高等机器学习

生成式模型

刘 畅

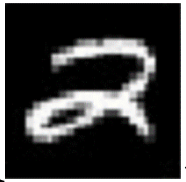
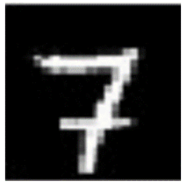
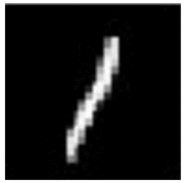
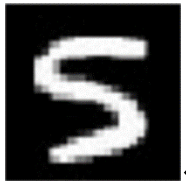
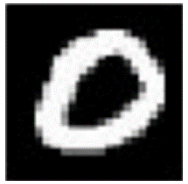
微软研究院

Microsoft

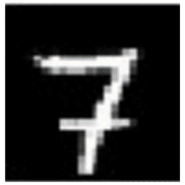
Generative Model: Overview

- Generative Models:
  Models that define $p(\text{data})$: $p(x)$ (unsupervised) or $p(x, y)$ (supervised).
  - By computing the p.d.f/p.m.f of $p(\text{data})$: data generation can be done in principle.
  - By specifying a generating process of data: the distribution $p(\text{data})$ is implicitly defined.

Unsupervised:

$\{x^{(1)}, \dots, x^{(N)}\} = \{$  ,  ,  ,  , $\dots$,  $\} \sim p(x)$

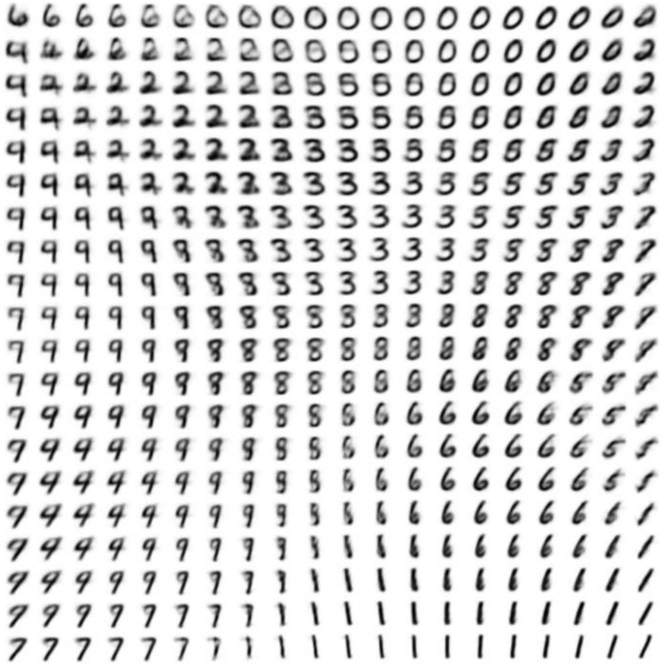
Supervised:

$\{(x^{(1)}, y^{(1)}), \dots, (x^{(N)}, y^{(N)})\} = \{($  $, \text{"2"}), \dots, ($  $, \text{"7"})\} \sim p(x, y)$

Generative Model: Overview

- What can generative models do:

  1. Generate new data.



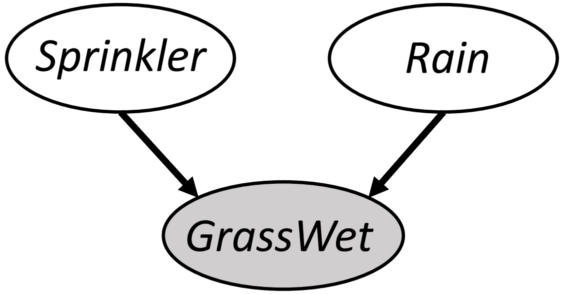
Generation $p(x)$ [KW14]

Conditional Generation
$p(x|y)$ [LWZZ18]

Generative Model: Overview

- What can generative models do:

  2. Infer unobserved variables.



Did it *Rain* if we see *GrassWet*?
-- Query $p(R|G=1)$ from $p(S,R,G)$.

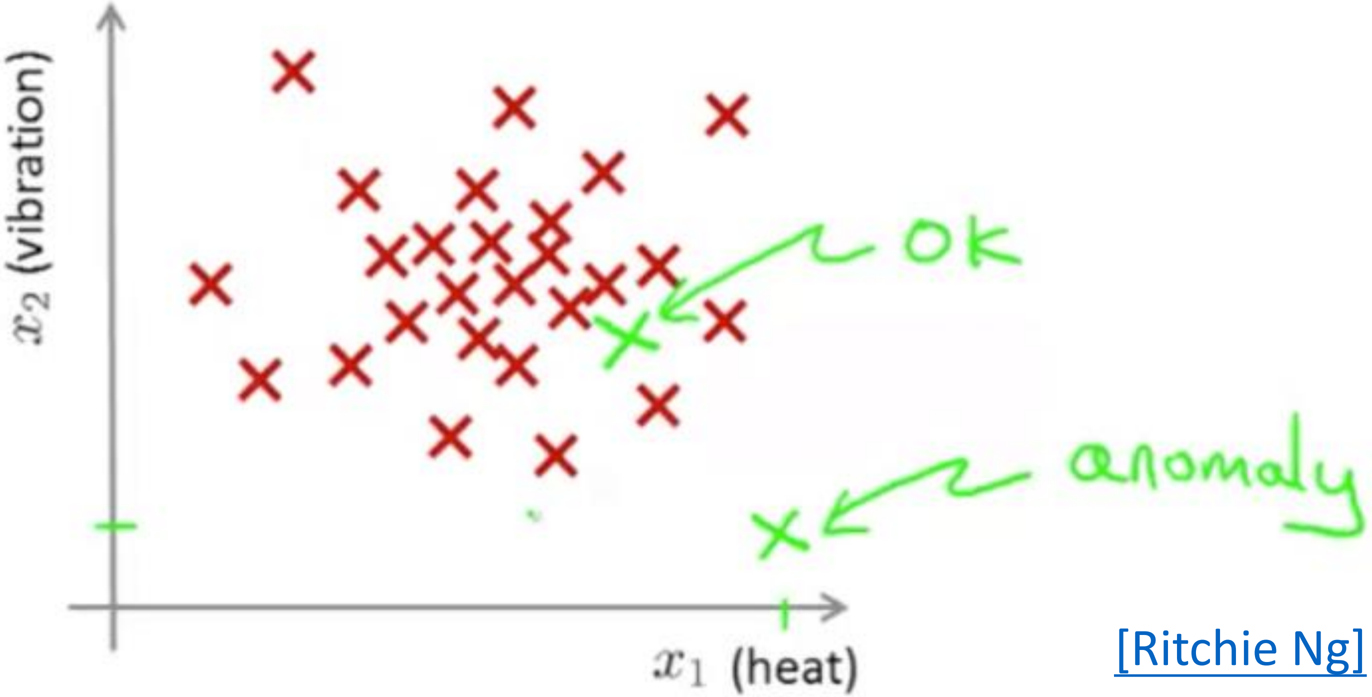
Missing Value Imputation (Completion) [OKK16].
-- Query $p(x_{\text{hidden}}|x_{\text{observed}})$ from $p(x_{\text{hidden}}, x_{\text{observed}})$.

Generative Model: Overview

- What can generative models do:

  3. Density estimation $p(x)$.

  - Uncertainty estimate.
  - Anomaly detection.



[Ritchie Ng]

Generative Model: Overview

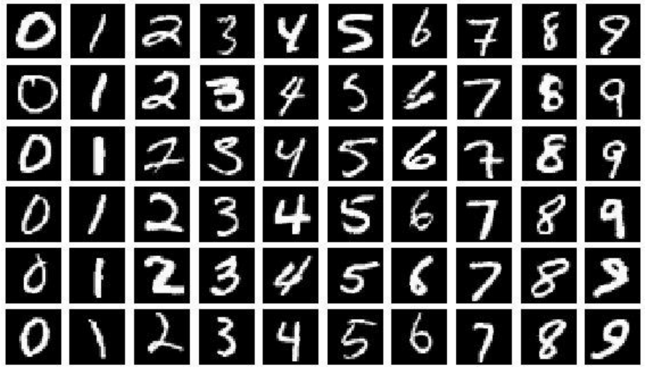
- What can generative models do:

4. Representation learning: semantic and concise (via latent variable z).

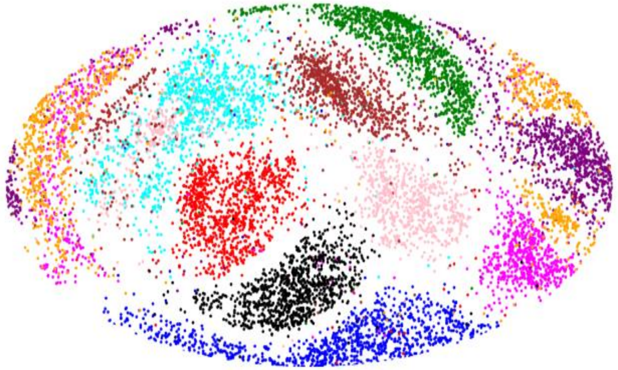
x (documents)

"ENGINES"	speed	product	introduced	designs
"ROYAL"	britain	queen	sir	earl
"ARMY"	commander	forces	war	general
"STUDY"	analysis	space	program	user
"PARTY"	act	office	judge	justice
"DESIGN"	size	glass	device	memory
"PUBLIC"	report	health	community	industry

z (topics) [PT13]



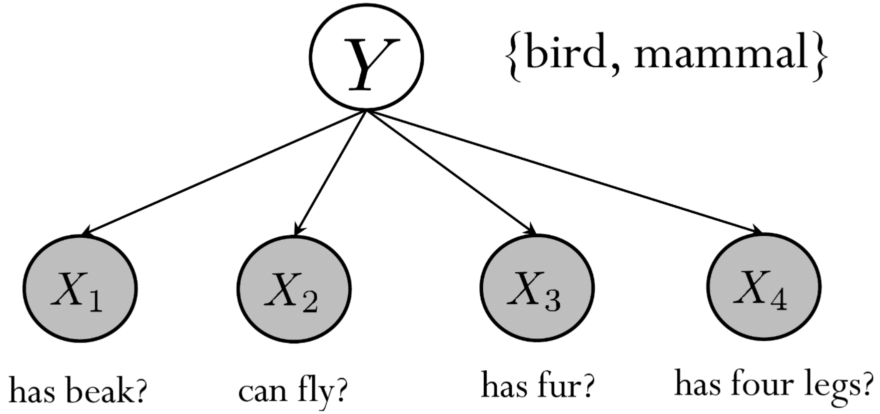
x (image)



