Generative Models

Distribution learning

Training Data(CelebA)

Model Samples (Karras et.al., 2018)

4 years of progression on Faces

Brundage et al., 2017

Image credits to Andrej Risteski

Distribution learning

BigGAN, Brock et al '18

Distribution learning

Conditional generative model P(zebra images| horse images)

Style Transfer

Input Image Monet Van Gogh

Image credits to Andrej Risteski

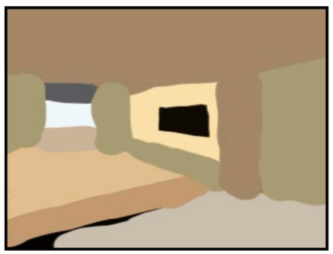
Distribution learning

Source actor

Target actor

Real-time reenactment

Generative model



Generate

Generative model
of realistic images

Stroke paintings to realistic images
[Meng, He, Song, et al., ICLR 2022]

"Ace of Pentacles"

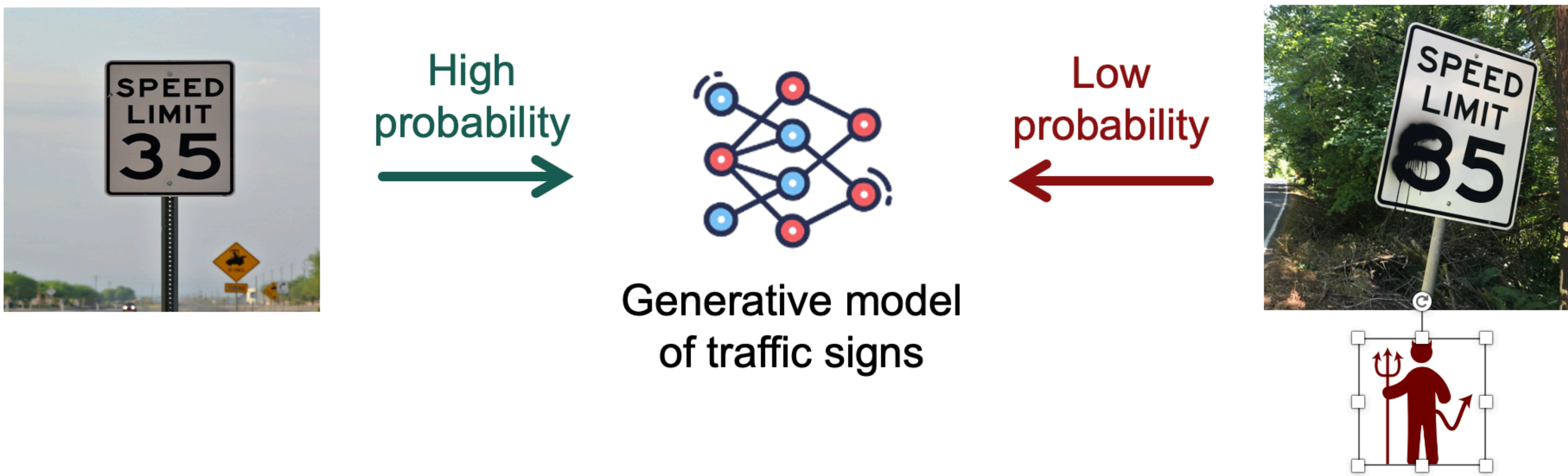
Generate

Generative model
of paintings

Language-guided artwork creation
https://chainbreakers.kath.io @RiversHaveWings

Slides credit to Yang Song

Generative model



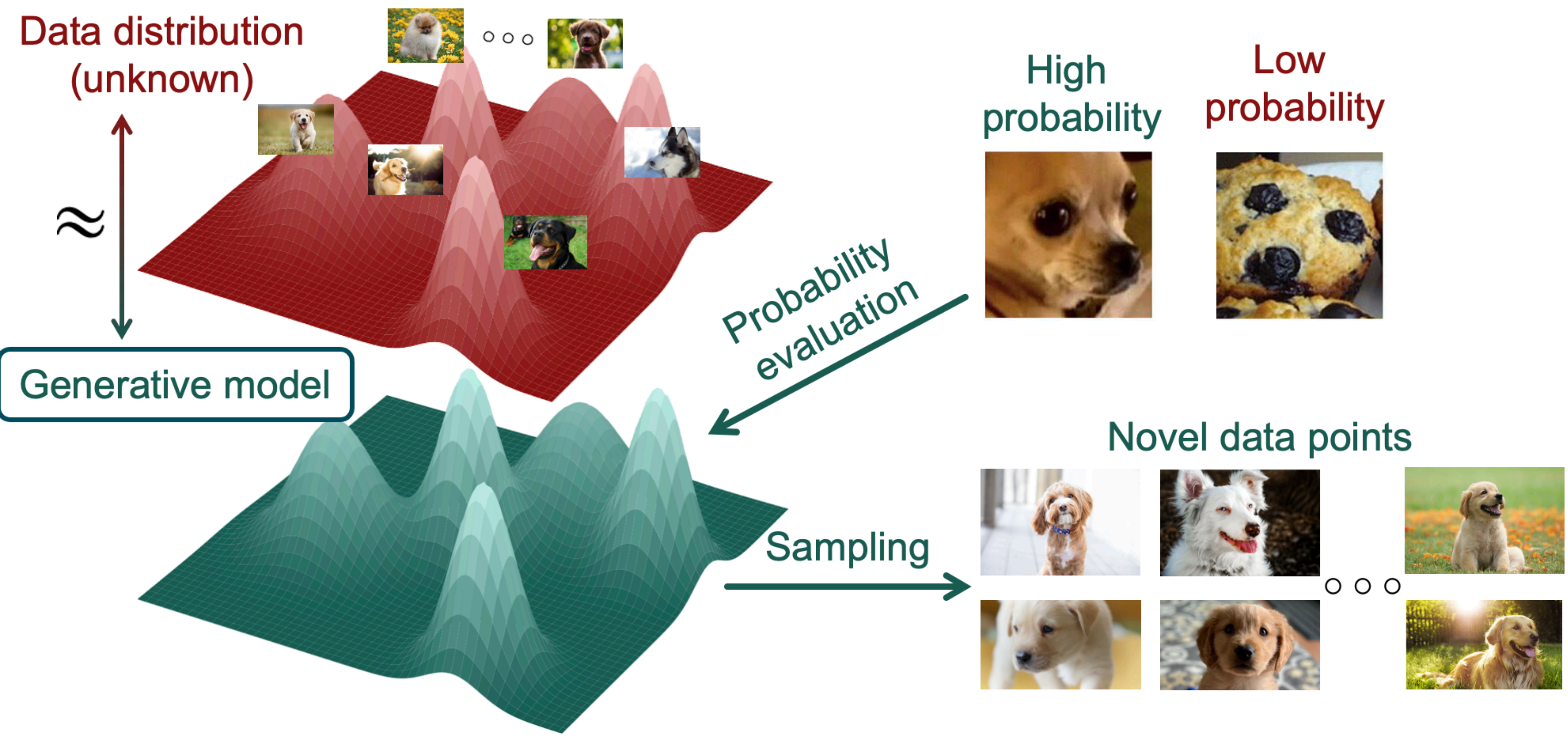
Outlier detection
[Song et al., ICLR 2018]

Slide credit to Yang Song

Desiderata for generative models

- **Probability evaluation**: given a sample, it is computationally efficient to evaluate the probability of this sample.
- **Flexible model family:** it is easy to incorporate any neural network models.
- **Easy sampling:** it is computationally efficient to sample a data from the probabilistic model.

Desiderata for generative models



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Taxonomy of generative models

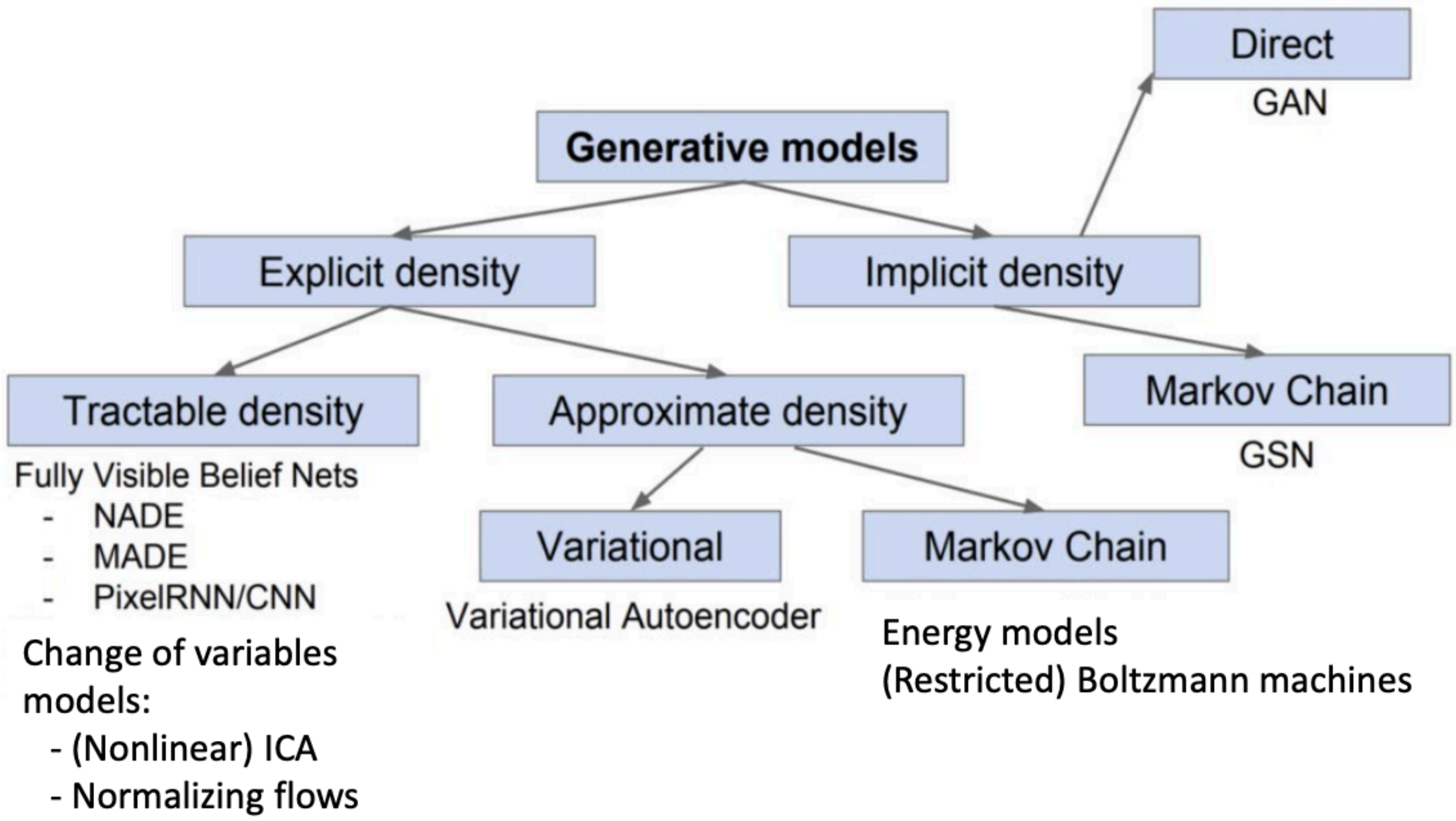
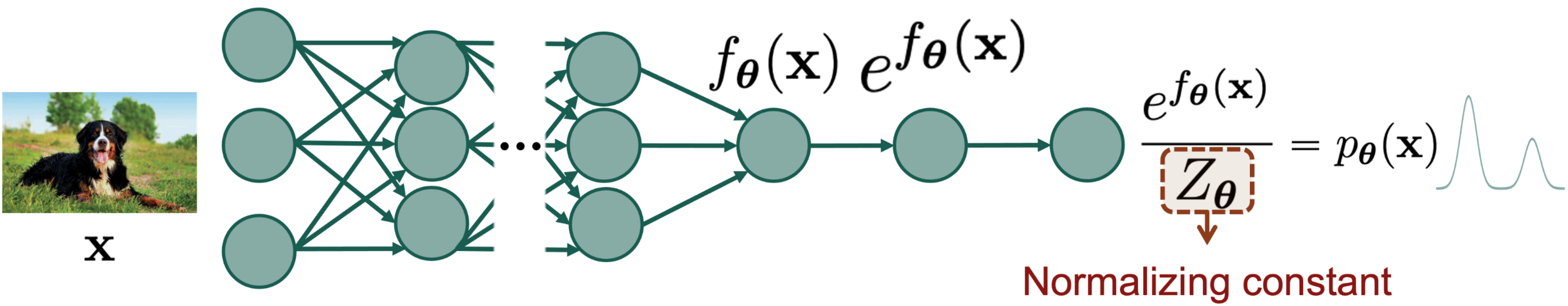


