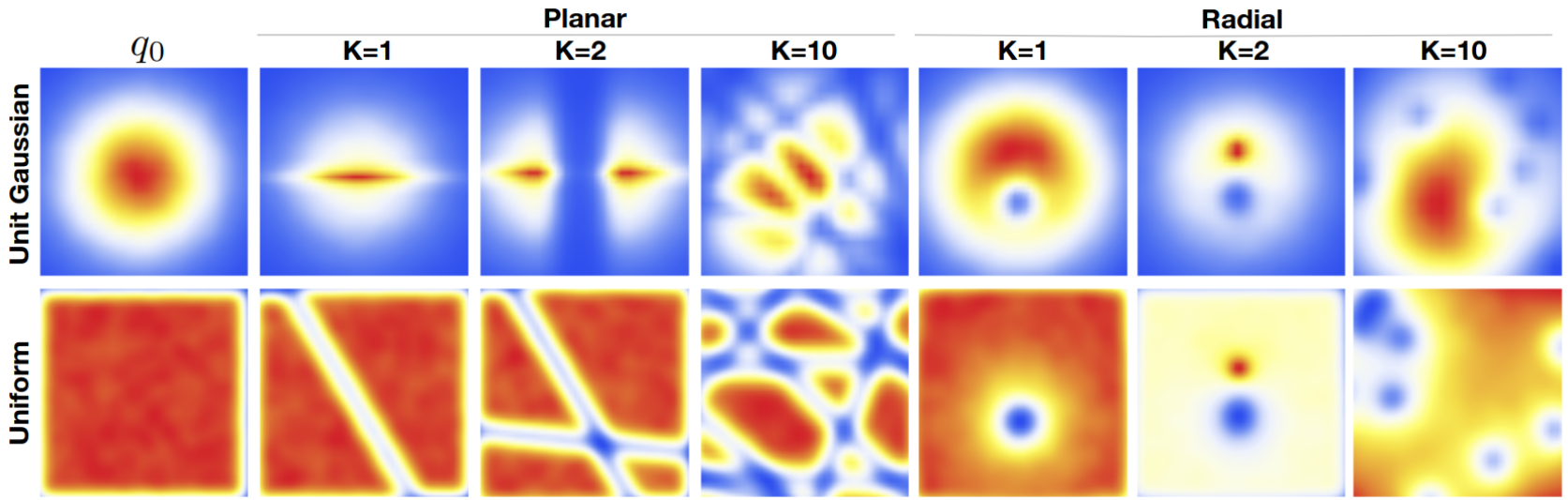

Figure: Illustration from Rezende and Mohamed, 2015 show the transformations obtained during a flow.

RealNVP (Dinh, Sohl-Dickstein, and Bengio, 2017)

$$\mathcal{T}_\theta(x[1{:}d], x[d{:}d_x]) = (x[1{:}d], x[d{:}d_x] \cdot e^{s(x[1:d];\theta)} + t(x[1{:}d];\theta)) \,, \quad (9)$$

where $s(\cdot;\theta), t(\cdot;\theta) : \mathbb{R}^d \to \mathbb{R}^{d_x - d}$ are typically neural networks.
The Jacobian of such flow is

$$\mathrm{J}_{\mathcal{T}_\theta}(x) = \begin{bmatrix} \mathrm{I}d & 0 \\ \dots & \mathrm{diag}(e^{s(x[1:d];\theta)}) \end{bmatrix} \,, \quad (10)$$

and thus $\log |\mathrm{J}_{\mathcal{T}_\theta}(x)| = \sum_{j=1}^{d_x - d} s(x[1{:}d];\theta)[j]$.

Illustration RNVP

Figure: Figure taken from Dinh, Sohl-Dickstein, and Bengio, 2017 illustrating generated samples from RealNVP on the Celeb dataset.

Problems with Normalizing flow

1. Considerable restriction on network architectures.
2. Manifold hypothesis: p_θ admits a density with respect to the ambient Lebesgue measure!