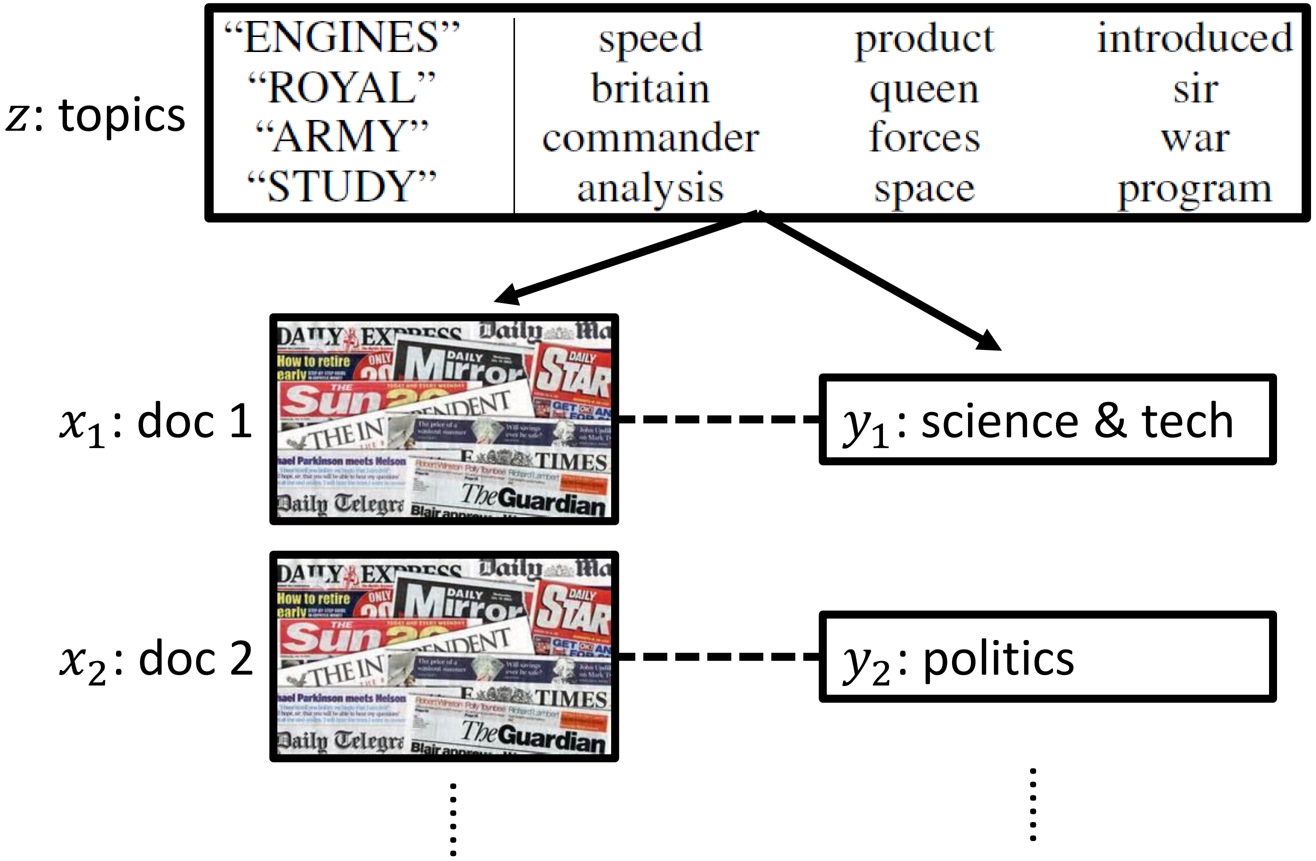
z (semantic regions) [DFD+18]

Generative Model: Overview

- What can generative models do:
  5. Supervised Learning: query $p(y|x)$ from $p(x,y)$.



Naive Bayes



Supervised LDA [MB08]

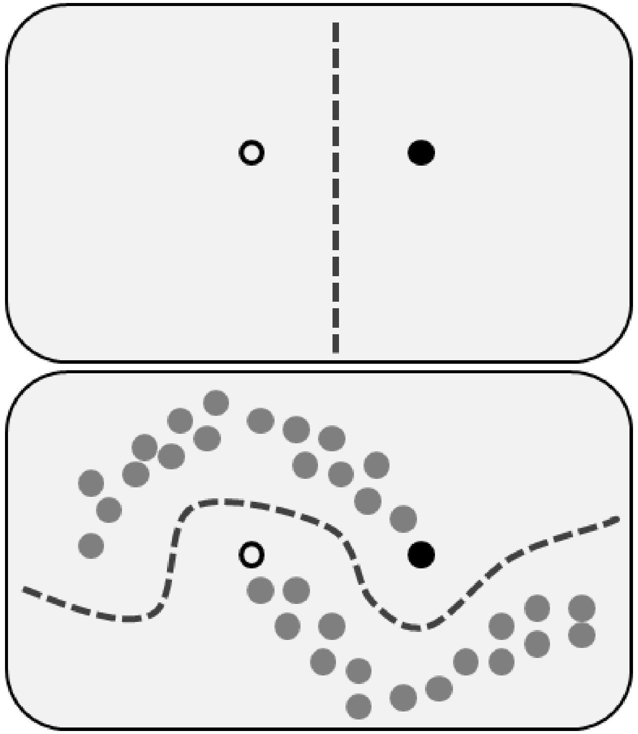
Generative Model: Overview

- What can generative models do:

  5. Supervised Learning: query $p(y|x)$ from $p(x,y)$.

     Semi-Supervised Learning:

     Unlabeled data $\{x^{(n)}\}$ can be utilized to learn a better $p(x,y)$.



Generative Model: Benefits

"What I cannot create, I do not understand." —*Richard Feynman*

- Natural for generation (*randomness/diversity, high-dimensional*).
- For representation learning: responsible and faithful knowledge of data.
- For supervised learning:
  - Leverage unlabeled data: semi-supervised learning.
  - Data-efficient: for logistic regression (discriminative) and naive Bayes (generative) [NJ01],

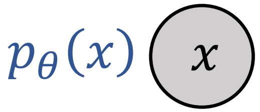
$$\epsilon_{\mathrm{Dis},N} \leq \epsilon_{\mathrm{Dis},\infty} + O\left(\sqrt{\frac{d}{N}}\right)$$

$$\epsilon_{\mathrm{Gen},N} \leq \epsilon_{\mathrm{Gen},\infty} + O\left(\sqrt{\frac{\log d}{N}}\right)$$

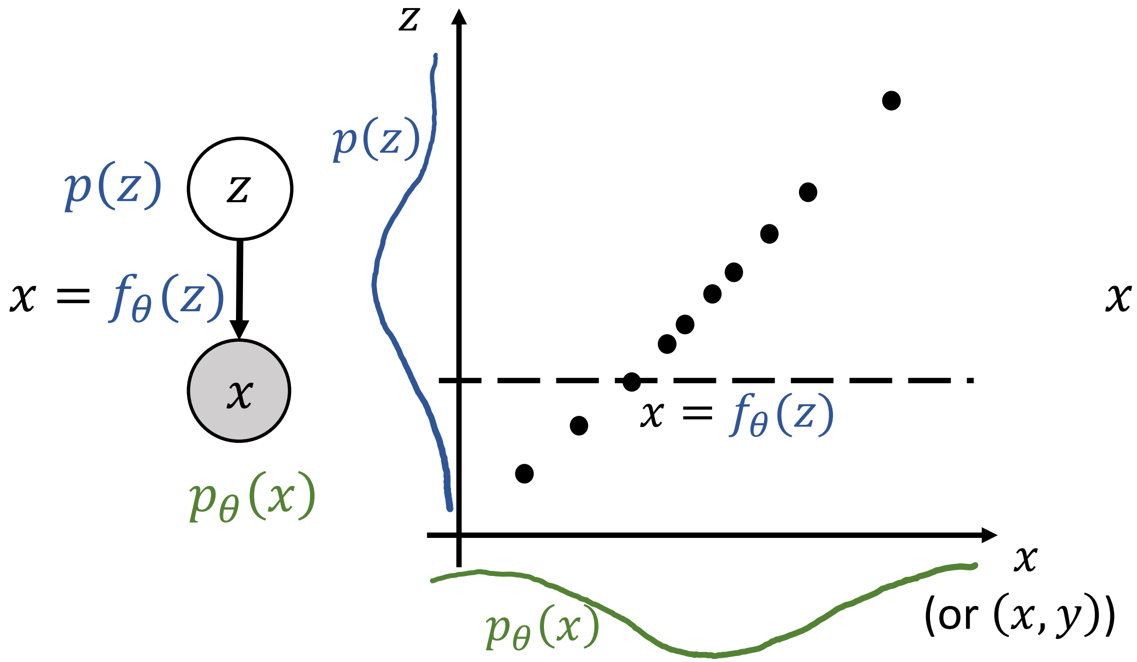
d: data dimension.
N: data size.