Image credits to Andrej Risteski

Key challenge for building generative models



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Key challenge for building generative models

Approximating the normalizing constant

- Variational auto-encoders [Kingma & Welling 2014, Rezende et al. 2014]
- Energy-based models [Ackley et al. 1985, LeCun et al. 2006]

✕ Inaccurate probability evaluation

Using restricted neural network models

- Autoregressive models [Bengio & Bengio 2000, van den Oord et al. 2016]
- Normalizing flow models [Dinh et al. 2014, Rezende & Mohamed 2015]

✕ Restricted model family

Generative adversarial networks (GANs)

- Model the generation process, not the probability distribution [Goodfellow et al. 2014]

✕ Cannot evaluate probabilities

Slide credit to Yang Song

Training generative models

- **Likelihood-based:** maximize the likelihood of the data under the model (possibly using advanced techniques such as variational method or MCMC):

$$\max_{\theta} \sum_{i=1}^{n} \log p_{\theta}(x_i)$$

- Pros:
  - **Easy training**: can just maximize via SGD.
  - **Evaluation**: evaluating the fit of the model can be done by evaluating the likelihood (on test data).

- Cons:
  - **Large models needed**: likelihood objectve is hard, to fit well need very big model.
  - **Likelihood entourages averaging:** produced samples tend to be blurrier, as likelihood encourages "coverage" of training data.

Training generative models

- **Likelihood-free:** use a **surrogate loss** (e.g., GAN) to train a discriminator to differentiate real and generated samples.

- Pros:
  - **Better objective, smaller models needed:** objective itself is learned - can result in visually better images with smaller models.

- Cons:
  - **Unstable training:** typically min-max (saddle point) problems.
  - **Evaluation:** no way to evaluate the quality of fit.

Generative Adversarial Nets

Implicit Generative Model

- **Goal:** a sampler $g(\cdot)$ to generate images
- A simple generator $g(z;\theta)$:
  - $z \sim N(0,I)$
  - $x = g(z;\theta)$ deterministic transformation

- Likelihood-free training:
  - Given a dataset from some distribution p_{data}
  - Goal: $g(z;\theta)$ defines a distribution, we want this distribution $\approx p_{data}$
  - Training: minimize $D(g(z;\theta), p_{data})$
    - D is some distance metric (not likelihood)
  - Key idea: ***Learn* a differentiable** D

GAN (Goodfellow et al., '14)

- Parameterize the discriminator $D(\,\cdot\,;\phi)$ with parameter ϕ

- **Goal:** learn ϕ such that $D(x;\phi)$ measures how likely x is from p_{data}
  - $D(x,\phi) = 1$ if $x \sim p_{data}$
  - $D(x,\phi) = 0$ if $x! \sim p_{data}$
  - a.k.a., a binary classifier
- GAN: use a neural network for $D(\,\cdot\,;\phi)$

- **Training:** need both negative and positive samples
  - Positive samples: just the training data
  - Negative samples: use our sampler $g(\,\cdot\,;z)$ (can provide infinite samples).

- **Overall objectives:**
  - Generator: $\theta* = \max_{\theta} D(g(z;\theta);\phi)$
  - Discriminator uses MLE Training:

    $\phi* = \max_{\phi} \mathbb{E}_{x\sim p_{data}}[\log D(x;\phi)] + \mathbb{E}_{\hat{x}\sim g(\cdot)}[\log(1 - D(\hat{x};\phi))]$

GAN (Goodfellow et al., '14)

- Generator $G(z;\theta)$ where $z \sim N(0,I)$
  - Generate realistic data
- Discriminator $D(x;\phi)$
  - Classify whether the data is real (from p_{data}) or fake (from G)
- Objective function:

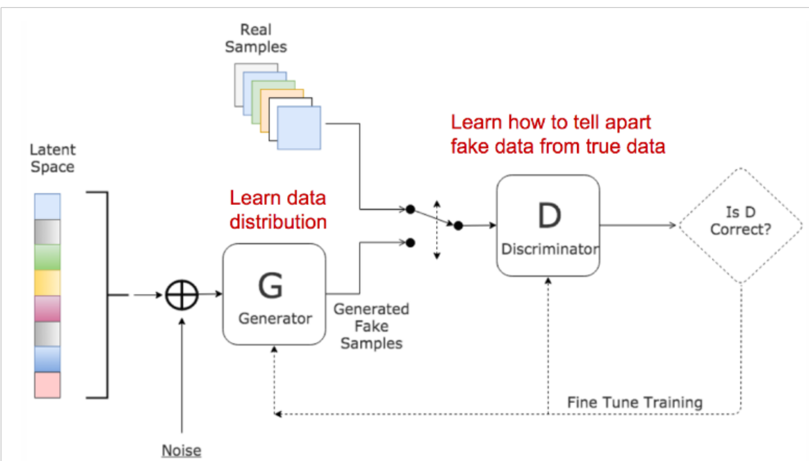
$$L(\theta,\phi) = \min_{\theta}\max_{\phi} \mathbb{E}_{x\sim p_{data}}\left[\log D(x;\phi)\right] + \mathbb{E}_{\hat{x}\sim G}\left[\log(1 - D(\hat{x};\phi))\right]$$

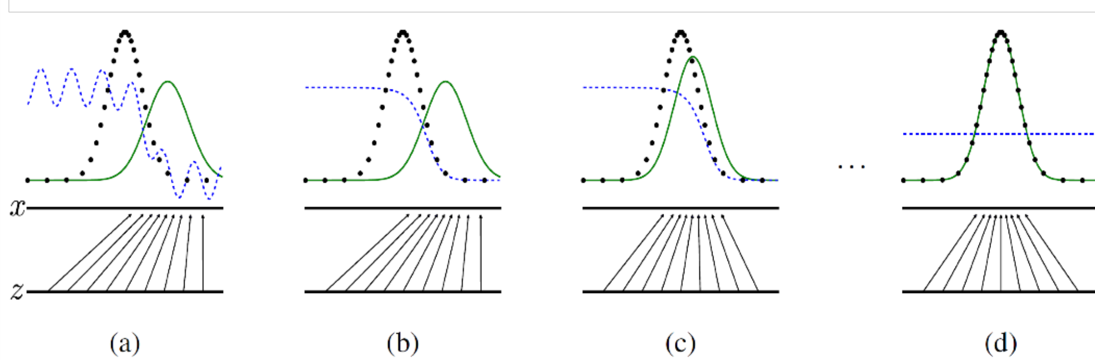
- Training procedure:
  - Collect dataset $\{(x,1)\,|\,x \sim p_{data}\} \cup \{(\hat{x},0) \sim g(z;\theta)\}$
  - Train discriminator
    $D : L(\phi) = \mathbb{E}_{x\sim p_{data}}\left[\log D(x;\phi)\right] + \mathbb{E}_{\hat{x}\sim G}\left[\log(1 - D(\hat{x};\phi))\right]$
  - Train generator $G : L(\theta) = \mathbb{E}_{z\sim N(0,I)}\left[\log D(G(z;\theta),\phi)\right]$
  - Repeat

GAN (Goodfellow et al., ‘14)

- Objective function:

$$L(\theta, \phi) = \min_{\theta} \max_{\phi} \mathbb{E}_{x \sim p_{data}} \left[\log D(x; \phi) \right] + \mathbb{E}_{\hat{x} \sim G} \left[\log(1 - D(\hat{x}; \phi)) \right]$$