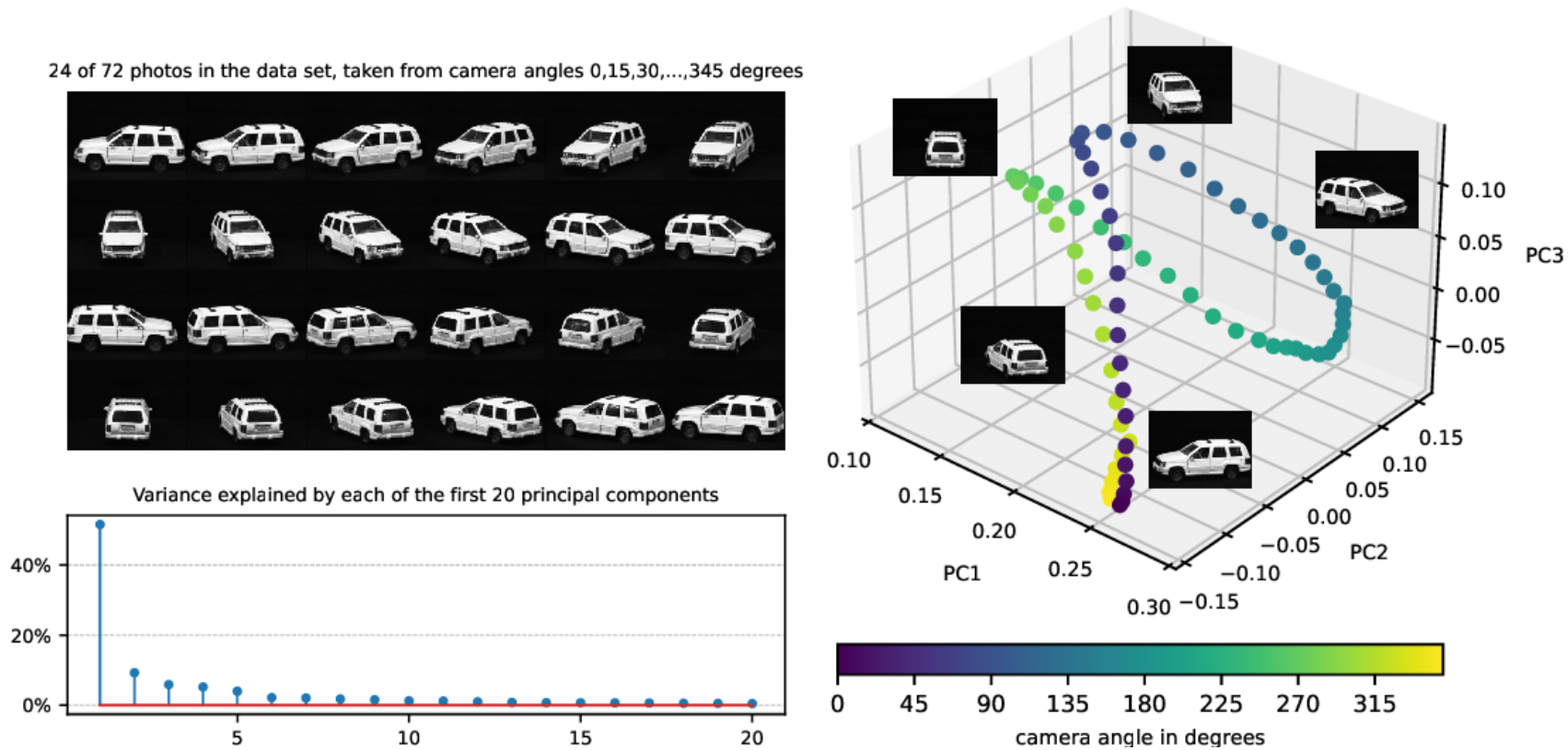

Figure: Taken from (Whiteley, Gray, and Rubin-Delanchy, 2024)

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Latent model

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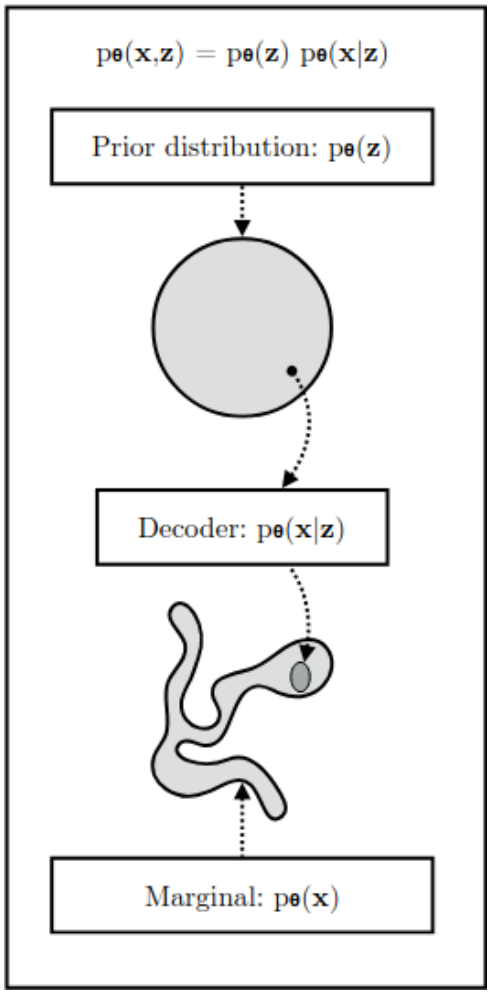

Figure: Illustration of the latent model [1].

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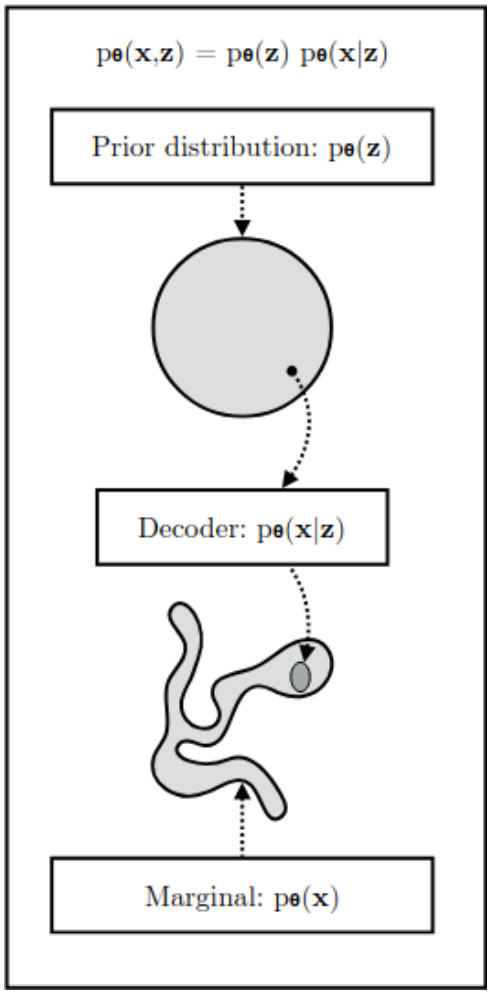
Gaussian Gaussian Latent model

We can consider

1. $\lambda = \mathcal{N}(0, \mathrm{I})$,
2. $p_\theta(\cdot|z) = \mathcal{N}(\mu_\theta(z), \sigma^2 \mathrm{I})$.

For $\mu_\theta(z) = Az$ we recover the (Probabilistic) PCA.
In general, μ_θ will be a Neural network.



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Can you calculate $\log p_\theta$?

For the VAE,

$$\log p_\theta(x) = \log \int p_\theta(x|z)\,\lambda(\mathrm{d}z)\,. \tag{11}$$

The answer is: Yes, but only for linear μ_θ!

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Can you estimate $\log p_\theta(x) = \log \int p_\theta(x|z)\,\lambda(\mathrm{d}z)$?

Naive MC:

1. Sample $Z_{1:K} \sim \lambda$
2. Approximate $p_\theta(x)$ by $K^{-1}\sum_{i=1}^{K} p_\theta(x|Z_i)$.

Problem: This estimation has high variance for realistic cases!

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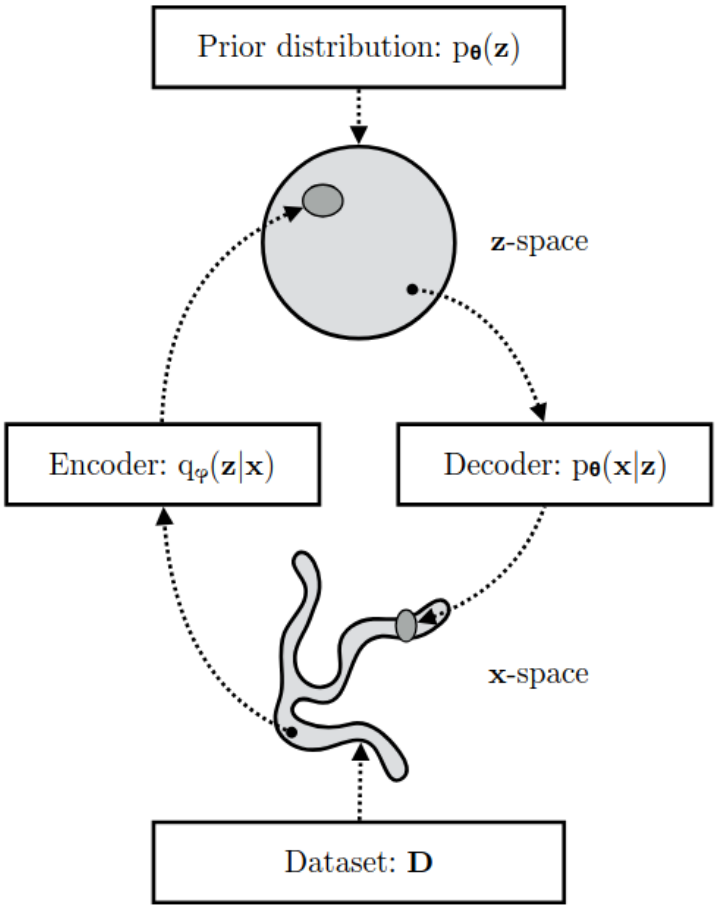