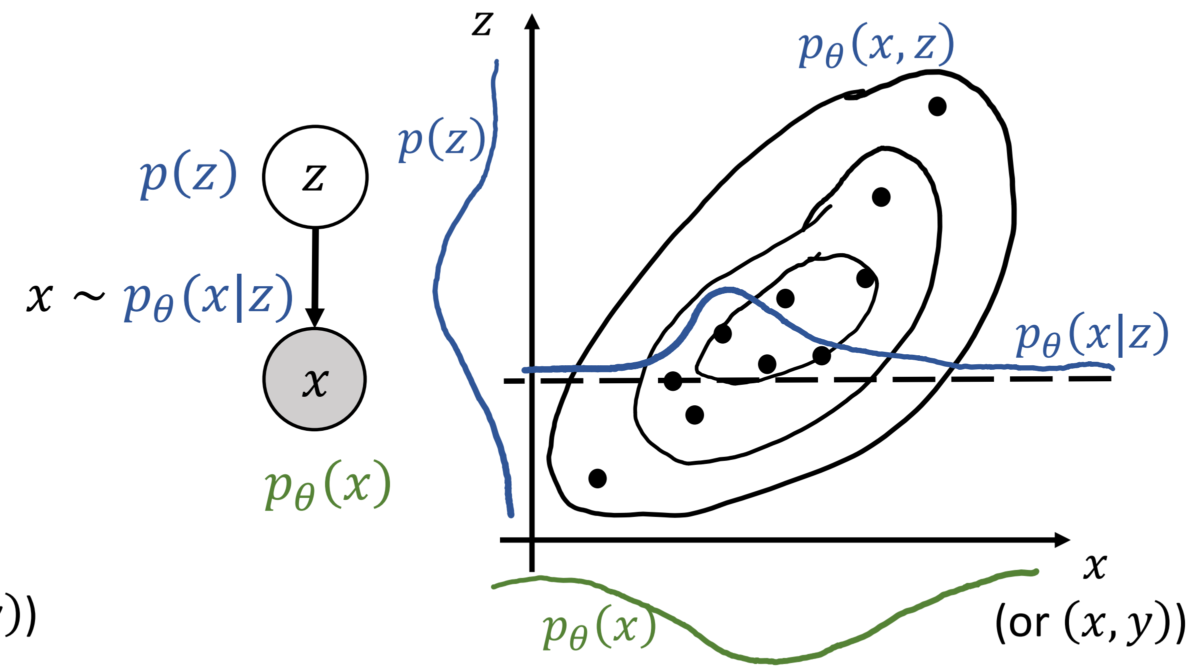
Generative Model: Taxonomy

- Plain Generative Models: Directly model $p(x)$; no latent variable.



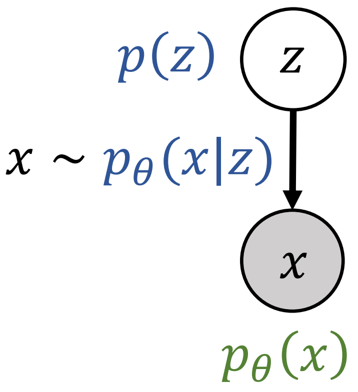
- Latent Variable Models:
  - Deterministic Generative Models: Dependency between x and z is *deterministic*: $x = f_\theta(z)$.
  - Probabilistic Graphical Models: Dependency between x and z is *probabilistic*: $(x, z) \sim p_\theta(x, z)$.

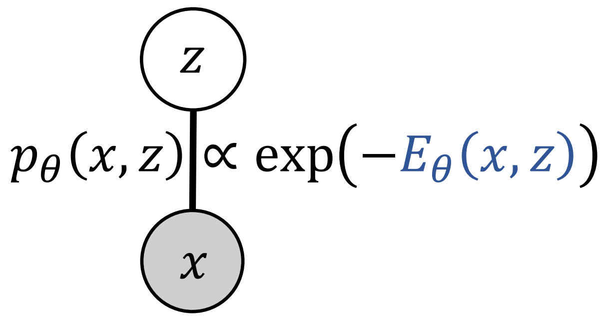




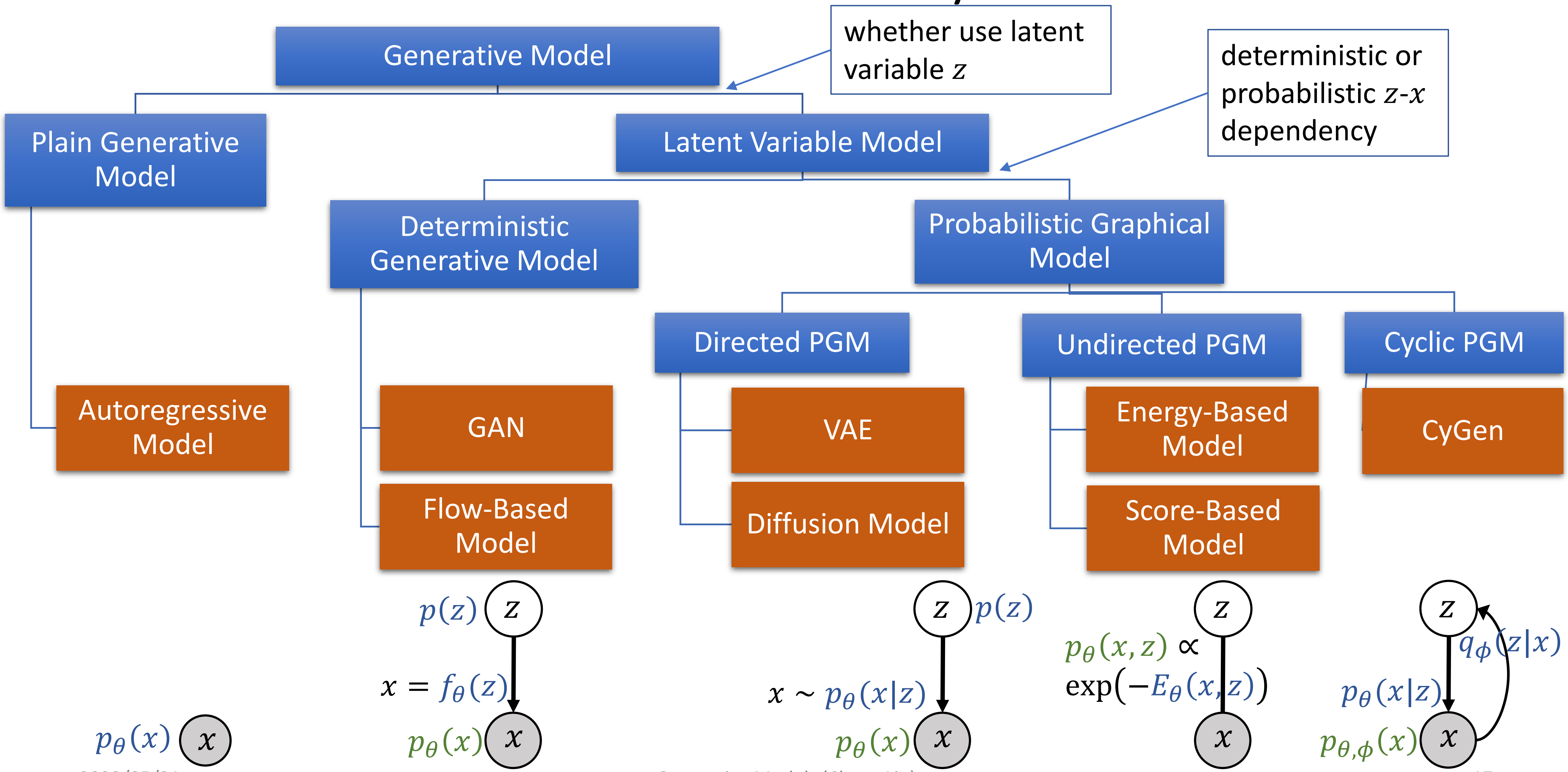
Generative Model: Taxonomy

- Latent Variable Models
  - Probabilistic Graphical Models (PGM):
    - Directed PGM:
      $p(x, z)$ specified by $p(z)$ and $p(x|z)$.
    - Undirected PGM:
      $p(x, z)$ specified by an Energy function:
      $p_\theta(x, z) \propto \exp\big(-E_\theta(x, z)\big)$.





Generative Model: Taxonomy



Outline

- Generative Models: Overview
- **Plain Generative Models**
    - Autoregressive Models
- Latent Variable Models
  - Deterministic Generative Models
    - Generative Adversarial Nets
    - Flow-Based Models
  - Probabilistic Graphical Models
    - Directed PGMs
      - Bayesian Inference (variational inference, MCMC)
      - Deep Bayesian Models (VAE)
    - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
    - Diffusion-Based Models

Plain Generative Models

- Directly model $p_\theta(x)$ (parameter θ) without latent variable.
- Easy to learn (no normalization issue of data likelihood) and use (data generation).
- Learning: **Maximum Likelihood Estimation (MLE)**.

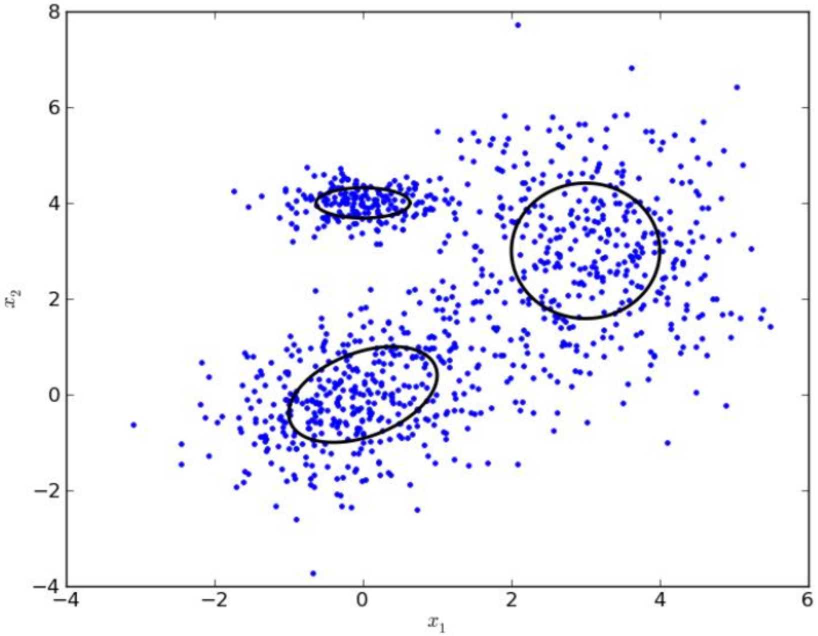
$$\theta^* = \arg\max_\theta \mathbb{E}_{\hat{p}(x)}[\log p_\theta(x)] = \arg\min_\theta \mathrm{KL}(\hat{p}, p_\theta)$$
$$\approx \arg\max_\theta \frac{1}{N} \sum_{n=1}^{N} \log p_\theta(x^{(n)}).$$

Kullback-Leibler divergence

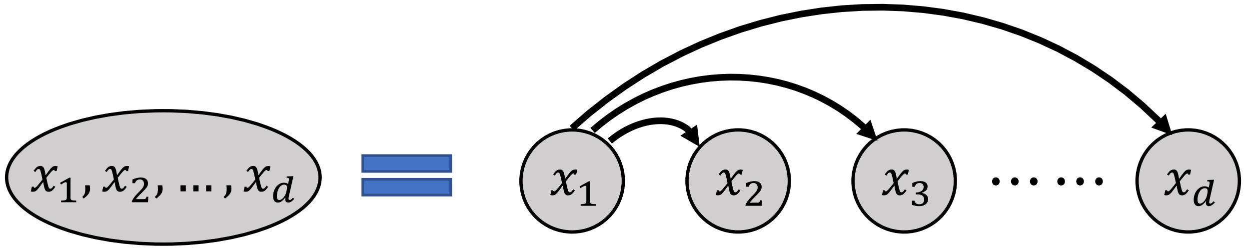
$$\mathrm{KL}(\hat{p}, p_\theta) := \mathbb{E}_{\hat{p}(x)}\left[\log \frac{\hat{p}(x)}{p_\theta(x)}\right]$$

- First example: Gaussian Mixture Model

$$p_\theta(x) = \sum_{k=1}^{K} \alpha_k \mathcal{N}(x|\mu_k, \Sigma_k),$$
$$\theta = (\alpha, \mu, \Sigma).$$



Autoregressive Models



$p(x_1, x_2, \dots, x_d)$ $\quad$ $p(x_1)\ p(x_2|x_1)\ p(x_3|x_1, x_2) \cdots p(x_d|x_{<d})$

Model $p(x)$ by each conditional $p(x_i|x_{<i})$ (i indices components).