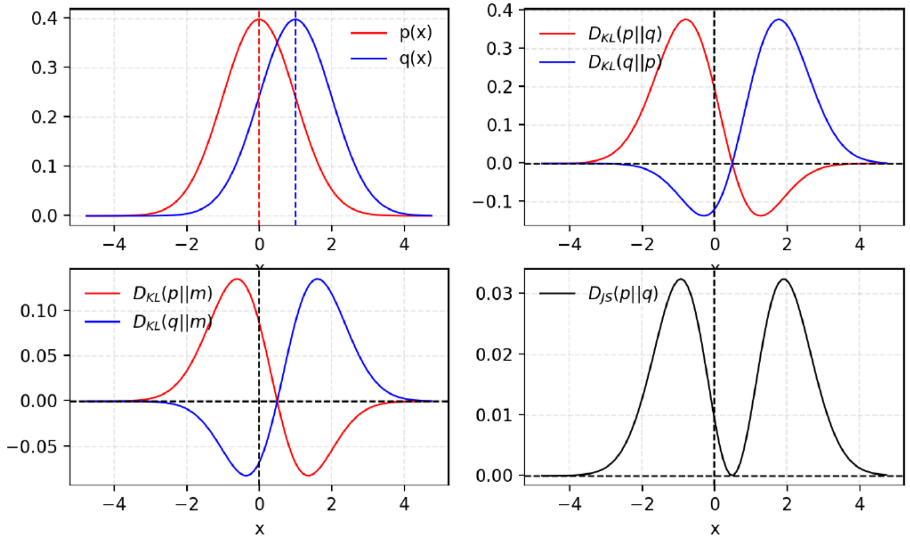




Math Behind GAN

Math Behind GAN

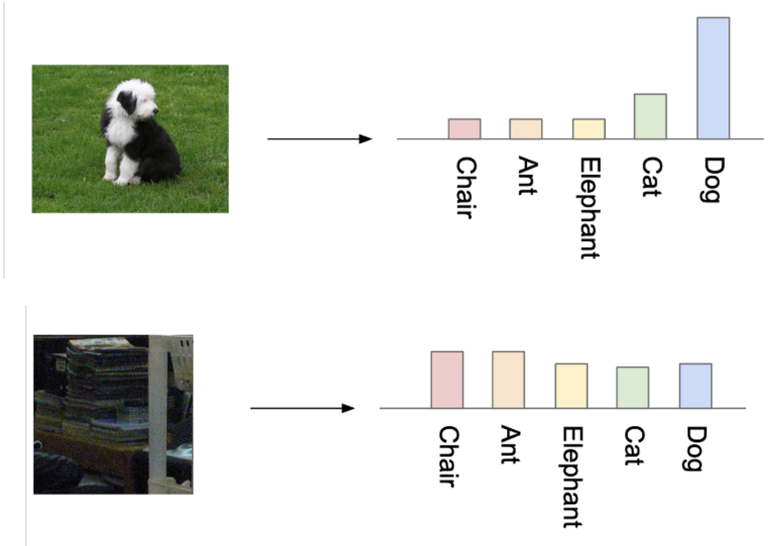
KL-Divergence and JS-Divergence



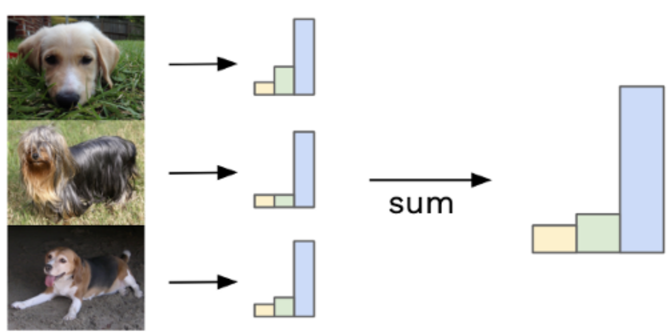
Math Behind GAN

Evaluation of GAN

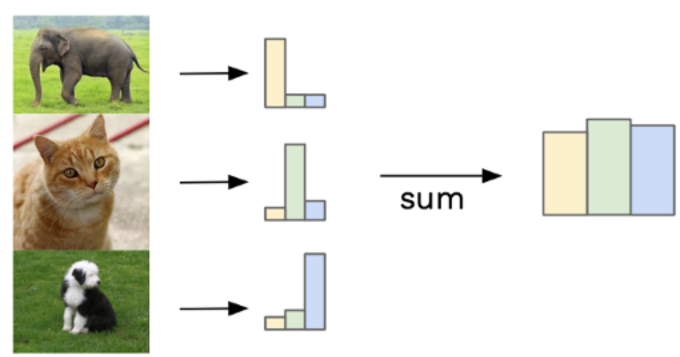
- No $p(x)$ in GAN.
- Idea: use a trained classifier $f(y \mid x)$:
- If $x \sim p_{data}$, $f(y|x)$ should have low entropy
  - Otherwise, $f(y \mid x)$ close to uniform.
- Samples from G should be diverse:
  - $p_f(y) = \mathbb{E}_{x \sim G}[f(y|x)]$ close to uniform.



Similar labels sum to give focussed distribution

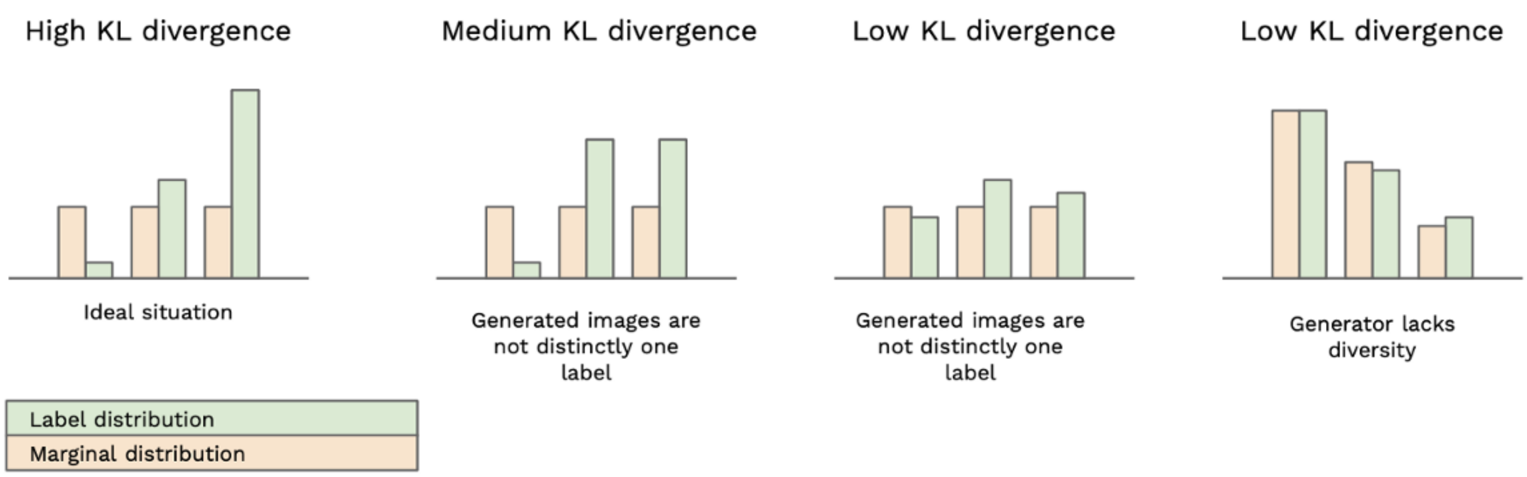


Different labels sum to give uniform distribution



Evaluation of GAN

- **Inception Score** (IS, Salimans et al. '16)
  - Use Inception V3 trained on ImageNet as $f(y\,|\,x)$
  - $IS = \exp\left(\mathbb{E}_{x\sim G}\left[KL(f(y\,|\,x)\,||\,p_f(y)))\right]\right)$
  - Higher the better



Comments on GAN

- Other evaluation metrics:
  - Fréchet Inception Distance (FID): Wasserstein distance between Gaussians

- Mode collapse:
  - The generator only generate a few type of samples.
  - Or keep oscillating over a few modes.

- Training instability:
  - Discriminator and generator may keep oscillating
  - Example: $-xy$, generator x, discriminatory y. NE: $x = y = 0$ but GD oscillates.
  - No stopping criteria.
  - Use Wsserstein GAN (Arjovsky et al. '17):
    $$\min_{G} \max_{f:\text{Lip}(f)\leq 1} \mathbb{E}_{x\sim p_{data}}\left[f(x)\right] - \mathbb{E}_{\hat{x}\sim p_G}[f(\hat{x})]$$
  - And need many other tricks…

Variational Autoencoder

Architecture

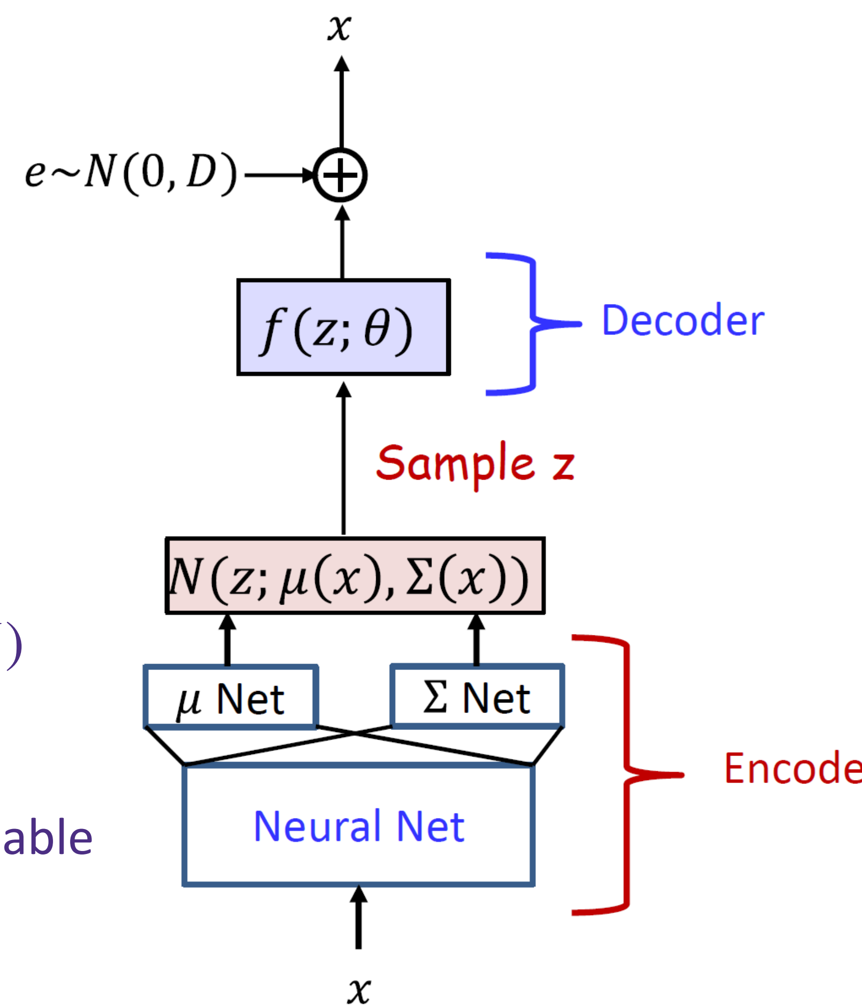
- Auto-encoder: $x \rightarrow z \rightarrow x$
- Encoder: $q(z \mid x; \phi) : x \rightarrow z$
- Decoder: $p(x \mid z; \theta) : z \rightarrow x$

- Isomorphic Gaussian:

$q(z \mid x; \phi) = N(\mu(x; \phi), \text{diag}(\exp(\sigma(x; \phi))))$

- Gaussian prior: $p(z) = N(0, I)$
- Gaussian likelihood: $p(x \mid z; \theta) \sim N(f(z; \theta), I)$