Figure: Overall view of the VAE.[1]

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The VAE solution (Diederik P. Kingma and Welling, 2013).

Introduce a parametric family of instrumental distribution $q_\phi(\cdot|x) \in \mathcal{P}(\mathbb{R}^{d_z})$ to reduce MC variance.

Make it match the true (intractable) posterior:

$$p_\theta(z|x) = \frac{p_\theta(x|z)\,\lambda(z)}{p_\theta(x)}\,. \qquad (12)$$

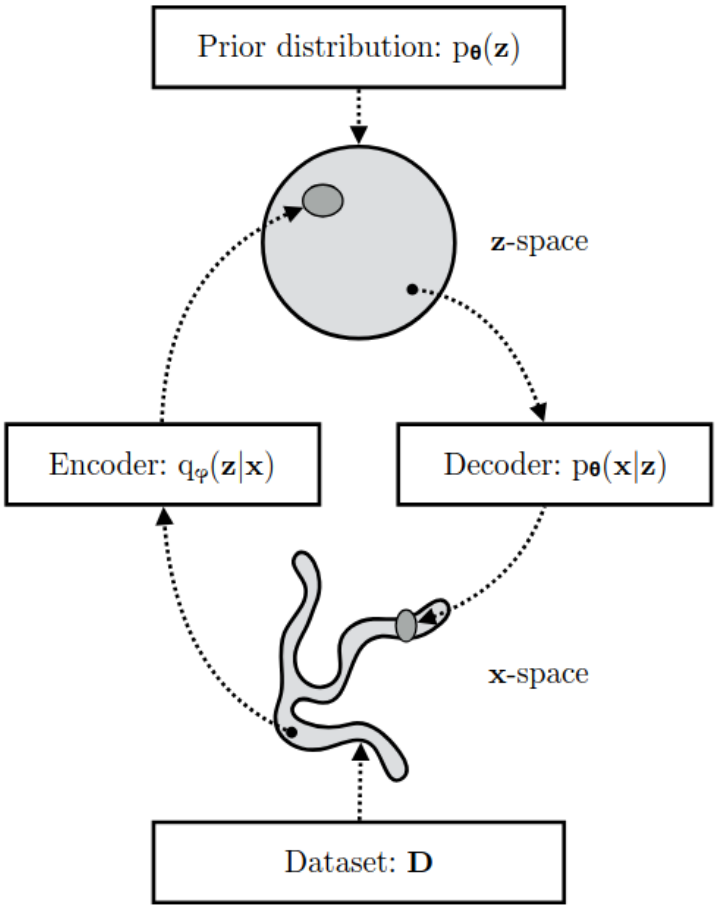

Figure: Overall view of the VAE.[1]

[1] Taken from Diederik P Kingma, Welling, et al., 2019.

Matching the posterior with Kullback Leibler

$$\mathsf{D}_{\mathsf{KL}}\left(q_\phi\left(\cdot|x\right)||p_\theta\left(\cdot|x\right)\right) = \int \log \frac{q_\phi\left(z|x\right)}{p_\theta\left(z|x\right)} q_\phi\left(z|x\right) \mathrm{d}z$$

Matching the posterior with Kullback Leibler

$$\begin{aligned}
\mathsf{D}_{\mathsf{KL}}\left(q_\phi\left(\cdot|x\right)||p_\theta\left(\cdot|x\right)\right) &= \int \log \frac{q_\phi\left(z|x\right)}{p_\theta\left(z|x\right)} q_\phi\left(z|x\right) \mathrm{d}z \\
&= \int \log \frac{q_\phi\left(z|x\right) p_\theta\left(x\right)}{p_\theta\left(x|z\right) \lambda(z)} q_\phi\left(z|x\right) \mathrm{d}z
\end{aligned}$$

Matching the posterior with Kullback Leibler

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\mathrm{D}_{\mathrm{KL}}\left(q_\phi\left(\cdot|x\right)||p_\theta\left(\cdot|x\right)\right) &= \int \log \frac{q_\phi\left(z|x\right)}{p_\theta\left(z|x\right)} q_\phi\left(z|x\right) \mathrm{d}z \\
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&= \log p_\theta\left(x\right) + \int \log \frac{q_\phi\left(z|x\right)}{p_\theta\left(x|z\right) \lambda(z)} q_\phi\left(z|x\right) \mathrm{d}z
\end{aligned}
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&= \log p_\theta\left(x\right) + \int \log \frac{q_\phi\left(z|x\right)}{\lambda(z)} q_\phi\left(z|x\right) \mathrm{d}z - \int \log p_\theta\left(x|z\right) q_\phi\left(z|x\right) \mathrm{d}z
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Evidence lower bound (ELBO)

$$
\begin{aligned}
m(\theta, \phi; x) &:= \log p_\theta\left(x\right) - \mathrm{D}_{\mathrm{KL}}\left(q_\phi\left(\cdot|x\right)||p_\theta\left(\cdot|x\right)\right) \\
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1. Maximize $m(\theta, \phi; x)$ in $\phi \Rightarrow$ Minimize $\mathrm{D}_{\mathrm{KL}}\left(q_\phi(\cdot|x) \,||\, p_\theta(\cdot|x)\right)$.

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We know $\log p_\theta(x) - \mathrm{D}_{\mathrm{KL}}\left(q_\phi(\cdot|x) \,||\, p_\theta(\cdot|x)\right)$ is intractable. Is $\mathbb{E}_{q_\phi(\cdot|x)}\left[\log p_\theta(x|Z)\right] - \mathrm{D}_{\mathrm{KL}}\left(q_\phi(\cdot|x) \,||\, \lambda\right)$ tractable?