- Full dependency can be restored.
- Conditionals are easier to model.
- Easy data generation:

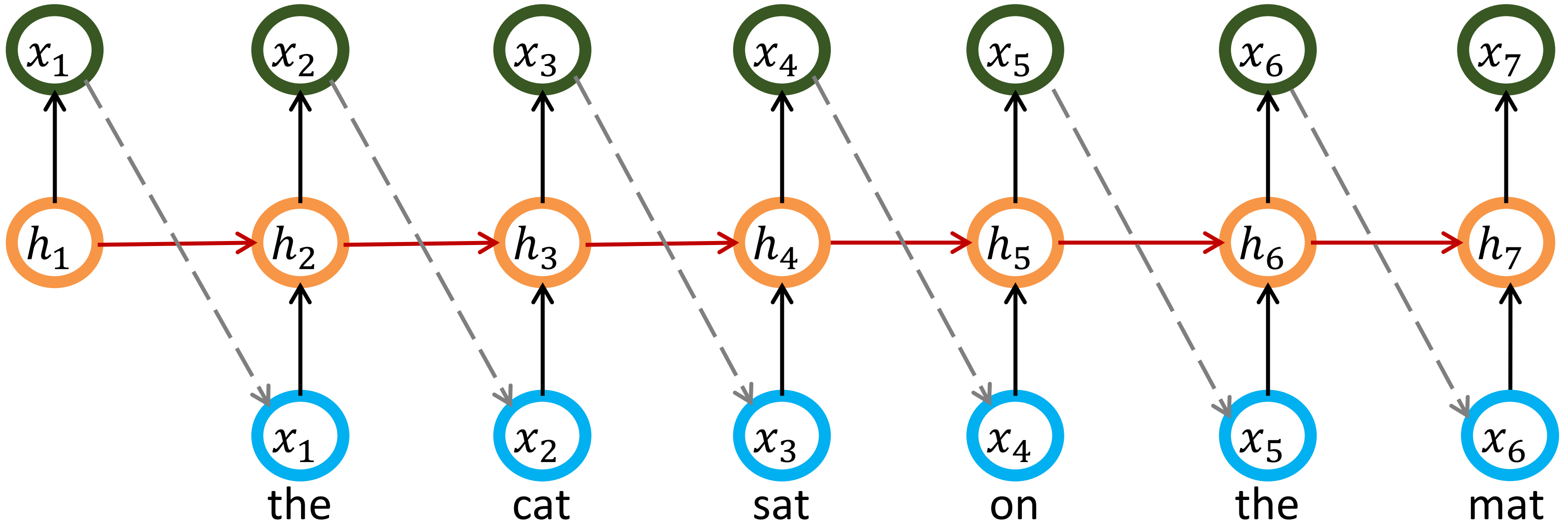
$$x \sim p(x) \Leftrightarrow x_1 \sim p(x_1), x_2 \sim p(x_2|x_1), \dots, x_d \sim p(x_d|x_1, \dots, x_{d-1}).$$

But **non-parallelizable**.

Autoregressive Models

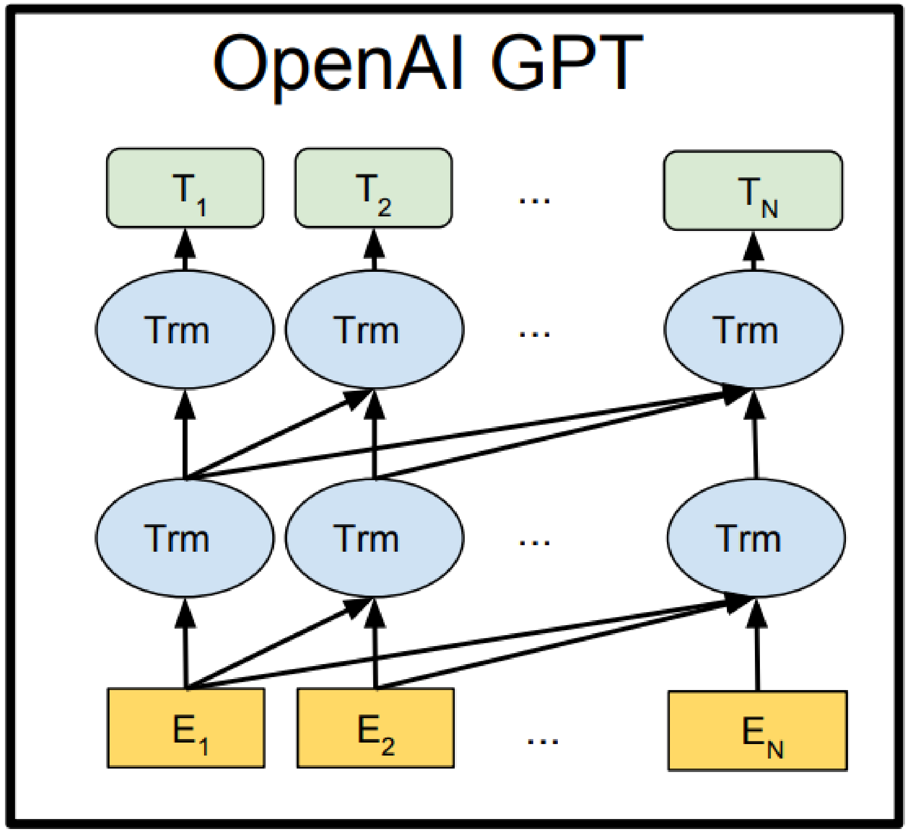
- A typical language model: Use a hidden state to represent the dependency on previous items.

$$p(\mathbf{x} = \text{“}\textit{the cat sat on the mat}\text{”})$$
$$= p(x_1 = \text{the})\ p(\text{cat}|x_1)\ \ p(\text{sat}|x_{1\ldots2})\ p(\text{on}|x_{1\ldots3})\ p(\text{the}|x_{1\ldots4})\ p(\text{mat}|x_{1\ldots5})\ p(\text{</s>}|x_{1\ldots6})$$



Autoregressive Models

- A typical language model: Use a hidden state to represent the dependency on previous items.



[DCLT18]

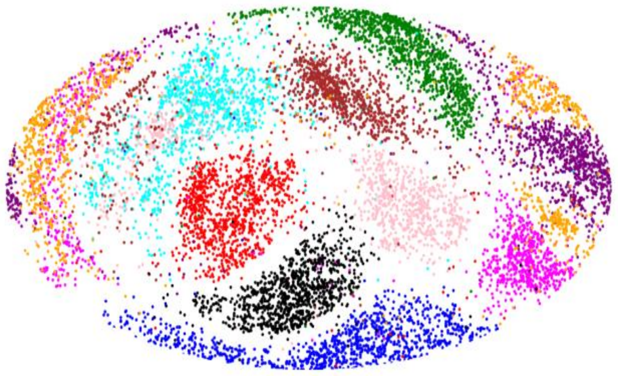
Outline

- Generative Models: Overview
- Plain Generative Models
    - Autoregressive Models
- **Latent Variable Models**
  - Deterministic Generative Models
    - Generative Adversarial Nets
    - Flow-Based Models
  - Probabilistic Graphical Models
    - Directed PGMs
      - Bayesian Inference (variational inference, MCMC)
      - Deep Bayesian Models (VAE)
    - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
    - Diffusion-Based Models

Latent Variable Models

- Latent Variable:
  - Abstract knowledge of data; enables various tasks.

Semantic Representation



Dimensionality Reduction

Knowledge Discovery

“ENGINES”	speed	product	introduced
“ROYAL”	britain	queen	sir
“ARMY”	commander	forces	war
“STUDY”	analysis	space	program
“PARTY”	act	office	judge
“DESIGN”	size	glass	device
“PUBLIC”	report	health	community

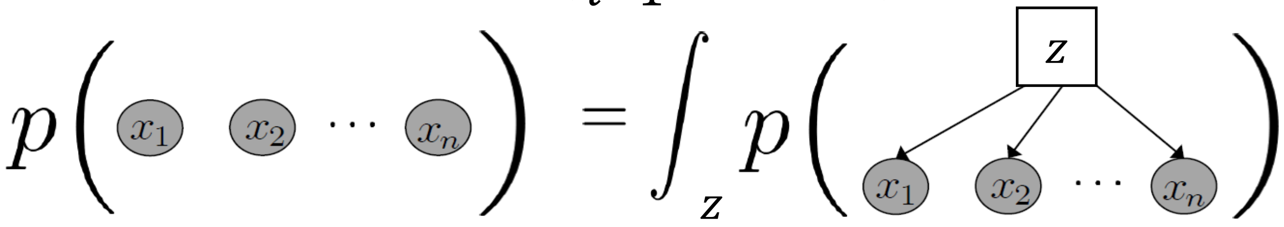
Manipulated Generation

Latent Variable Models

- Latent Variable:
  - Compact representation of dependency.