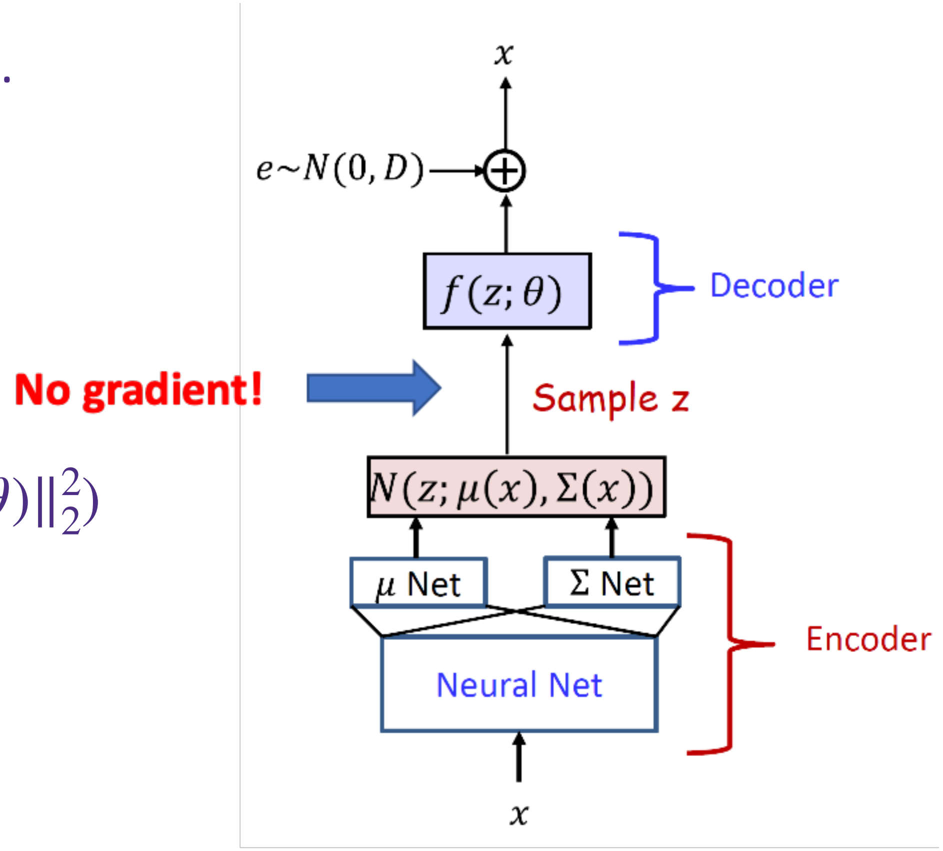
- Probabilistic model interpretation: latent variable model.



VAE Training

- Training via optimizing ELBO
  - $L(\phi, \theta; x) = \mathbb{E}_{z \sim q(z|x;\phi)}[\log p(z|x;\theta)] - KL\left(q(z|x;\phi)\,||\,p(z)\right)$
  - Likelihood term + KL penalty

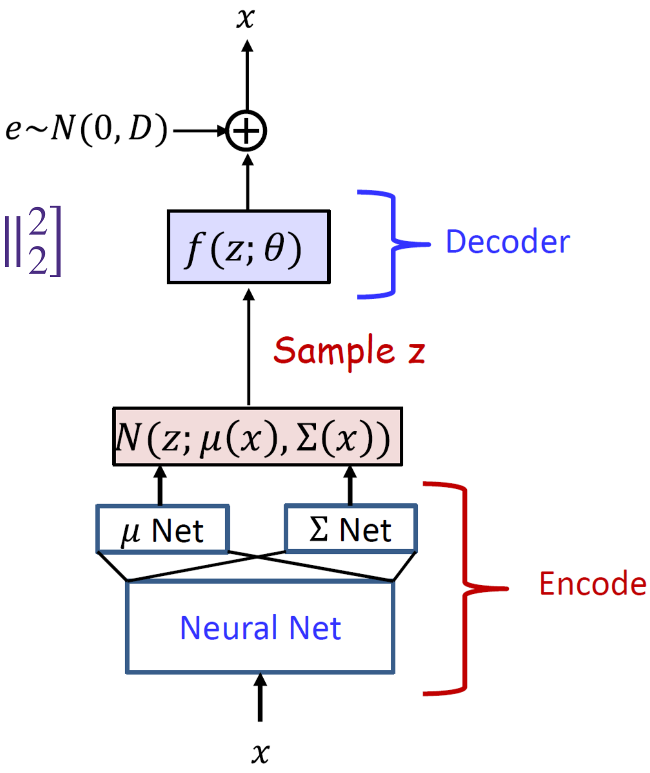
- KL penalty for Gaussians has closed form.
- Likelihood term (reconstruction loss):
  - Monte-Carlo estimation
  - Draw samples from $q(z|x;\phi)$
  - Compute gradient of θ:
    - $x \sim N(f(z;\theta); I)$
    - $p(x) = \frac{1}{\sqrt{2\pi}} \exp(-\frac{1}{2}\|x - f(z;\theta)\|_2^2)$



VAE Training

- Likelihood term (reconstruction loss):
  - Gradient for ϕ . Loss: $L(\phi) = \mathbb{E}_{z\sim q(z;\phi)}\left[\log p(x\,|\,z)\right]$
  - Reparameterization trick:
    - $z \sim N(\mu,\Sigma) \Leftrightarrow z = \mu + \epsilon, \epsilon \sim N(0,\Sigma)$
  - $L(\phi) \propto \mathbb{E}_{z\sim q(z|\phi)}\left[\|f(z;\theta) - x\|_2^2\right]$

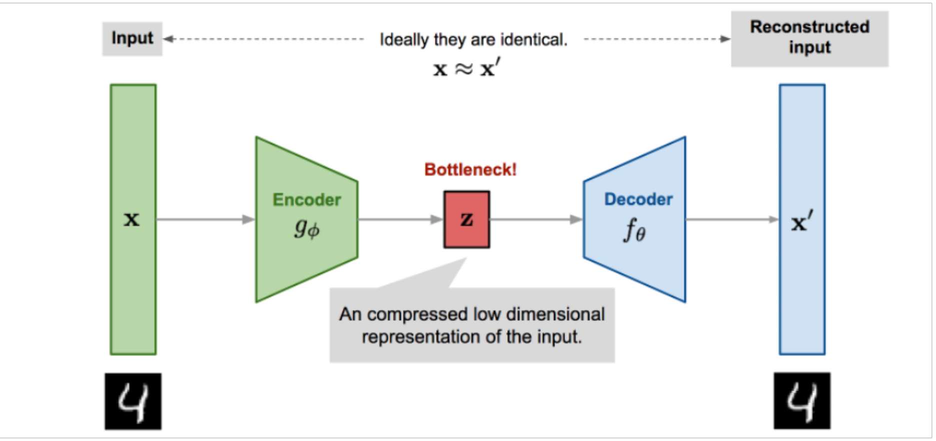
    $\propto \mathbb{E}_{\epsilon\sim N(0,I)}\left[\|f(\mu(x;\phi) + \sigma(x;\phi)\cdot\epsilon;\theta) - x\|_2^2\right]$
  - Monte-Carlo estimate for $\nabla L(\phi)$

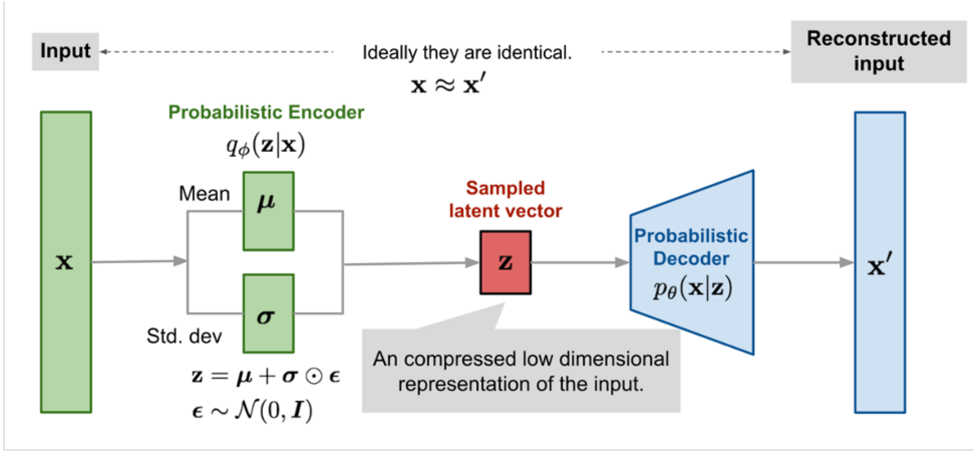


- End-to-end training

VAE vs. AE

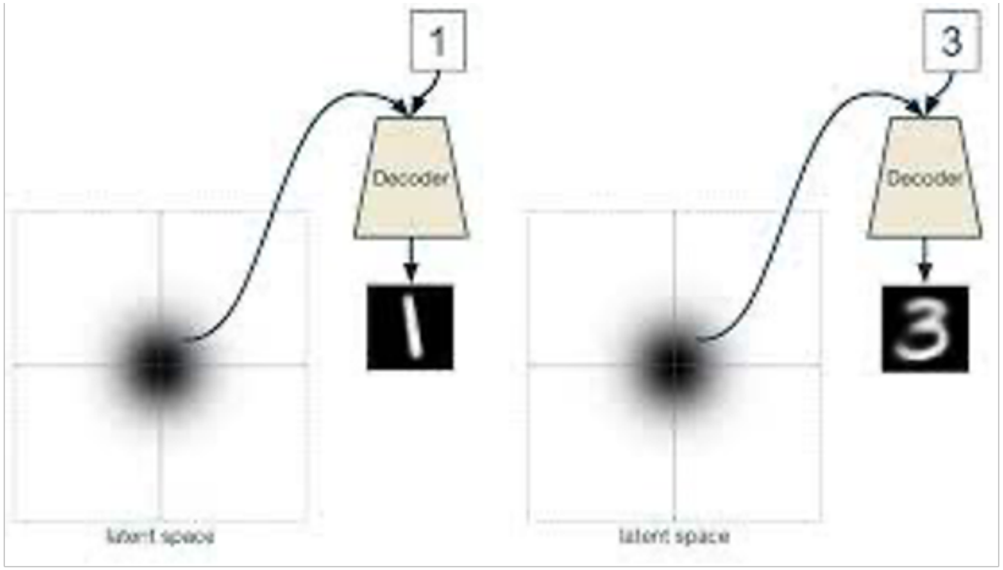
- AE: classical unsupervised representation learning method.
- VAR: a probabilistic model of AE
  - AE + Gaussian noise on z
  - KL penalty: L_2 constraint on the latent vector z





Conditioned VAE

- Semi-supervised learning: some labels are also available



conditioned generation

Comments on VAE

- Pros:
  - Flexible architecture
  - Stable training

- Cons:
  - Inaccurate probability evaluation (approximate inference)