Calculating the ELBO

$$\mathbb{E}_{q_\phi(\cdot|x)}\left[\log p_\theta\left(x|Z\right)\right] - \mathrm{D}_{\mathrm{KL}}\left(q_\phi\left(\cdot|x\right)||\lambda\right)$$

Calculating the ELBO

$$\mathbb{E}_{q_\phi(\cdot|x)}\left[\log p_\theta\left(x|Z\right)\right] - \mathrm{D}_{\mathrm{KL}}\left(q_\phi\left(\cdot|x\right)||\lambda\right)$$

Gaussian Gaussian Latent model

Consider

1. $\lambda = \mathcal{N}(0, \mathrm{I})$,
2. $p_\theta\left(\cdot|z\right) = \mathcal{N}(\mu_\theta(z), \sigma^2\mathrm{I})$,
3. $q_\phi\left(\cdot|x\right) = \mathcal{N}(\mu_\phi(x), \Sigma_\phi(x))$.

Here, we consider $\Sigma_\phi(x) = \mathrm{diag}(\sigma^2_\phi(\mathrm{x}))$ where $\sigma^2_\phi(x) \in \mathbb{R}^{d_z}$.

Calculating the ELBO

$$\mathbb{E}_{q_\phi(\cdot|x)}\left[\log p_\theta\left(x|Z\right)\right] - \mathrm{D}_{\mathrm{KL}}\left(q_\phi\left(\cdot|x\right)||\lambda\right)$$

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$$\mathrm{D}_{\mathrm{KL}}\left(q_\phi\left(\cdot|x\right)||\lambda\right) = \frac{1}{2}\left[\|\mu_\phi(x)\|^2 + \mathrm{tr}(\Sigma_\phi(x)) + \log|\Sigma_\phi(x)| - d_z\right] \quad (13)$$

Calculating the ELBO

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$$\mathbb{E}_{q_\phi(\cdot|x)}\left[\log p_\theta\left(x|Z\right)\right] = \mathbb{E}_{q_\phi(\cdot|x)}\left[-\frac{1}{2\sigma^2}\|x - \mu_\theta(Z)\|^2\right] + cte. \quad (14)$$

The reparametrization trick for $\mathbb{E}_{q_\phi(\cdot|x)}\left[-\frac{1}{2\sigma^2}\|x-\mu_\theta(Z)\|^2\right]$

$$q_\phi(\cdot|x) = \mathcal{N}(\mu_\phi(x), diag(\sigma_\phi^2(x))).$$

One way of sampling:

1. Sample $\epsilon \sim \mathcal{N}(0, \mathrm{I})$
2. Set $Z = \mu_\phi(x) + \sigma_\phi(x) \odot \epsilon$.

Thus,

$$\mathbb{E}_{q_\phi(\cdot|x)}\left[-\frac{1}{2\sigma^2}\|x-\mu_\theta(Z)\|^2\right] = \mathbb{E}_{\mathcal{N}(0,\mathrm{I})}\left[-\frac{1}{2\sigma^2}\|x-\mu_\theta(\mu_\phi(x)+\sigma_\phi(x)\odot\epsilon)\|^2\right]$$

We can approximate with MC

$$\begin{aligned}&\mathbb{E}_{\mathcal{N}(0,\mathrm{I})}\left[-\frac{1}{2\sigma^2}\|x-\mu_\theta(\mu_\phi(x)+\sigma_\phi(x)\odot\epsilon)\|^2\right]\\ &\approx K^{-1}\sum_{k=1}^{K}-\frac{1}{2\sigma^2}\|x-\mu_\theta(\mu_\phi(x)+\sigma_\phi(x)\odot\epsilon_k)\|^2\end{aligned}$$

where $\epsilon_k \sim \mathcal{N}(0, \mathrm{I})$.

Calculating the ELBO: Recap

$$\mathbb{E}_{q_\phi(\cdot|x)}\left[\log p_\theta\left(x|Z\right)\right] - \mathrm{D}_{\mathrm{KL}}\left(q_\phi\left(\cdot|x\right)||\lambda\right)$$

Gaussian Gaussian Latent model

Consider

1. $\lambda = \mathcal{N}(0, \mathrm{I})$,
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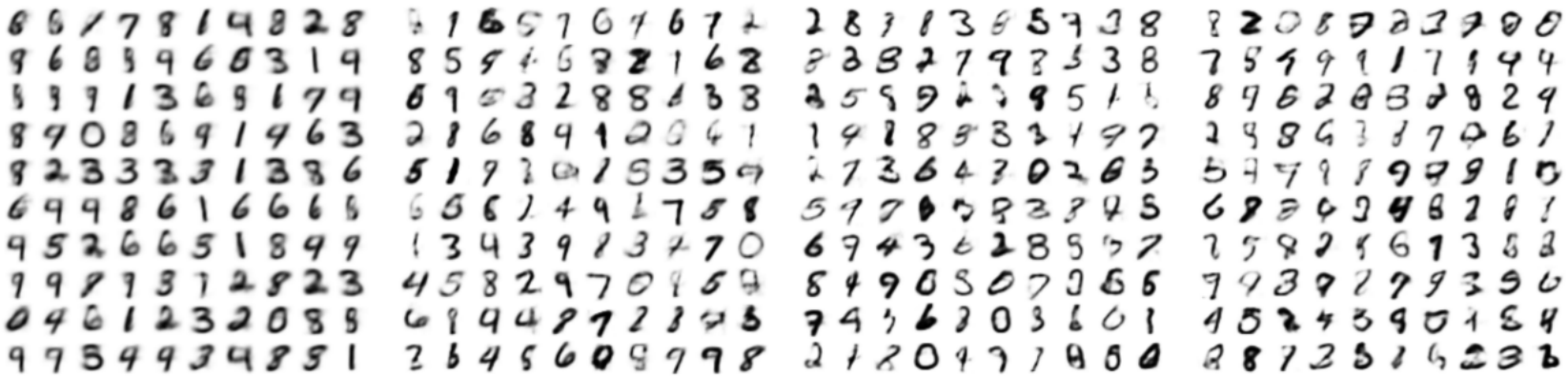
$$\mathbb{E}_{q_\phi(\cdot|x)}\left[\log p_\theta\left(x|Z\right)\right] \approx K^{-1}\sum_{k=1}^{K} -\frac{1}{2\sigma^2}\|x - \mu_\theta(\mu_\phi(x) + \sigma_\phi(x)\odot\epsilon_k)\|^2 + cte. \quad (16)$$

We can calculate gradients!

VAE on MNIST



(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

Figure: MNIST with different latent dimension.

1. VAE are good encoders! (Encode + Decode generalizes well!) ✓
2. Sampling from the prior fails for high dimensional latent models! x

$$Z \sim \lambda\,, \quad X \sim p_\theta\left(\cdot|Z\right)$$

[8] Taken from Diederik P. Kingma and Welling, 2013.