    De Finetti's Theorem (1955): if $(x_1, x_2, \dots)$ are *infinitely exchangeable*, then $\exists$ r.v. z and $p(\cdot\,|z)$ s.t. $\forall n$,

$$p(x_1, \dots, x_n) = \int \left(\prod_{i=1}^{n} p(x_i|z) \right) p(z)\,\mathrm{d}z\,.$$



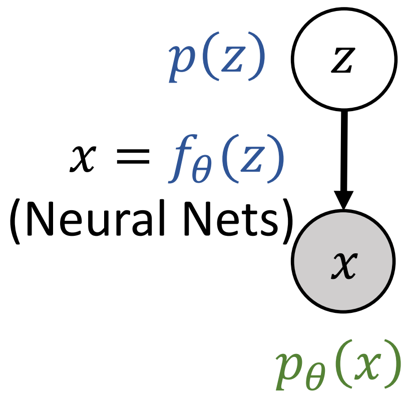
Infinite exchangeability:

For all n and permutation σ, $p(x_1, \dots, x_n) = p\big(x_{\sigma(1)}, \dots, x_{\sigma(n)}\big)$.

Outline

- Generative Models: Overview
- Plain Generative Models
  - Autoregressive Models
- **Latent Variable Models**
  - **Deterministic Generative Models**
    - **Generative Adversarial Nets**
    - Flow-Based Models
  - Probabilistic Graphical Models
    - Directed PGMs
      - Bayesian Inference (variational inference, MCMC)
      - Deep Bayesian Models (VAE)
    - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
    - Diffusion-Based Models

Generative Adversarial Nets



- Deterministic $f_\theta : z \mapsto x$, modeled by a neural network.
  - \+ Flexible modeling ability.
  - \+ Good generation performance.
  - \- Hard to infer z of a data point x.
  - \- Unavailable p.d.f/p.m.f $p_\theta(x)$.
  - \- Mode-collapse.
- Learning: $\min_\theta \mathrm{discr}\big(\hat{p}(x), p_\theta(x)\big)$.
  - discr. = $\mathrm{KL}(\hat{p}, p_\theta) \Longrightarrow$ MLE: $\max_\theta \mathbb{E}_{\hat{p}}[\log p_\theta]$, but the p.d.f/p.m.f $p_\theta(x)$ is unavailable!
  - discr. = Jensen-Shannon divergence [GPM+14].
  - discr. = Wasserstein distance [ACB17].

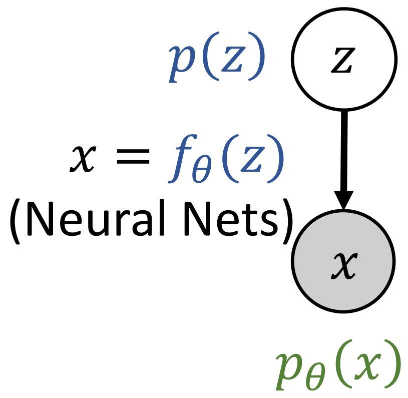
Generative Adversarial Nets

- Learning: $\min_\theta \mathrm{discr}\big(\hat{p}(x), p_\theta(x)\big)$.
  - GAN [GPM+14]: discr. = Jensen-Shannon divergence.

$$\mathrm{JS}(\hat{p}, p_\theta) := \frac{1}{2}\left(\mathrm{KL}\left(\hat{p}, \frac{p_\theta + \hat{p}}{2}\right) + \mathrm{KL}\left(p_\theta, \frac{p_\theta + \hat{p}}{2}\right)\right)$$

$$= \frac{1}{2}\max_{T(\cdot)} \mathbb{E}_{\hat{p}(x)}\big[\log \sigma\big(T(x)\big)\big] + \underbrace{\mathbb{E}_{p_\theta(x)}\Big[\log\Big(1 - \sigma\big(T(x)\big)\Big)\Big]}_{=\mathbb{E}_{p(z)}\left[\log\left(1-\sigma\left(T\left(f_\theta(z)\right)\right)\right)\right]} + \log 2\,.$$

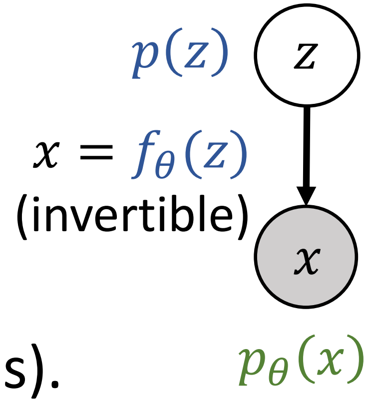
  - $\sigma\big(T(x)\big)$ is the discriminator; T implemented as a neural network.
  - Expectations can be estimated by samples.



Outline

- Generative Models: Overview
- Plain Generative Models
    - Autoregressive Models
- **Latent Variable Models**
    - **Deterministic Generative Models**
        - Generative Adversarial Nets
        - **Flow-Based Models**
    - Probabilistic Graphical Models
        - Directed PGMs
            - Bayesian Inference (variational inference, MCMC)
            - Deep Bayesian Models (VAE)
        - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
        - Diffusion-Based Models

Flow-Based Models



- Deterministic and invertible $f_\theta : z \mapsto x$.
  - + Available density function!

$$p_\theta(x) = p\left(z = f_\theta^{-1}(x)\right) \left|\frac{\partial f_\theta^{-1}}{\partial x}\right| \quad \text{(rule of change of variables).}$$

Jacobian determinant, $\left(\frac{\partial f_\theta^{-1}}{\partial x}\right)_{ij} := \frac{\partial \left(f_\theta^{-1}\right)_i}{\partial x_j}$.

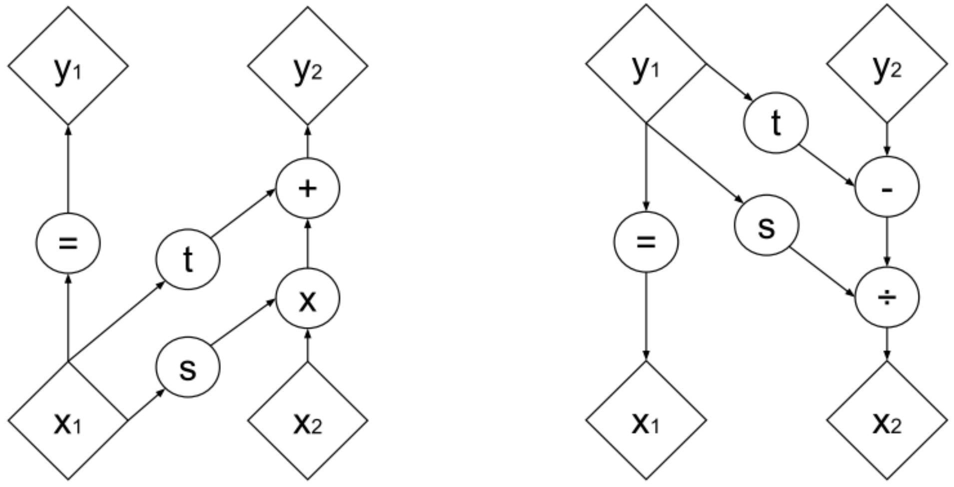
  - + Easy inference: $z = f_\theta^{-1}(x)$.
  - - Redundant representation: dim. z = dim. x.
  - - Restricted f_θ: deliberative design; either f_θ or f_θ^{-1} computes costly.
- Learning: $\min_\theta \mathrm{KL}\left(\hat{p}(x), p_\theta(x)\right) \Longrightarrow$ MLE: $\max_\theta \mathbb{E}_{\hat{p}(x)}[\log p_\theta(x)]$.
- Examples:
  - NICE [DKB15], RealNVP [DSB17], MAF [PPM17], GLOW [KD18].
  - Also used for variational inference [RM15, KSJ+16].

Flow-Based Models

- RealNVP [DSB17]
  - Building block: **Coupling**: $y = g(x)$,

$$\begin{cases} y_{1:d} & = x_{1:d} \\ y_{d+1:D} & = x_{d+1:D} \odot \exp\big(s(x_{1:d})\big) + t(x_{1:d}) \end{cases}$$

$$\Leftrightarrow \begin{cases} x_{1:d} & = y_{1:d} \\ x_{d+1:D} & = \big(y_{d+1:D} - t(y_{1:d})\big) \odot \exp\big(-s(y_{1:d})\big), \end{cases}$$



(a) Forward propagation (b) Inverse propagation

where s and t: $\mathbb{R}^{D-d} \to \mathbb{R}^{D-d}$ are general functions for scale and translation.

  - Jacobian Determinant: $\left|\frac{\partial g}{\partial x}\right| = \exp\left(\sum_{j=1}^{D-d} s_j(x_{1:d})\right)$.
  - Partitioning x using a binary mask b:

- Continuous normalizing flow [GCB+18].

$$\partial_t z_t = f_t(z_t) \Longrightarrow \frac{\mathrm{d}}{\mathrm{d}t} \log p_t(z_t) = -\nabla \cdot f_t(z_t) = -\mathrm{tr}\left(\frac{\partial f_t}{\partial z}\right).$$

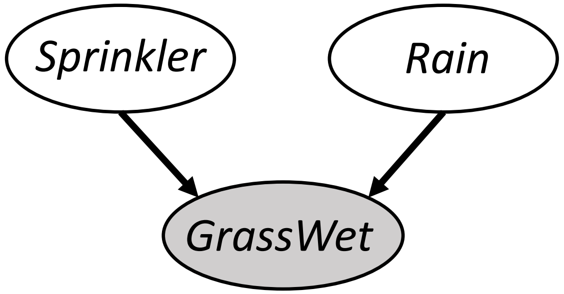
  - Use ODE solver for fwd/bwd map and $\log p_{t_1}\big(z(t_1)\big) = \log p_{t_0}\big(z(t_0)\big) - \int_{t_0}^{t_1} \mathrm{tr}\left(\frac{\partial f_t}{\partial z}\right) \mathrm{d}t$.

Outline

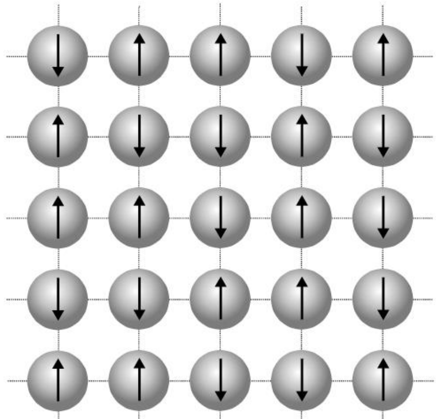
- Generative Models: Overview
- Plain Generative Models
    - Autoregressive Models
- Latent Variable Models
    - Deterministic Generative Models
        - Generative Adversarial Nets
        - Flow-Based Models
    - **Probabilistic Graphical Models**
        - Directed PGMs
            - Bayesian Inference (variational inference, MCMC)
            - Deep Bayesian Models (VAE)
        - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
        - Diffusion-Based Models

Classical Probabilistic Graphical Models

- Generally, they may or may not have latent variables.
- Intuitively: represent variable **relations** by a graph.
- Formally: a way to represent a joint distribution by making **conditional independence (CI)** assumptions.