Normalizing Flows

Intuition about easy to sample

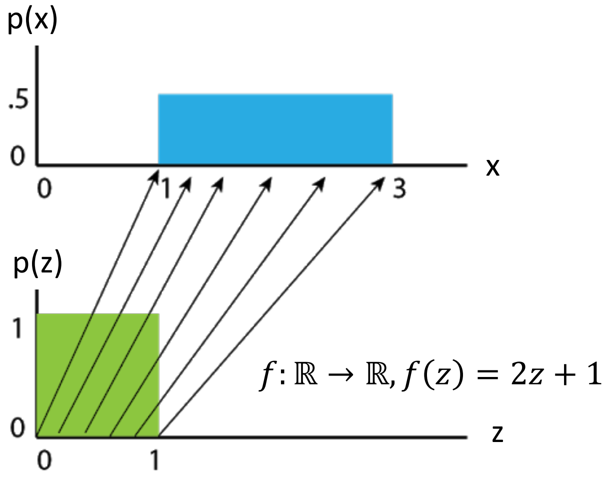
- Goal: design $p(x)$ such that
  - Easy to sample
  - Tractable likelihood (density function)

- 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 $p(x) = ?$



Intuition about tractable density

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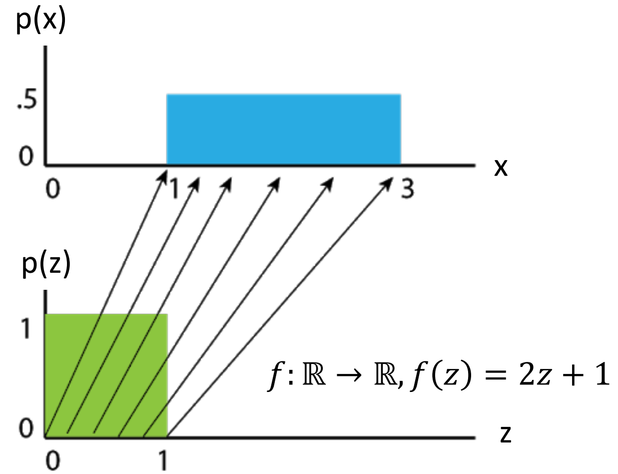


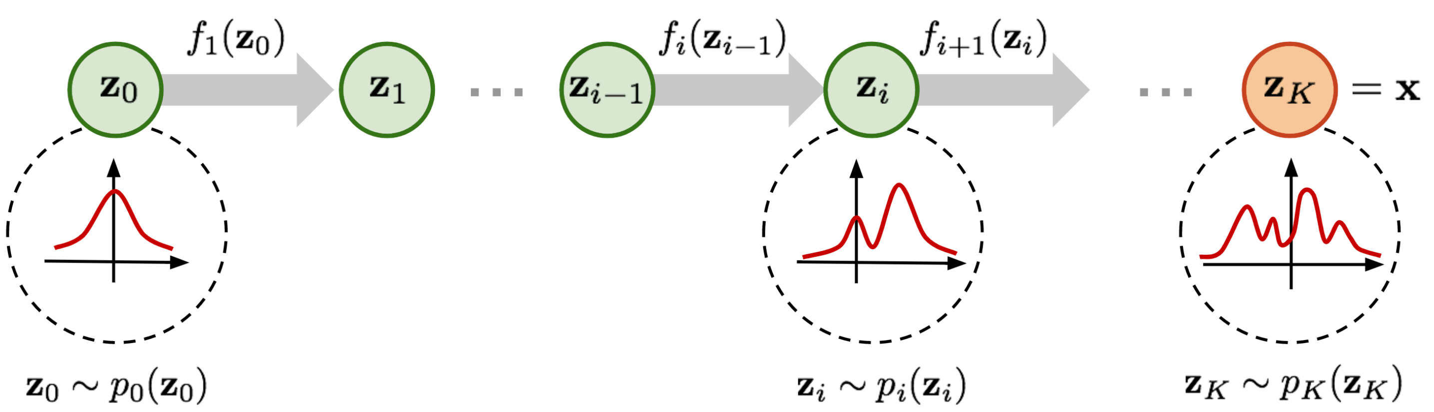
- Uniform: $z \sim$ Unif$[0,1]$
  - Density $p(z) = 1$
  - $x = 2z + 1$, then $p(x) = 1/2$
    - $x = az + b$, then $p(x) = 1/|a|$ (for $a \neq 0$)
  - $x = f(z), p(z)|\frac{dz}{dx}| = |f'(z)|^{-1}p(z)$
    - Assume $f(z)$ is a bijection

Change of variable

- Suppose $x = f(z)$ for some general non-linear $f(\cdot)$
  - The linearized change in volume is determined by the Jacobian of $f(\cdot)$:
  - $$\frac{\partial f(z)}{\partial z} = \begin{bmatrix} \frac{\partial f_z(x)}{\partial z_1} & \cdots & \frac{\partial f_1(z)}{\partial z_d} \\ \cdots & \cdots & \cdots \\ \frac{\partial f_d(z)}{\partial z_1} & \cdots & \frac{\partial f_d(z)}{\partial z_d} \end{bmatrix}$$
- Given a bijection $f(z) : \mathbb{R}^d \to \mathbb{R}^d$
  - $z = f^{-1}(x)$
  - $$p(x) = p(f^{-1}(x)) \left| \det\left(\frac{\partial f^{-1}(x)}{\partial x}\right) \right| = p(z) \left| \det\left(\frac{\partial f^{-1}(x)}{\partial x}\right) \right|$$
  - 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

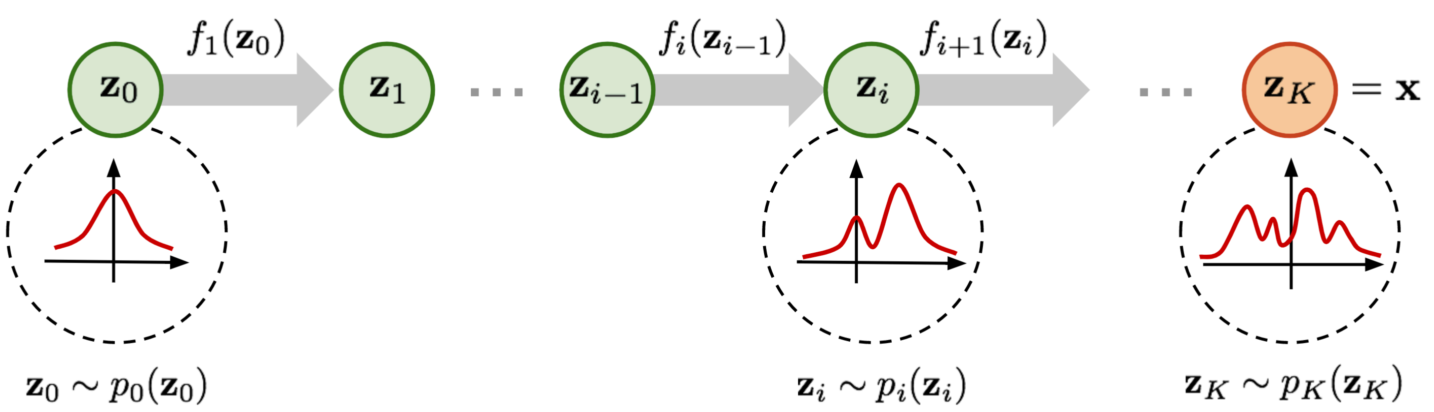
- Idea
  - Sample z_0 from an "easy" distribution, e.g., standard Gaussian
  - Apply K bijections $z_i = f_i(z_{i-1})$
  - The final sample $x = f_K(z_K)$ has tractable desnity
- Normalizing Flow
  - $z_0 \sim N(0,I), z_i = f_i(z_{i-1}), x = Z_K$ where $x, z_i \in \mathbb{R}^d$ and f_i is invertible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



Normalizing Flow

- 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

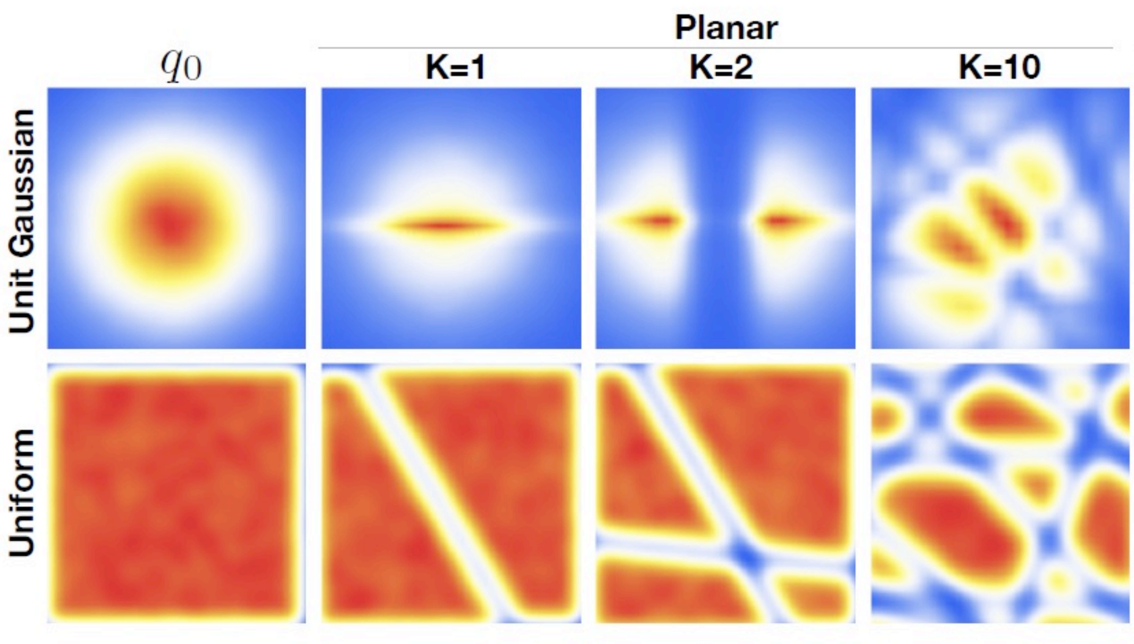
- Naive flow model requires extremely expensive computation
  - Computing determinant of $d \times d$ matrices
- Idea:
  - Design a good bijection $f_i(z)$ such that the determinant is easy to compute

Plannar Flow

- Technical tool: Matrix Determinant Lemma:
  - $\det(A + uv^\top) + (1 + v^\top A^{-1} u) \det A$
- Model:
  - $f_\theta(z) + z + u \odot h(w^\top z + b)$
  - $h(\cdot)$ chosen to be $\tanh(\cdot)(0 < h'(\cdot) < 1)$
  - $\theta = [u, w, b], \det\left(\frac{\partial f}{\partial z}\right) = \det(I + h'(w^\top z + b) u w^\top) = 1 + h'(w^\top z + b) u^\top w$
  - 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
  - Suppose $x_i = f_i(z)$ only depends on $z_{\leq i}$