Outline

Bypassing log density completely: Duality

Riesz representation theorem

Every positive linear functional L in $C_c(\mathbb{R}^{d_x})$ can be represented by $L(f) = \mathbb{E}_\mu [f(X)]$ for some $\mu \in \mathcal{P}$.

Maybe, for some divergences, we can bypass calculating log densities by some duality theorem!

For us a duality theorem for a given divergence D allows to evaluate the divergence D between p_0 and p_1 by just considering their effect on functions in a given class!

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Duality for the KL

Theorem (Donsker and Varadhan, 1983)

Let $(q, p) \in \mathcal{P}$, such that $p \ll q$ and $q \ll p$. Then,

$$\mathrm{D}_{\mathrm{KL}}\left(q||p\right) = \sup_{f \in \mathcal{G}_q} \mathbb{E}_q\left[f\right] - \log \mathbb{E}_p\left[\exp(f)\right] \ , \tag{17}$$

where $\mathcal{G}_q$ is the set of measurable g such that $\mathbb{E}_q\left[\exp(g)\right] < \infty$.
Furthermore, equality hold if and only if $f = \log \frac{\mathrm{d}q}{\mathrm{d}p}$.

Duality for Jensen-Shannon

Theorem (Jensen Shannon duality Goodfellow et al., 2014)

Let $(q, p) \in \mathcal{P}$, such that $p \ll q$ and $q \ll p$. Define the Jensen-Shannon entropy as,

$$\mathrm{D}_{\mathrm{JS}}\left(q||p\right) = \frac{1}{2}\left(\mathrm{D}_{\mathrm{KL}}\left(q||p\right) + \mathrm{D}_{\mathrm{KL}}\left(p||q\right)\right) \ . \tag{18}$$

Then,

$$2\,\mathrm{D}_{\mathrm{JS}}\left(q||p\right) = \sup_{D \in \mathcal{C}\ell} \mathbb{E}_q\left[\log D(X)\right] + \mathbb{E}_p\left[\log(1 - D(X))\right] + \log(4)\ , \tag{19}$$

where $\mathcal{C}\ell$ is the set of measurable functions from $\mathbb{R}^{d_x} \to [0, 1]$.

Minimize $\sup_{D \in \mathcal{C}\ell} \mathbb{E}_q [\log D(X)] + \mathbb{E}_p [\log(1 - D(X))]$ $\Leftrightarrow$ Minimize $\mathrm{D}_{\mathrm{JS}}(q||p)$.

The GAN framework

1. Approximate $\mathcal{C}\ell$ by the set of classifiers defined by a Neural network architecture $\mathcal{D}_\phi = \{D_\phi : \mathbb{R}^{d_x} \to [0,1]\}_\phi$.
2. Generative model: $Z \in \mathbb{R}^{d_z} \sim \lambda$, apply a Neural net $X = f_\theta(Z)$, and p_θ the law of X.
3. Train it in two steps:

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   - For fixed ϕ, set $\theta^* = \arg\min_\theta \mathbb{E}_q [\log D_\phi(X)] + \mathbb{E}_\lambda [\log(1 - D_\phi(f_\theta(Z)))]$

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   b. For fixed ϕ, set
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A closer look at GAN training

1. $\phi = \arg\max_\phi \overbrace{\mathbb{E}_\pi \left[\log D_\phi(X)\right] + \mathbb{E}_\lambda \left[\log(1 - D_\phi(f_\theta(Z)))\right]}^{-Cross-entropy}$
   This is equivalent to training a classifier to distinguish between real data $X_r \sim \pi$ from fake data $X_f \sim p_\theta$.
2. $\theta = \arg\min_\theta \mathbb{E}_\pi \left[\log D_\phi(X)\right] + \mathbb{E}_\lambda \left[\log(1 - D_\phi(f_\theta(Z)))\right]$ We are now training the generator to "fool" the classifier by minimizing the cross-entropy.

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   This is equivalent to training a classifier to distinguish between real data $X_r \sim \pi$ from fake data $X_f \sim p_\theta$.
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"In the proposed adversarial nets framework, the generative model is pitted against an adversary: a discriminative model that learns to determine whether a sample is from the model distribution or the data distribution. The generative model can be thought of as analogous to a team of counterfeiters, trying to produce fake currency and use it without detection, while the discriminative model is analogous to the police, trying to detect the counterfeit currency. Competition in this game drives both teams to improve their methods until the counterfeits are indistiguishable from the genuine articles."[9]

[9] from Goodfellow et al., 2014

Original GANs

1. No restriction on architecture ✓
2. No restriction on dimension of the latent space ✓
3. Training requires two networks x
4. Adversarial loss $\rightarrow$ unstable training x
5. Mode collapse x

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An evolution: Wasserstein GANs

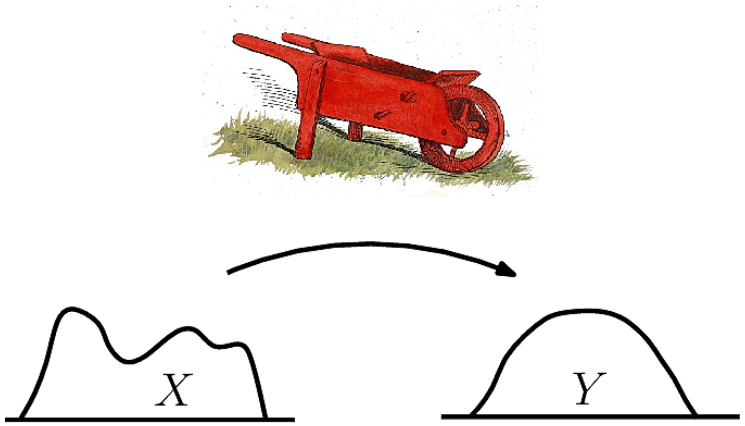


Figure: The earth mover problem

Wasserstein distance

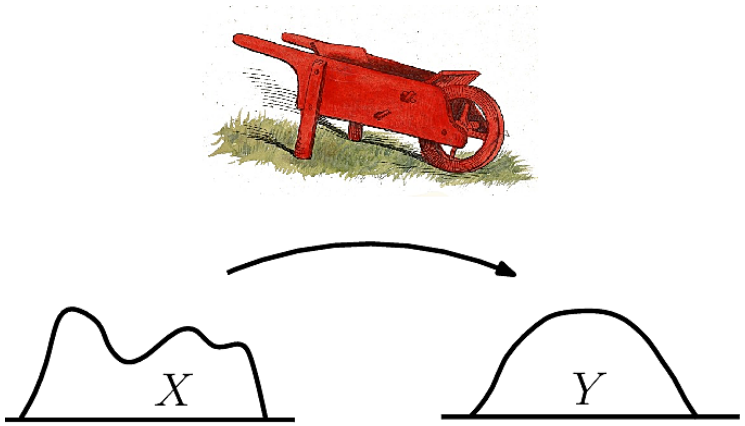
Let $(q, p) \in (\mathcal{P}(\mathbb{R}^{d_x}))^2$, define the set of coupling distributions

$$C(q,p) = \{v \in \mathcal{P}(\mathbb{R}^{d_x} \times \mathbb{R}^{d_x}) | q(A) = v(A \times \mathbb{R}^{d_x}), p(A) = v(\mathbb{R}^{d_x} \times A)\} .$$