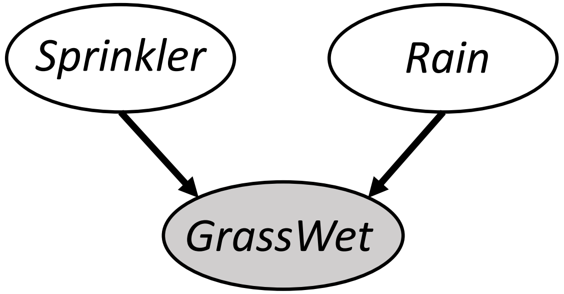
$$p(S, R, G) = p(S)p(R)p(G|S, R)$$



$$p(x) \propto \exp \underbrace{\left(-\sum_{(i,j)\in\mathcal{E}} J\left(x_i, x_j\right) - \sum_i H(x_i)\right)}_{\text{Energy function } -E(x)}$$

Directed Probabilistic Graphical Models

- Represented by a **Directed Acyclic Graph** (DAG).
- Synonyms: Bayesian/belief/causal network.

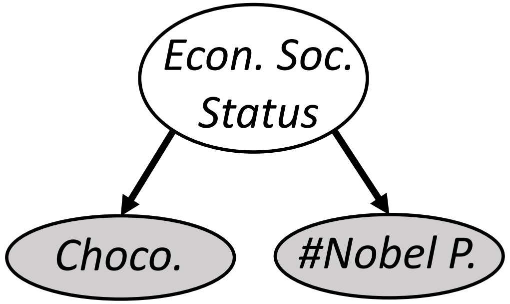


$$p(S, R, G) = p(S)p(R)p(G|S, R)$$

CI assumptions:
- $S \perp R$ since $p(S, R) = p(S)p(R)$.
- $S\ ! \perp R|G$ since $p(S, R|G) \neq p(S|G)p(R|G)$ in general.

Markovianess

Faithfulness



$$p(E, C, N) = p(E)p(C|E)p(N|E)$$

CI assumptions:
- $C \perp N|E$ since $p(C, N|E) = p(C|E)p(N|E)$.
- $C\ ! \perp N$ since $p(C, N) \neq p(C)p(N)$ in general.

Directed Probabilistic Graphical Models

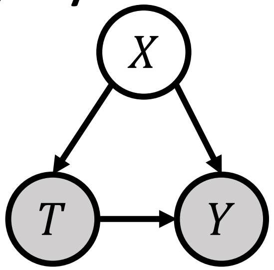
As a language of causality

- Formal definition of causality:
  *"two variables have a causal relation, if **intervening** the cause may change the effect, but not vice versa"* [Pearl09, PJS17].
  - **Intervention**: change the value of a variable by leveraging mechanisms and changing variables out of the considered system.
- Example: for the Altitude and average Temperature of a city, $A \to T$.
  - Running a huge heater (intv. T) does not lower A.
  - Raising the city by a huge elevator (intv. A) lowers T.
- Causality contains more information than observation (== static/observational data, joint distribution, CIs).
  - Both $p(A)p(T|A)$ ($A \to T$) and $p(T)p(A|T)$ ($T \to A$) can describe $p(A,T)$,
  - but they give different outcomes under intervention.

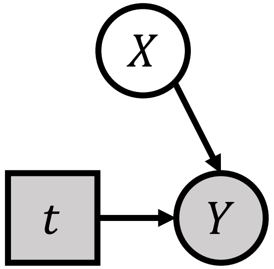
Directed Probabilistic Graphical Models

As a language of causality

- Pearl's surgery: describing intervention.



Intervening T with t



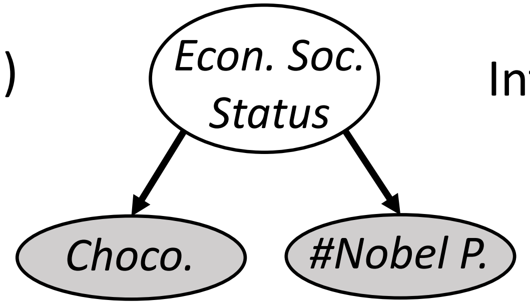
$$p(Y|t) = \int p(Y|X,t)p(X|t)\,\mathrm{d}X$$

do-operation

$$p(Y|do(t)) = \tilde{p}(Y|t) = \int p(Y|X,t)p(X)\,\mathrm{d}X$$

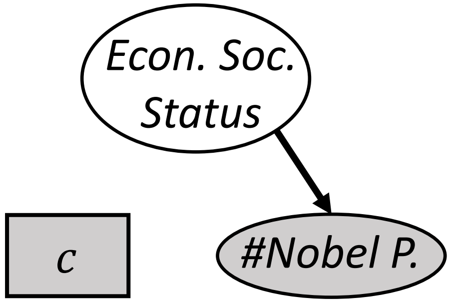
- Explaining spurious correlation:

(Confounding bias)



$$C \not\perp N$$

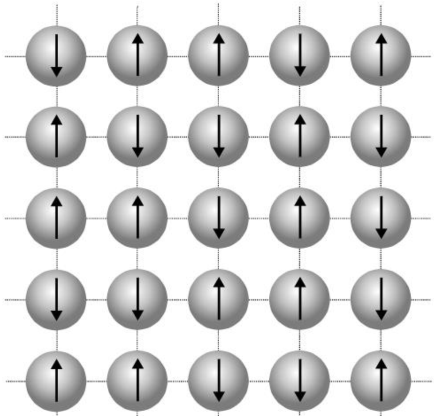
Intervening *Choco.* with c



$$p(N|do(c)) = p(N)$$

Undirected Probabilistic Graphical Models

- For **symmetric** relations (e.g., image pixels), it is **unnatural** to assign a direction.
  - Side effect: there would be undesired or arbitrary CI assertions.
- Represent the relation by an **undirected** graph.
  - **Synonyms**: Markov random field, energy-based model.
  - $A \perp B \mid \mathbf{S}$: every path between A and B contains a node in $\mathbf{S}$.
  - **Markovianess** (Hammersley-Clifford theorem):
    p satisfies graph CI properties if it factorizes as one term per maximal *clique* (fully connected subgraph).

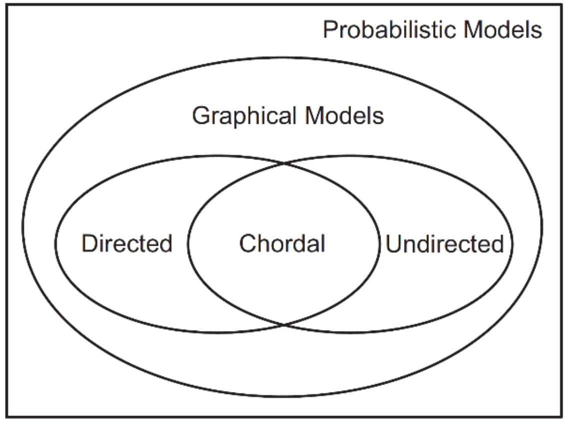


Ising model

Markovianess

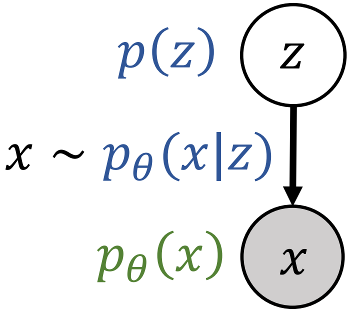
$$p(x) \propto \exp \underbrace{\left(-\sum_{(i,j)\in\mathcal{E}} J(x_i, x_j) - \sum_i H(x_i)\right)}_{\text{Energy function } -E(x)}$$

Probabilistic Graphical Models

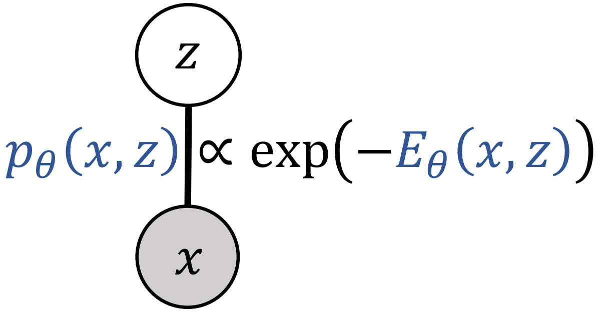


- Directed and Undirected PGMs cover **different** distributions.
- Not all PGMs are generative
  (e.g., Bayesian neural networks, conditional random fields).
- Classical PGMs do emphasize the "graph" information.
- Deep PGMs often have simple graphs, and focus on learning the edge relation:
  Dependency between x and z is *probabilistic*: $(x, z) \sim p_\theta(x, z)$.

Directed PGM:



Undirected PGM:



Outline

- Generative Models: Overview
- Plain Generative Models
    - Autoregressive Models
- Latent Variable Models
    - Deterministic Generative Models
        - Generative Adversarial Nets
        - Flow-Based Models
    - Probabilistic Graphical Models
        - **Directed PGMs**
            - Bayesian Inference (variational inference, MCMC)
            - Deep Bayesian Models (VAE)
        - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
        - Diffusion-Based Models

Directed PGMs

Bayesian models

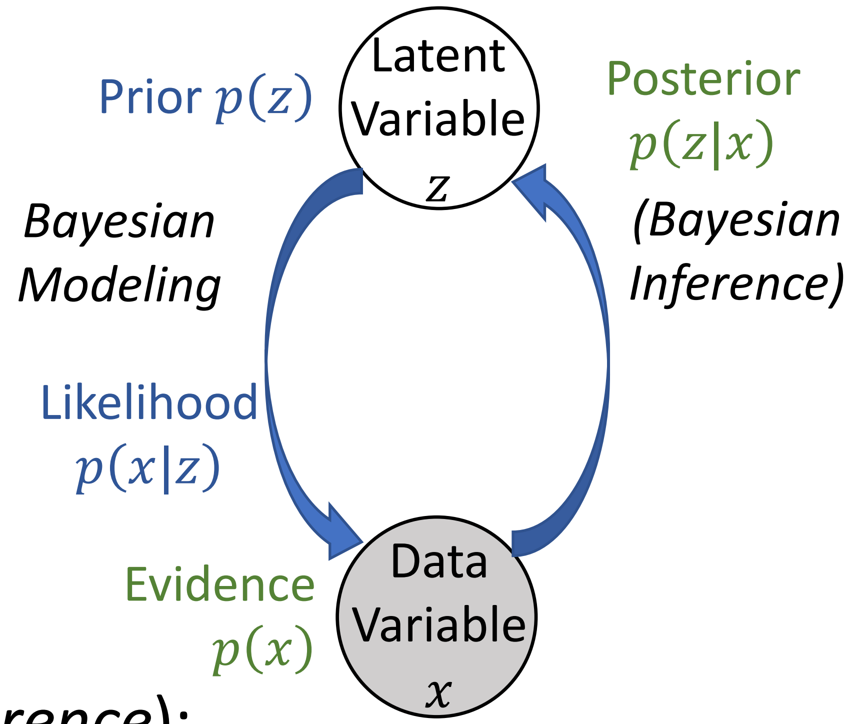
- Model structure (*Bayesian Modeling*):
  - *Prior* $p(z)$: *initial* belief of z.
  - *Likelihood* $p(x|z)$: dependence of x on z.
- Learning: MLE.