Energy-Based Models

Energy-based Models

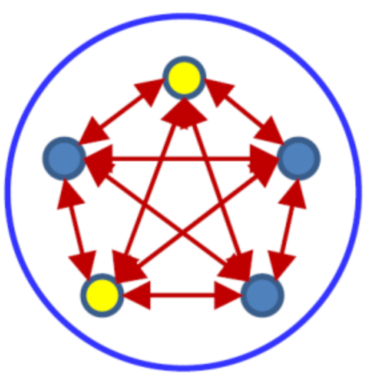
- Goal of generative models:
  - a probability distribution of data: $P(x)$

- Requirements
  - $P(x) \geq 0$ (non-negative)
  - $\int_x P(x)dx = 1$

- Energy-based model:
  - Energy function: $E(x;\theta)$, parameterized by θ
  - $P(x) = \frac{1}{z}\exp(-E(x;\theta))$ (why exp?)
  - $z = \int_z \exp(-E(x;\theta))dx$

Boltzmann Machine

- Generative model
  - $E(y) = -\frac{1}{2}y^\top W y$
  - $P(y) = \frac{1}{z}\exp(-\frac{E(y)}{T})$, T: temperature hyper-parameter
  - W: parameter to learn
- When y_i is binary, patterns are affecting each other through W



$$z_i = \frac{1}{T}\sum_j w_{ji}s_j$$

$$\boxed{P(s_i = 1|s_{j\neq i}) = \frac{1}{1+e^{-z_i}}}$$

Boltzmann Machine: Training

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

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

  - Maximum log-likelihood:

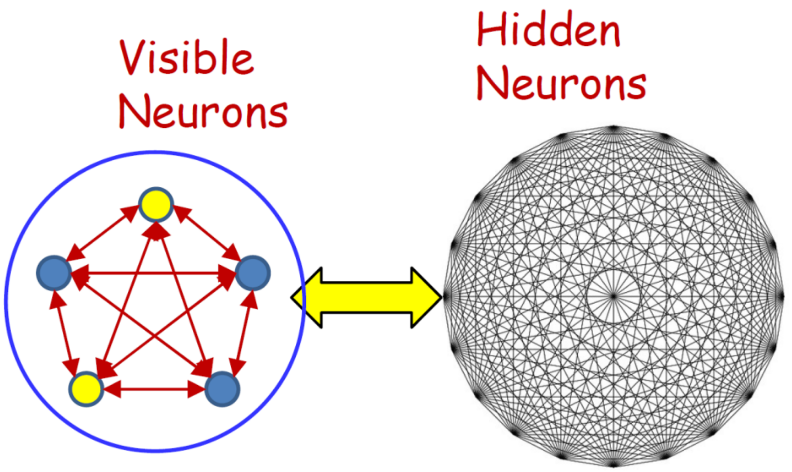
$$L(W) = \frac{1}{N}\sum_{y \in D} \frac{1}{2} y^\top W y - \log \sum_{y'} \exp(\frac{1}{2} y'^\top W y')$$

Boltzmann Machine: Training

Boltzmann Machine: Training

Boltzmann Machine with Hidden Neurons

- Visible and hidden neurons:
    - y: visible, h: hidden
- $P(y) = \sum_h P(y, v)$

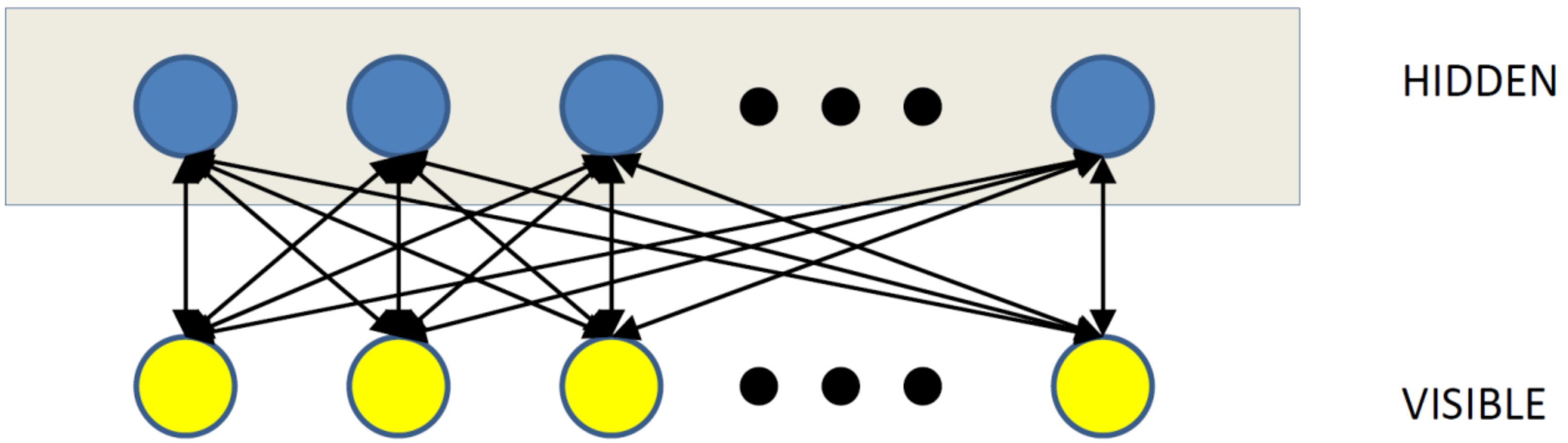


Boltzmann Machine with Hidden Neurons: Training

Boltzmann Machine with Hidden Neurons: Training

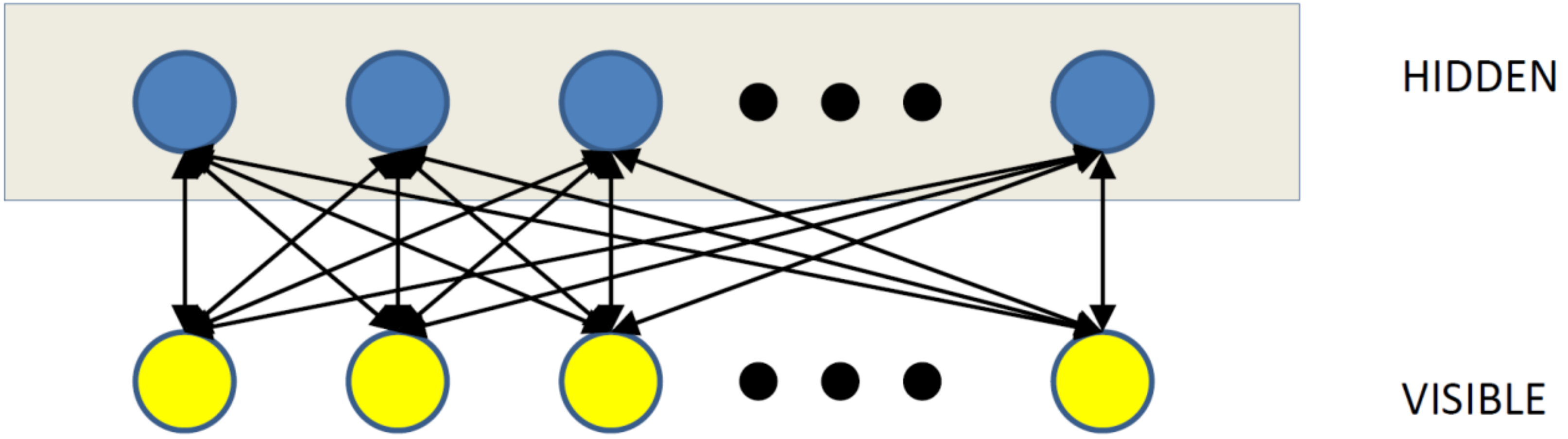
Restricted Bolzmann Machine

- A structured Boltzmann Machine
  - Hidden neurons are only connected to visible neurons
  - No intra-layer connections
  - Invented by Paul Smolensky in ’89
  - Became more practical after Hinton invested fast learning algorithms in mid 2000



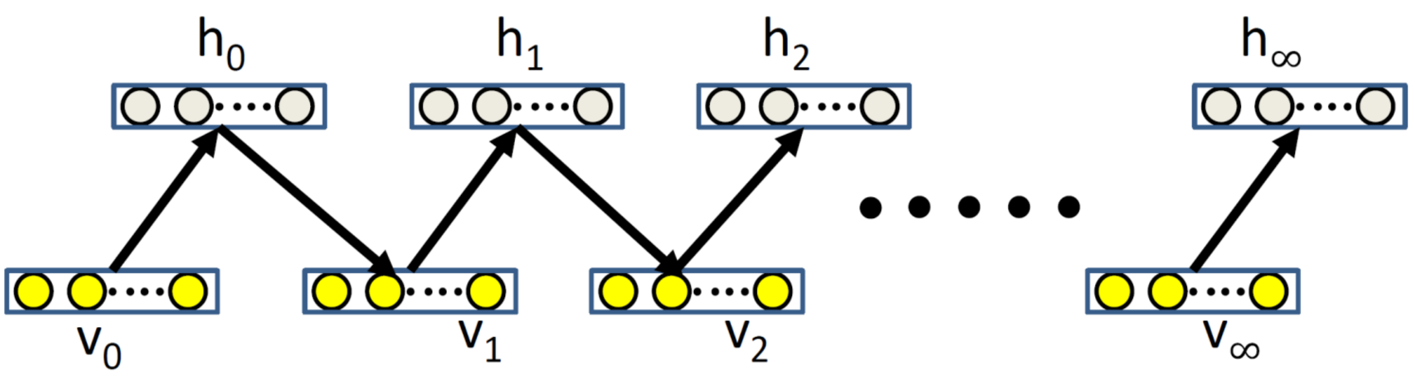
Restricted Bolzmann Machine

- Computation Rules
  - Iterative sampling
  - Hidden neurons h_i: $z_i = \sum_j w_{ij} v_j$, $P(h_i \mid v) = \dfrac{1}{1 + \exp(-z_i)}$
  - Visible neurons v_j: $z_j = \sum_i w_{ij} h_i$, $P(v_j \mid h) = \dfrac{1}{1 + \exp(-z_j)}$