The Wasserstein distance is defined as

$$\mathcal{W}(q,p) = \inf_{v \in C(q,p)} \int \|x-y\| v(\mathrm{d}x, \mathrm{d}y) = \inf_{v \in C(q,p)} \mathbb{E}_{(X_0,X_1)\sim v} \left[\|X_0 - X_1\|\right] . \tag{20}$$

[9] Taken from `https://sbl.inria.fr/`.



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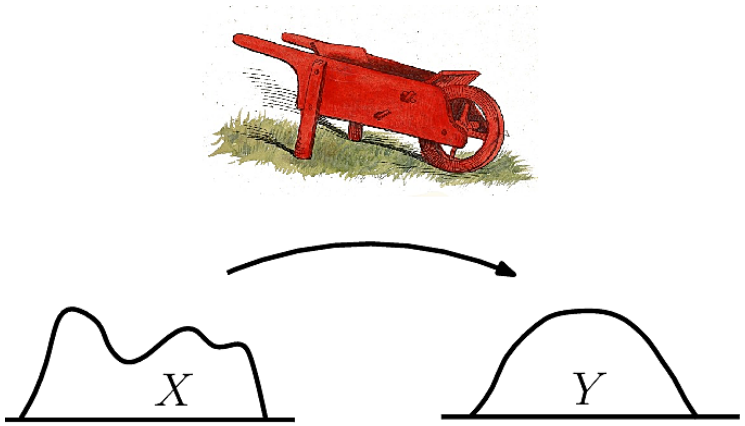

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Theorem (Kantorovich-Rubinstein theorem (see (Villani, 2021)))

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where $\mathrm{Lip}_1 := \{f : \mathbb{R}^{d_x} \to \mathbb{R} || f(x) - f(y)| \leq \|x - y\|\}$.

In Arjovsky, Chintala, and Bottou, 2017 proposes changing $\mathrm{D}_{\mathrm{JS}}(\pi||p_\theta)$ by $\mathcal{W}(\pi, p_\theta)$ in the training of GANs.

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No more mode collapse

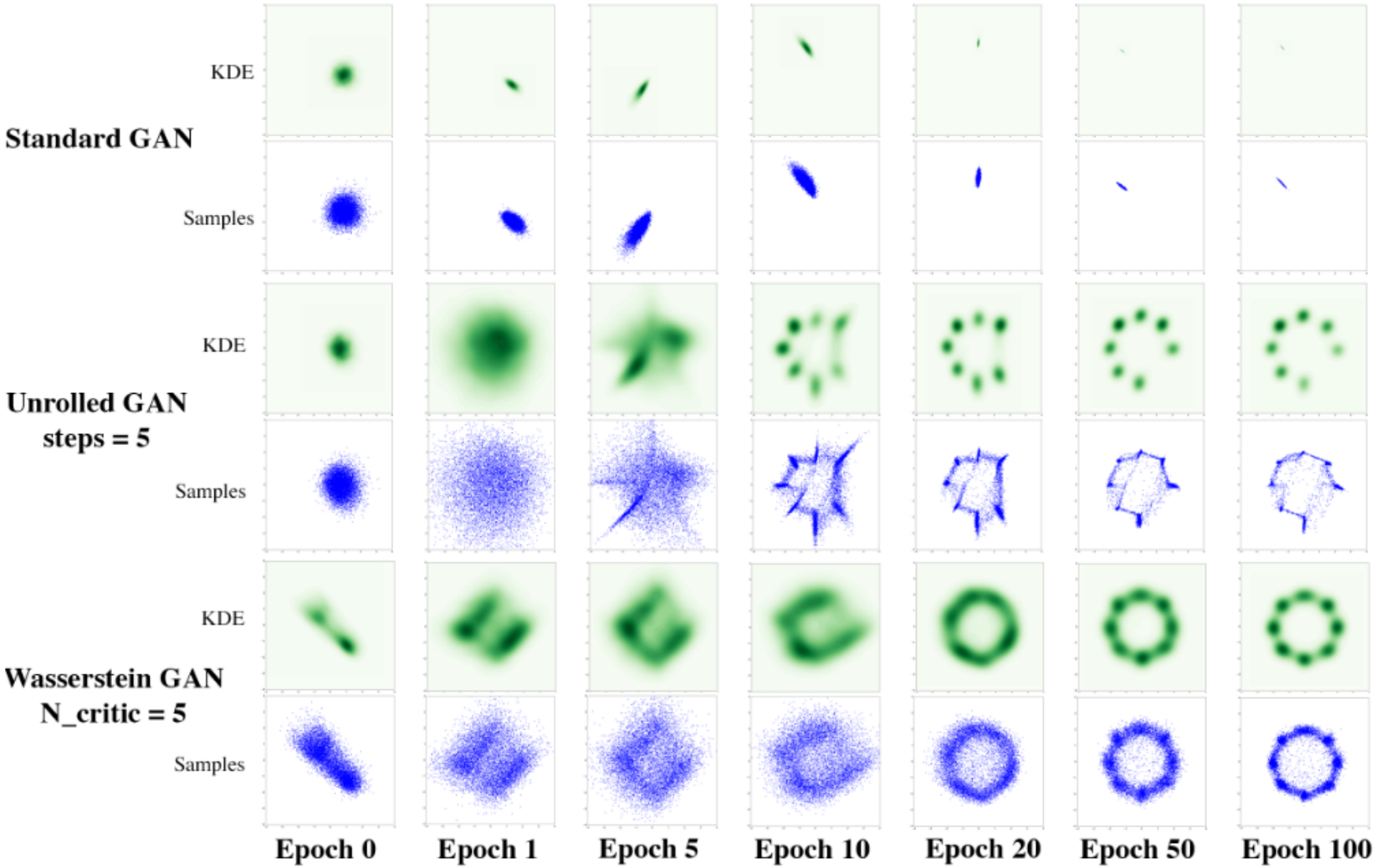

Figure: Comparison between GAN and Wasserstein GANs taken from Arjovsky, Chintala, and Bottou, 2017.