  $\theta^* = \arg\max_\theta \mathbb{E}_{\hat{p}(x)}[\log p_\theta(x)]$,

  Evidence $p(x) = \int p(z, x) \, \mathrm{d}z$.
- Feature/representation learning (*Bayesian Inference*):

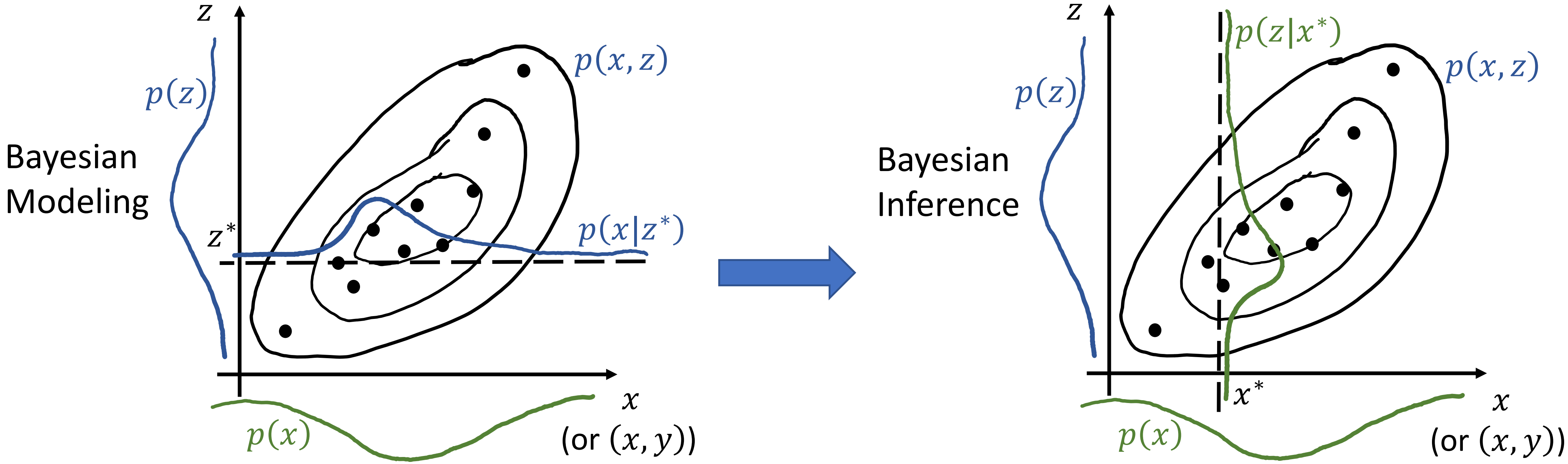
  Posterior $p(z|x) = \frac{p(z,x)}{p(x)} = \frac{p(z)p(x|z)}{\int p(z,x) \, \mathrm{d}z}$ (Bayes' rule)

  represents the *updated* information that observation x conveys to latent z.



Bayesian Inference

Estimate the posterior $p(z|x)$.



Bayes' rule: $\quad$ *Posterior* $p(z|x) = \frac{p(x,z)}{p(x)} = \frac{p(x,z)}{\int p(x,z)\,\mathrm{d}z} \propto p(x,z) = p(z)p(x|z).$

Bayesian Inference

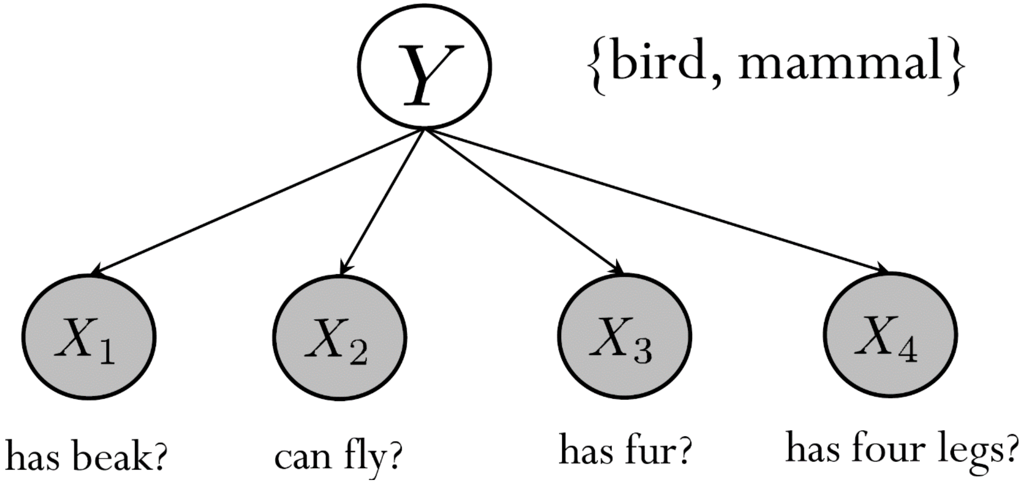
Estimate the posterior $p(z|x)$.

- Infer unobserved variables from observation.

Naive Bayes: $z = y$.

$$p(y=0|x)$$
$$= \frac{p(x|y=0)p(y=0)}{p(x|y=0)p(y=0) + p(x|y=1)p(y=1)}.$$

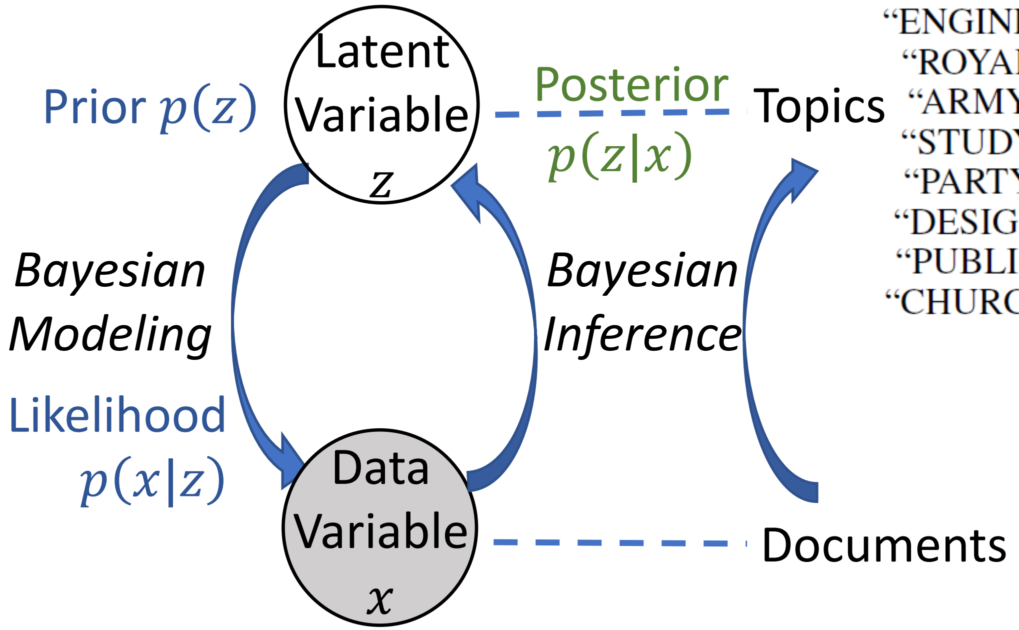
$f(x) = \arg\max_y p(y|x)$ achieves the lowest error $\int p\big(y = (1 - f(x)) \mid x\big)\, p(x)\, \mathrm{d}x$.



Bayesian Inference

Estimate the posterior $p(z|x)$.

- Extract knowledge/representation from data.



"ENGINES"	speed	product	introduced	designs	fuel
"ROYAL"	britain	queen	sir	earl	died
"ARMY"	commander	forces	war	general	military
"STUDY"	analysis	space	program	user	research
"PARTY"	act	office	judge	justice	legal
"DESIGN"	size	glass	device	memory	engine
"PUBLIC"	report	health	community	industry	conference
"CHURCH"	prayers	communion	religious	faith	historical

Bayesian Inference

Estimate the posterior $p(z|x)$.

$$p(z|x) = \frac{p(x,z)}{\boxed{p(x)}} = \frac{p(x,z)}{\boxed{\int p(x,z)\,\mathrm{d}z}}$$

Intractable!

Bayesian Inference

- Variational inference (VI)

  Use a *tractable* variational distribution $q(z)$ to approximate $p(z|x)$:
  $$\min_{q \in \mathcal{Q}} \mathrm{KL}\big(q(z), p(z|x)\big).$$
  Tractability: known density function, or samples are easy to draw.
  - Parametric VI: use a parameter ϕ to represent $q_\phi(z)$.
  - Particle-based VI: use a set of particles $\{z^{(i)}\}_{i=1}^N$ to represent $q(z)$.
- Monte Carlo (MC)
  - Draw samples from $p(z|x)$.
  - Typically done by simulating a *Markov chain* (i.e., MCMC) for tractability.

Bayesian Inference: Variational Inference

"Feed two birds with one scone."