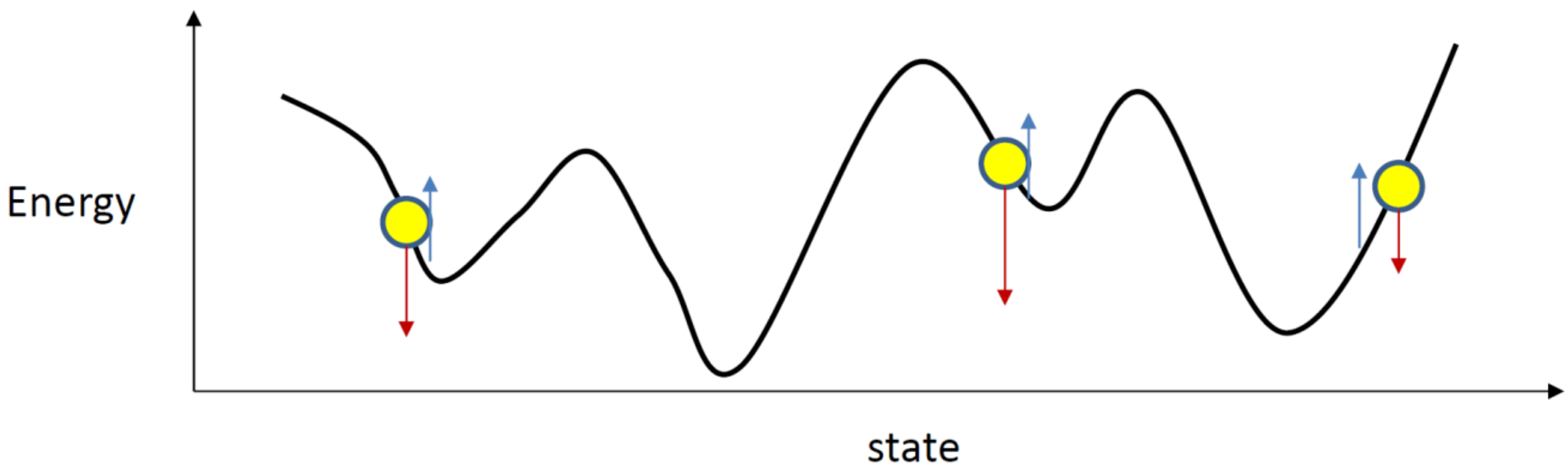
Restricted Bolzmann Machine

- Sampling:
  - Randomly initialize visible neurons v_0
  - Iterative sampling between hidden neurons and visible neurons
  - Get final sample (v_∞, h_∞)



Restricted Bolzmann Machine

- Maximum likelihood estimated:
- $\nabla_{w_{ij}} L(W) = \frac{1}{N_P K} \sum_{v \in P} v_{0i} h_{0j} - \frac{1}{M} \sum v_{\infty i} h_{\infty j}$
- No need to lift up the entire energy landscape!
  - Raising the neighborhood of desired patterns is sufficient

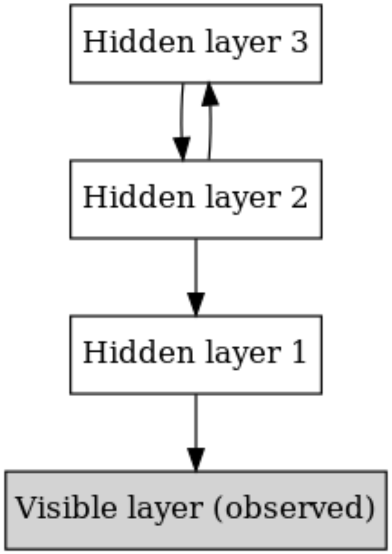


Deep Bolzmann Machine

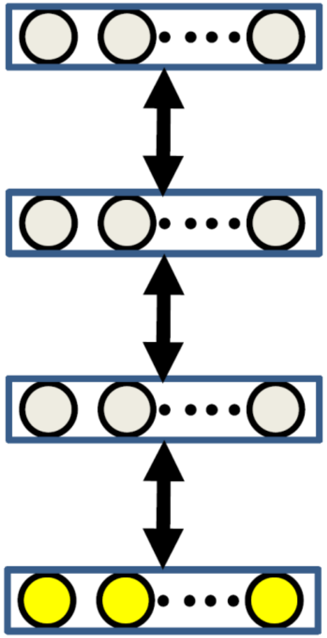
- Can we have a **deep** version of RBM?
  - Deep Belief Net ('06)
  - Deep Boltzmann Machine ('09)

- Sampling?
  - Forward pass: bottom-up
  - Backward pass: top-down

- Deep Bolzmann Machine
  - The very first deep generative model
  - Salakhudinov & Hinton

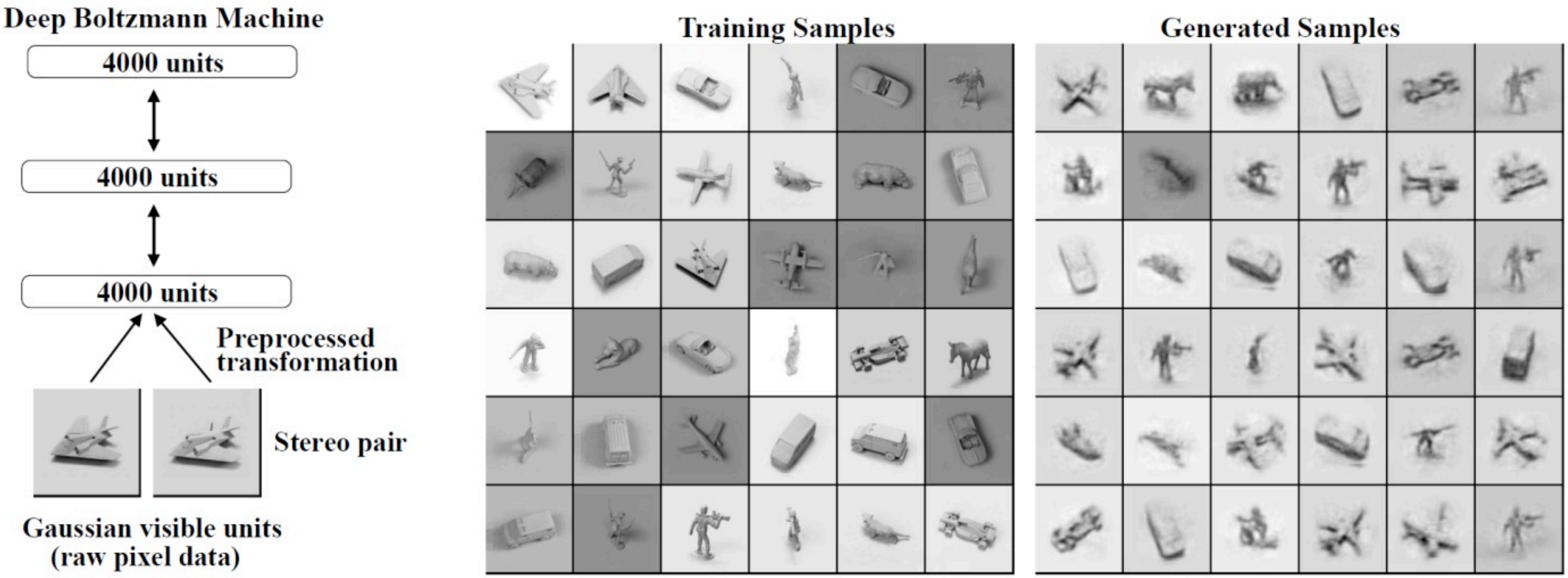


deep belief net



Deep Boltzmann Machine

Deep Bolzmann Machine



Summary

- Pros: powerful and flexible
  - An arbitrarily complex density function $p(x) = \frac{1}{z}\exp(-E(x))$
- Cons: hard to sample / train
  - Hard to sample:
    - MCMC sampling
  - Partition function
    - No closed-form calculation for likelihood
    - Cannot optimize MLE loss exactly
    - MCMC sampling

Score-Based Models and Diffusion Models

Recap: Boltzmann Machine Training

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

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

  - Maximum log-likelihood:

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

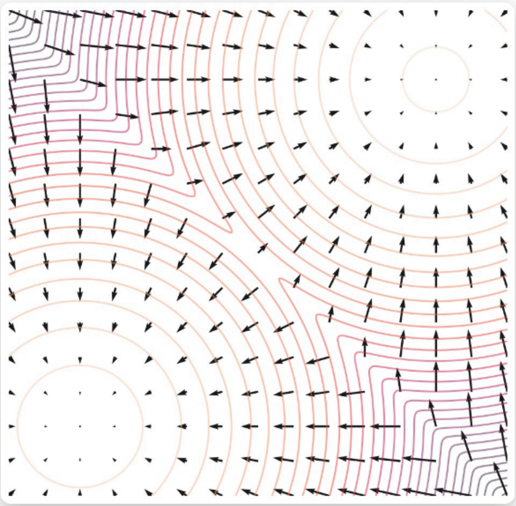
Can we avoid calculating the gradient of normalizing constant ($\nabla_x Z_\theta$)?

Score Matching

- 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 $\nabla_x \log p_{data}(x)$?



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

Score Matching

Score Matching

Sliced Score Matching

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

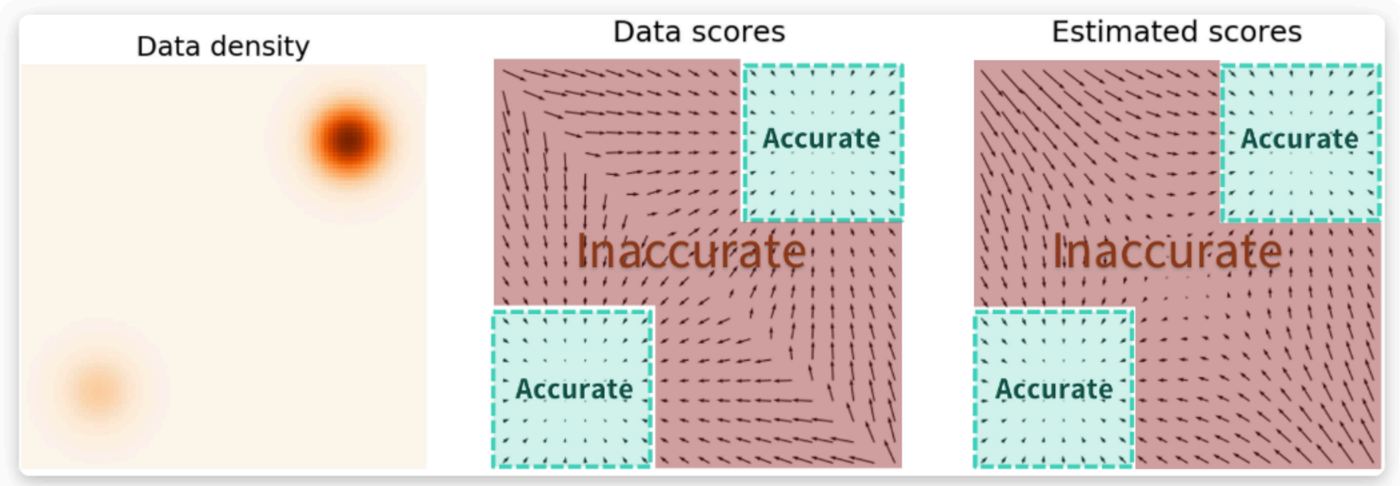
Score Matching: Langevin Dynamics

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

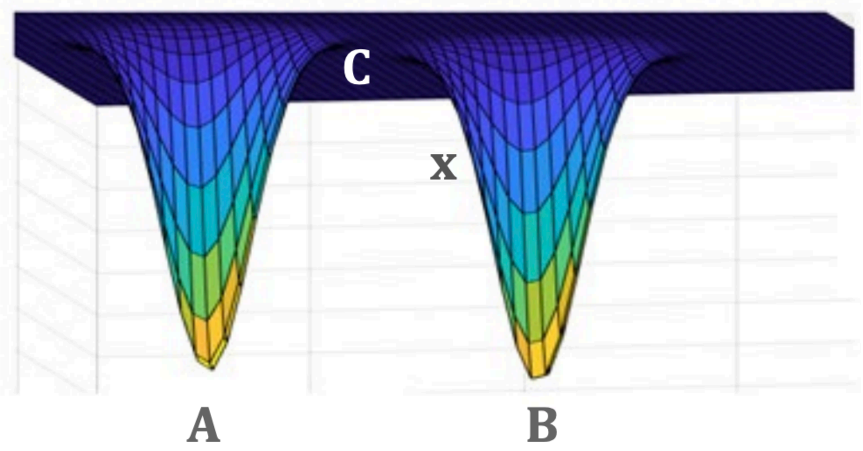
Stationary (equilibrium distribution): p(x)

Practical Issues

- 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 $x' = x + z$.