Wasserstein GANs

1. Same pros as the GANs ✓
2. No more mode collapse ✓
3. Growing literature on how to constraint Lipschitz norm of neural net ✓
4. still SOTA (state of the art) in some image tasks ✓
5. Training still requires some care !

Figure: Uncurated images from StyleGAN Karras, Laine, and Aila, 2019.

Outline

Noising and Denoising

Figure: $X_0 \sim \pi$.

Figure: $X_t = X_0 + \sigma_t Z_t$. [10]1

Suppose we have an increasing noise schedule

$$\sigma : [0, T] \to \sigma_t \in \mathbb{R}_* \ .$$

Can we reverse the procedure?

[1] $Z_t \perp X_0$, $Z_t \sim \mathcal{N}(0, \mathrm{I})$.

Noising and Denoising

Suppose we have an increasing noise schedule

$$\sigma : [0, T] \to \sigma_t \in \mathbb{R}_* \ .$$

1. Noising kernel:

$$p_{t|0}(x_t|x_0) = \mathcal{N}(x_t; x_0, \sigma_t^2 \mathrm{I}) \ ,$$

2. Marginal:

$$p_t(x_t) = \int p_{t|0}(x_t|x_0)\pi(\mathrm{d}x_0) \ .$$

Our goal is to go backwards:

$$p_T \to p_{T-\Delta t} \to \cdots \to p_0 \ .$$

Figure: $X_0 \sim \pi$.

Figure:
$X_t = X_0 + \sigma_t Z_t$. [12]1

Generative models by score matching Y. Song et al., 2021

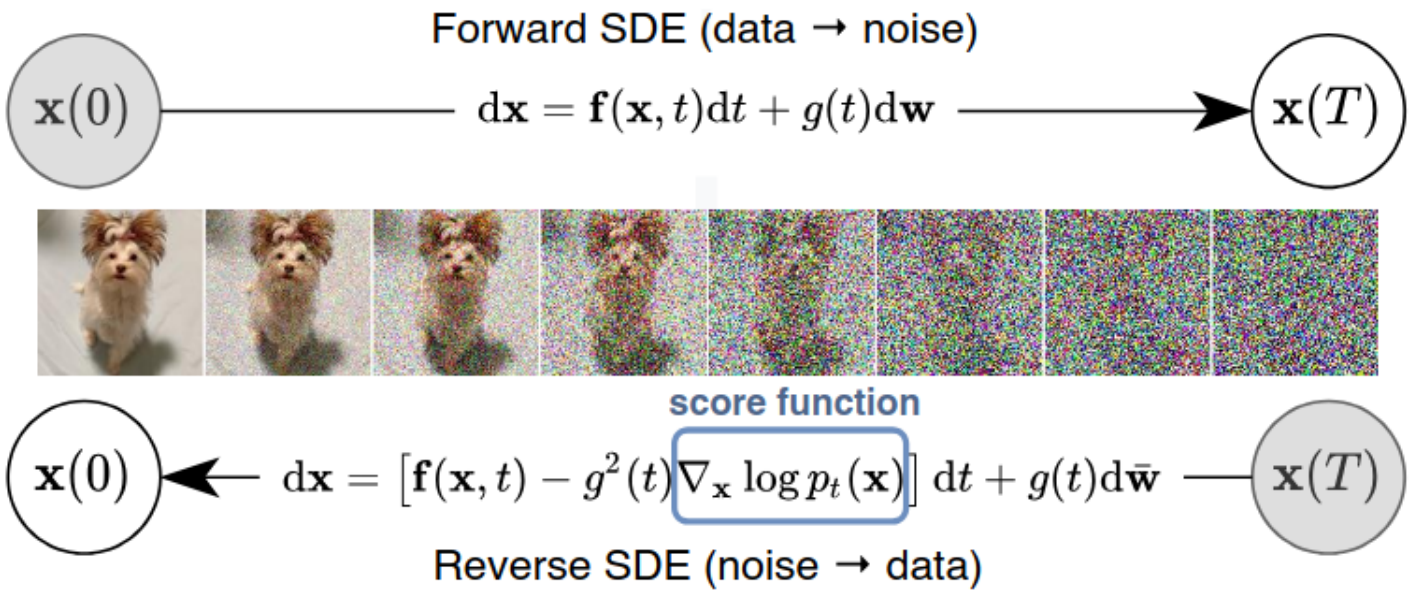

Figure: Illustration of noising and denoising with SDEs.

Our p_t is the time t marginal of the SDE

$$\mathrm{d}x = \sqrt{\frac{d\sigma_t^2}{dt}}\, dw \ .$$

It admits the backward decomposition

$$\mathrm{d}x = -\frac{d\sigma_t^2}{dt} \nabla \log p_t(x) d_t + \sqrt{\frac{d\sigma_t^2}{dt}}\, d\bar{w} \ .$$

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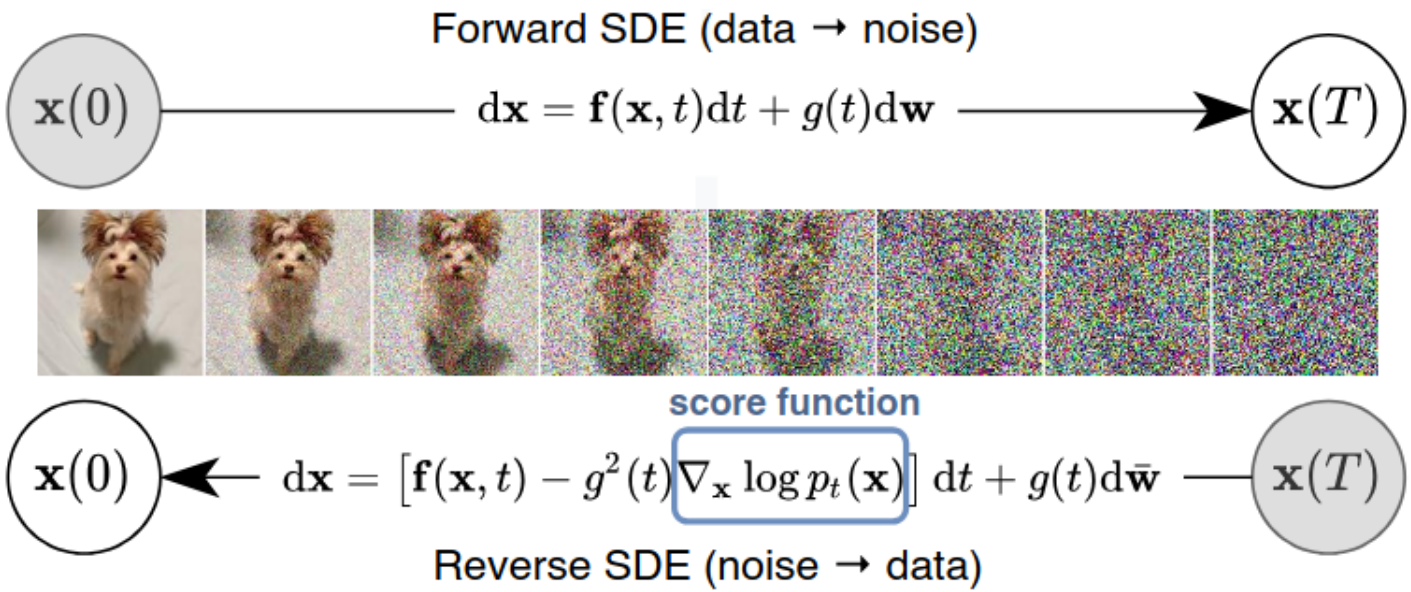