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

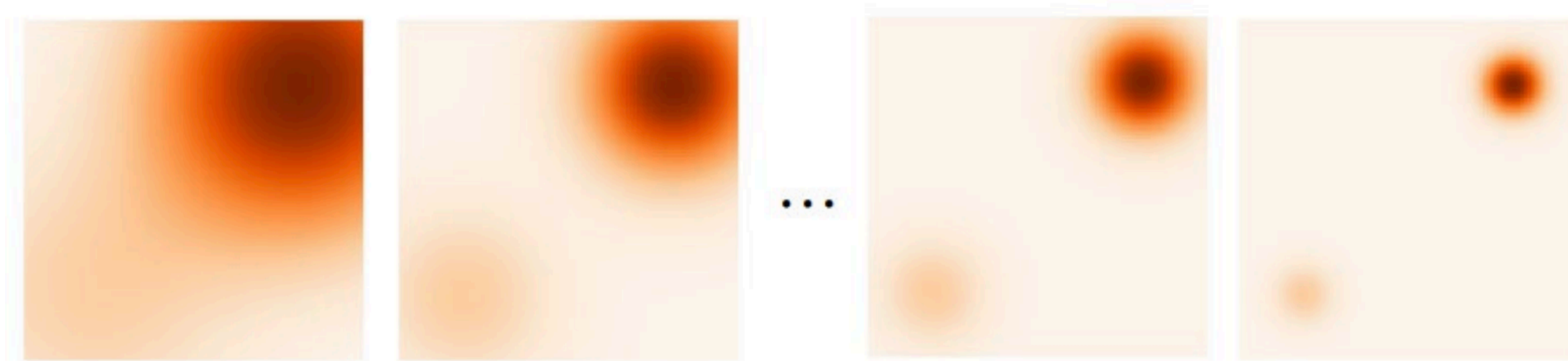


Figure by Stefano Ermon.

Annealing: Denoising Score Matching

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

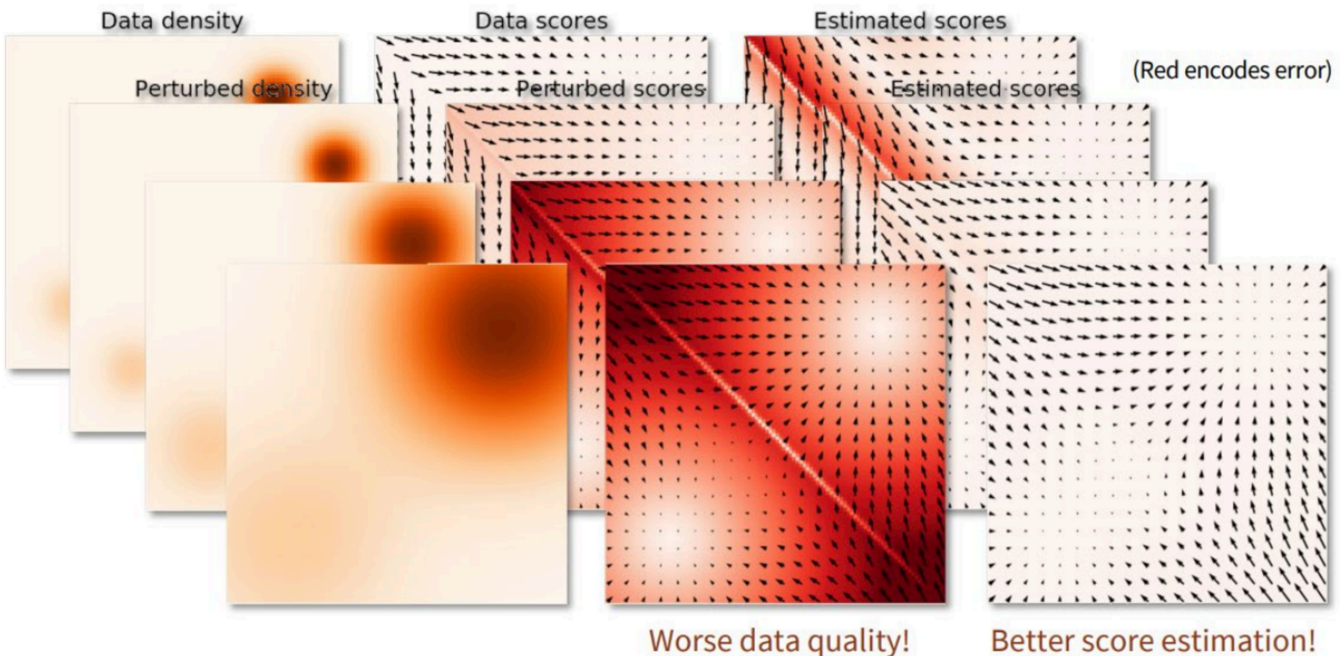


Figure by Stefano Ermon.

Annealed Langevin Dynamics

Algorithm 1 Annealed Langevin dynamics.

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

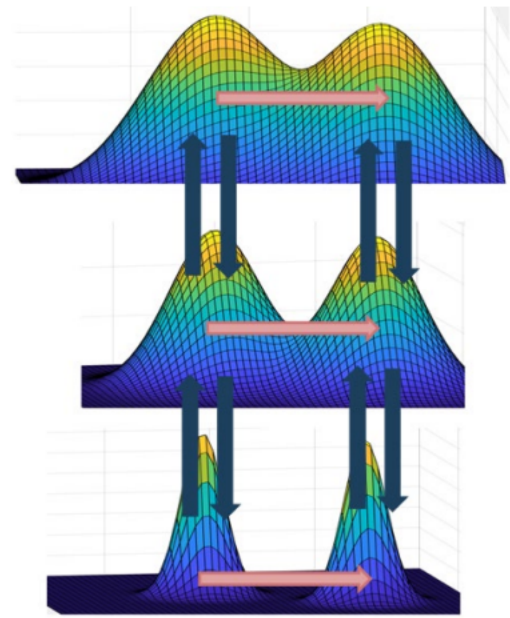
```
Initialize x̃_0
for i ← 1 to L do
    α_i ← ε · σ_i^2 / σ_L^2          ▷ α_i is the step size.
    for t ← 1 to T do
        Draw z_t ∼ N(0, I)
        x̃_t ← x̃_{t-1} + (α_i/2) s_θ(x̃_{t-1}, σ_i) + √α_i z_t
    end for
    x̃_0 ← x̃_T
end for
return x̃_T
```

$\alpha_i \leftarrow \epsilon \cdot \sigma_i^2/\sigma_L^2$

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

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

Figure from Song-Ermon '19

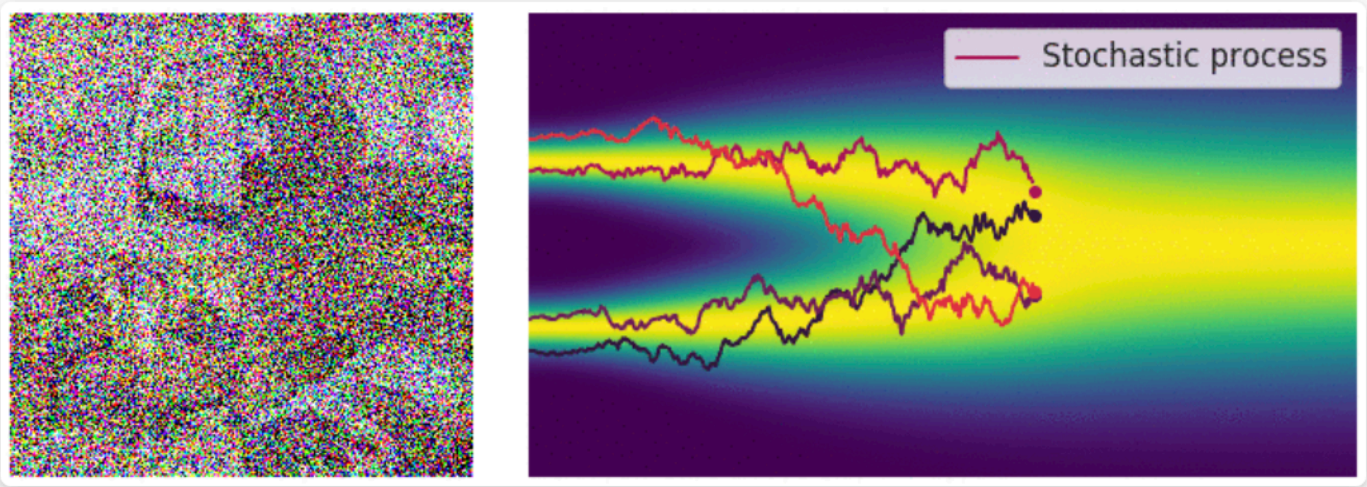


Diffusion Models

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

Perturbing Data with an SDE

- Let the number of noise scales approaches infinity!

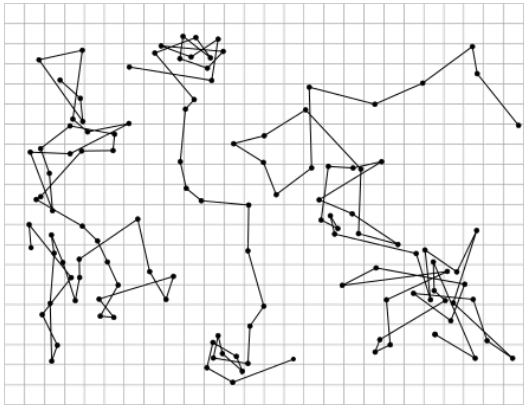


Perturbing data to noise with a continuous-time stochastic process.

Stochastic Differential Equations

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

- 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:

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

- 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

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

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

- 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.