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$\nabla \log p_t(x)$ and denoising

$$\begin{aligned}
\nabla_{x_t} \log p_t(x_t) &= \frac{\nabla_{x_t} p_t(x_t)}{p_t(x_t)} = \frac{\int \nabla_{x_t} p_{t|0}(x_t|x_0)\pi(\mathrm{d}x_0)}{p_t(x_t)} \\
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&= \int \nabla \log p_{t|0}(x_t|x_0) \frac{p_{t|0}(x_t|x_0)\pi(\mathrm{d}x_0)}{p_t(x_t)} \\
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\end{aligned}$$

$\nabla \log p_{t|0}(x_t|x_0) = -\sigma_t^{-2}(x_t - x_0)$, thus

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Denoising and score

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Learning the score from data $\Leftrightarrow$ Learn a denoiser from data.

$$L_{sm}(\theta) = \mathbb{E}_{t \sim \text{Unif}([0,T])}\left[\gamma_t^2 \mathbb{E}_{X_0 \sim \pi, Z \sim \mathcal{N}(0,\text{I})}\left[\|X_0 - D_\theta(X_0 + \sigma_t Z, \sigma_t)\|^2\right]\right] \; .$$

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But $\mathbb{E}\left[\|X_0 - \mathbb{E}\left[X_0|X_t\right]\|^2\right] = \min_{g \text{ measurable}} \mathbb{E}\left[\|X_0 - g(X_t)\|^2\right]$.

Learning the score from data $\Leftrightarrow$ Learn a denoiser from data.

$$L_{sm}(\theta) = \mathbb{E}_{t \sim \text{Unif}([0,T])}\left[\gamma_t^2 \mathbb{E}_{X_0 \sim \pi, Z \sim \mathcal{N}(0,\text{I})}\left[\|X_0 - D_\theta(X_0 + \sigma_t Z, \sigma_t)\|^2\right]\right] \ .$$

Backward simulation

Suppose we have a trained denoiser $D_\theta(x, \sigma_t)$.
We now have to simulate from

$$\mathrm{d}x = \frac{d\sigma_t^2}{dt}\sigma_t^{-2}(x - D_\theta(x, \sigma_t))d_t + \sqrt{\frac{d\sigma_t^2}{dt}}d\bar{w} \ .$$

We should in theory start from p_T.

But $\mathrm{D_{KL}}\left(p_T || \mathcal{N}(0, \sigma_T^2 \mathrm{I})\right) \leq \sigma_T^{-2}\mathbb{E}\left[\|X_0\|^2\right]$.

With an appropriate choice of σ_T, we can start from $\mathcal{N}(0, \sigma_T^2 \mathrm{I})$.

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With an appropriate choice of σ_T, we can start from $\mathcal{N}(0, \sigma_T^2 \mathrm{I})$.

Backward simulation; Naive discretization

We have to simulate from

$$\mathrm{d}x = \frac{d\sigma_t^2}{dt}\sigma_t^{-2}(x - D_\theta(x, \sigma_t))d_t + \sqrt{\frac{d\sigma_t^2}{dt}}d\bar{w} \ .$$

We consider the rather crude approximation

$$X_{t-1} = X_t + \frac{(\sigma_{t-1}^2 - \sigma_t^2)}{\sigma_t^2}(X_t - D_\theta(X_t, \sigma_t)) + \sqrt{\sigma_t^2 - \sigma_{t-1}^2}Z_t$$

Backward simulation; Naive discretization

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Algorithm 3 Backward sampling

procedure SAMPLING
Input: N.
Output: X_0.
  $X_N \sim \mathcal{N}(0, \mathrm{I})$.
  for $i = N-1, \cdots, 0$ **do**
    $t_i = (i/N)T$
    $Z_i \sim \mathcal{N}(0, \mathrm{I})$.
    $X_i = X_{i+1} + \frac{(\sigma^2_{t_i} - \sigma^2_{t_{i+1}})}{\sigma^2_{t_{i+1}}}(X_{i+1} - D_\theta(X_{i+1}, \sigma_{t_{i+1}})) + \sqrt{\sigma^2_{t_{i+1}} - \sigma^2_{t_i}} Z_i$.
  end for
  Return: X_0
end procedure

This is a very naive sampler. There are much better samplers, see Karras, Aittala, et al., 2022 or J. Song, Meng, and Ermon, 2021.

Illustration

Figure: Illustration on the Celeb dataset from Y. Song et al., 2021.

1. SOTA in most image tasks ✓
2. No mode collapse ✓
3. No adversarial training ✓
4. Easier to condition on text (for example) ✓
5. Easy to conditiong à-posteriori ✓
6. Sampling requires more Neural function evaluations (NFE) x

If you want to learn more about Normalizing flows

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Algorithm 4 Backward sampling

procedure SAMPLING
Input: N.
Output: X_0.
  $X_N \sim \mathcal{N}(0, \mathrm{I})$.
  for $i = N-1, \cdots, 0$ **do**
    $t_i = (i/N)T$
    $Z_i \sim \mathcal{N}(0, \mathrm{I})$.
    $X_i = X_{i+1} + \frac{\sigma_{t_i}^2 - \sigma_{t_{i+1}}^2}{\sigma_{t_{i+1}}^2}(X_{i+1} - D_\theta(X_{i+1}, \sigma_{t_{i+1}})) + \sqrt{\frac{\sigma_{t_i}^2}{\sigma_{t_{i+1}}^2}\left(\sigma_{t_{i+1}}^2 - \sigma_{t_i}^2\right)} Z_i$.
  end for
  Return: X_0
end procedure