- To do Bayesian inference by: $\min_{q \in \mathcal{Q}} \mathrm{KL}\big(q(z), p(z|x)\big)$,

  $\mathrm{KL}\big(q(z), p_\theta(z|x)\big)$ is hard to compute…

  Note $\quad \log p_\theta(x) = \mathcal{L}_\theta[q(z)] + \mathrm{KL}\big(q(z), p_\theta(z|x)\big)$,

  where $\quad \mathcal{L}_\theta[q(z)] \coloneqq \mathbb{E}_{q(z)}[\log p_\theta(z, x)] - \mathbb{E}_{q(z)}[\log q(z)]$,

  so $\quad \min_{q \in \mathcal{Q}} \mathrm{KL}\big(q(z), p(z|x)\big) \Leftrightarrow \max_{q \in \mathcal{Q}} \mathcal{L}_\theta[q(z)]$.

  The $\mathcal{L}_\theta[q(z)] = \mathbb{E}_{q(z)}[\log p_\theta(z, x)] - \mathbb{E}_{q(z)}[\log q(z)]$ is easier to compute.

Bayesian Inference: Variational Inference

"Feed two birds with one scone."

- In model learning: $\mathbb{E}_{\hat{p}(x)}[\log p_\theta(x)] = \frac{1}{N}\sum_{n=1}^{N} \log p_\theta(x^{(n)})$.
  - Introduce a *variational distribution* $q(z)$:

$$\log p_\theta(x) = \mathcal{L}_\theta[q(z)] + \mathrm{KL}\big(q(z), p_\theta(z|x)\big),$$

$$\text{where } \mathcal{L}_\theta[q(z)] \coloneqq \mathbb{E}_{q(z)}[\log p_\theta(z, x)] - \mathbb{E}_{q(z)}[\log q(z)].$$

    - $\mathcal{L}_\theta[q(z)] \leq \log p_\theta(x)$ ➔ **Evidence Lower BOund (ELBO)**!
    - $\mathcal{L}_\theta[q(z)]$ is easier to estimate.
  - (Variational) Expectation-Maximization Algorithm:

    (a) E-step: Let $\mathcal{L}_\theta[q(z)] \approx \log p_\theta(x)$, that is $\overbrace{\min_{q \in \mathcal{Q}} \mathrm{KL}\big(q(z), p_\theta(z|x)\big)}^{\text{Bayesian Inference}}$;

    (b) M-step: $\max_\theta \mathcal{L}_\theta[q(z)]$.

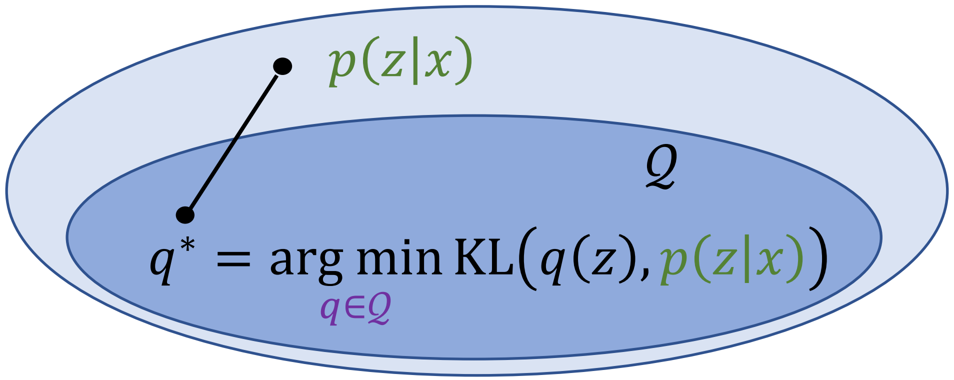
    - Classical EM: take $q(z) = p_\theta(z|x)$ (i.e., with exact inference).

Bayesian Inference: Variational Inference

- **Parametric variational inference**: use a parameter ϕ to represent $q_\phi(z)$.

$$\max_{\phi} \left(\mathcal{L}_\theta[q_\phi(z)] = \mathbb{E}_{q_\phi(z)}[\log p_\theta(z, x)] - \mathbb{E}_{q_\phi(z)}[\log q_\phi(z)] \right).$$

  - Main Challenge:
    - $\mathcal{Q}$ should be as large/general/flexible as possible,
    - while enables practical optimization of the ELBO.



Bayesian Inference: Variational Inference

- **Parametric variational inference**: use a parameter ϕ to represent $q_\phi(z)$.

$$\max_\phi \left(\mathcal{L}_\theta[q_\phi(z)] = \mathbb{E}_{q_\phi(z)}[\log p_\theta(z,x)] - \mathbb{E}_{q_\phi(z)}[\log q_\phi(z)] \right).$$

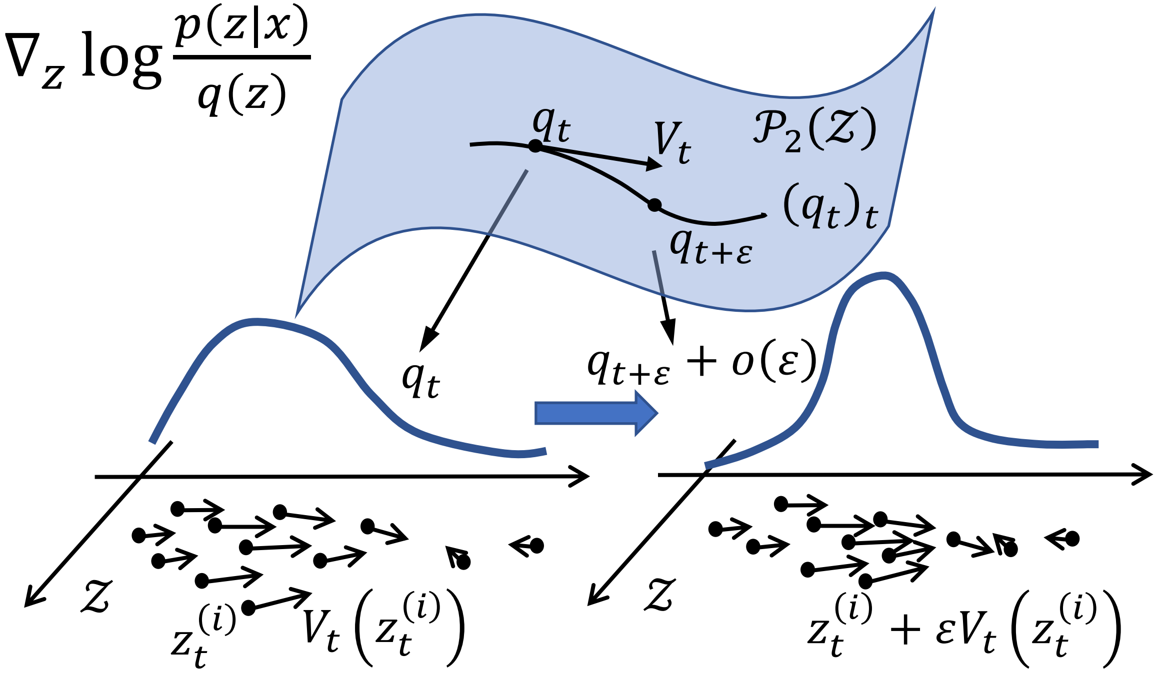
  - **Explicit variational inference**: specify the form of the density function $q_\phi(z)$.
    - Model-specific $q_\phi(z)$ design: $\mathcal{L}_\theta[q_\phi(z)]$ has closed form (e.g., [SJJ96] for SBN, [BNJ03] for LDA).
    - [GHB12, HBWP13, RGB14]: model-agnostic $q_\phi(z)$ (e.g., mixture of Gaussians).
    - [RM15, KSJ+16]: define $q_\phi(z)$ by a flow-based generative model.
  - **Implicit variational inference**: define $q_\phi(z)$ by a GAN-like generative model.
    - More flexible but more difficult to optimize.
    - Density ratio estimation: [MNG17, SSZ18a].

$$\mathcal{L}_\theta[q_\phi(z)] = \mathbb{E}_{q_\phi(z)}[\log p_\theta(x|z)] - \mathbb{E}_{q_\phi(z)}\left[\log \frac{q_\phi(z)}{p(z)}\right].$$

    - Gradient Estimation $\nabla \log q_\phi(z)$: [VLBM08, LT18, SSZ18b].

Bayesian Inference: Variational Inference

- **Particle-based variational inference**:
  - Use particles $\{z^{(i)}\}_{i=1}^N$ to represent $q(z)$.
  - To minimize $\mathrm{KL}\big(q(z), p(z|x)\big)$, find a proper dynamics $\frac{\mathrm{d}z_t}{\mathrm{d}t} = V_t(z_t)$ on the particles that decreases $\mathrm{KL}\big(q(z), p(z|x)\big)$ fastest.
  - One choice of V_t: $-\mathrm{grad}_q \mathrm{KL}\big(q(z), p(z|x)\big) = \nabla_z \log \frac{p(z|x)}{q(z)}$ on the 2-Wasserstein space.
    - Wasserstein space: an abstract space of distributions.
    - Wasserstein tangent vector $\Longleftrightarrow$ vector field.



Bayesian Inference: Variational Inference

- **Particle-based variational inference**: use particles $\{z^{(i)}\}_{i=1}^{N}$ to represent $q(z)$.

$$V := \mathrm{grad}_q \mathrm{KL}\big(q(z), p(z|x)\big) = \nabla_z \log \frac{p(z|x)}{q(z)}.$$

$$z^{(i)} \leftarrow z^{(i)} + \varepsilon V\big(z^{(i)}\big).$$

$V\big(z^{(i)}\big) \approx$

- SVGD [LW16]: $\sum_j K_{ij} \nabla_{z^{(j)}} \log p\big(z^{(j)} \big| x\big) + \sum_j \nabla_{z^{(j)}} K_{ij}$
- Blob [CZW+18]: $\nabla_{z^{(i)}} \log p\big(z^{(i)} \big| x\big) - \frac{\sum_j \nabla_{z^{(i)}} K_{ij}}{\sum_k K_{ik}} - \sum_j \frac{\nabla_{z^{(i)}} K_{ij}}{\sum_k K_{jk}}$.
- GFSD [LZC+19]: $\nabla_{z^{(i)}} \log p\big(z^{(i)} \big| x\big) - \frac{\sum_j \nabla_{z^{(i)}} K_{ij}}{\sum_k K_{ik}}$.
- GFSF [LZC+19]: $\nabla_{z^{(i)}} \log p\big(z^{(i)} \big| x\big) + \sum_{j,k} (K^{-1})_{ik} \nabla_{z^{(j)}} K_{kj}$.

$= \sum_j \big(z^{(i)} - z^{(j)}\big) K_{ij}$
for Gaussian Kernel:
Repulsive force!

Outline

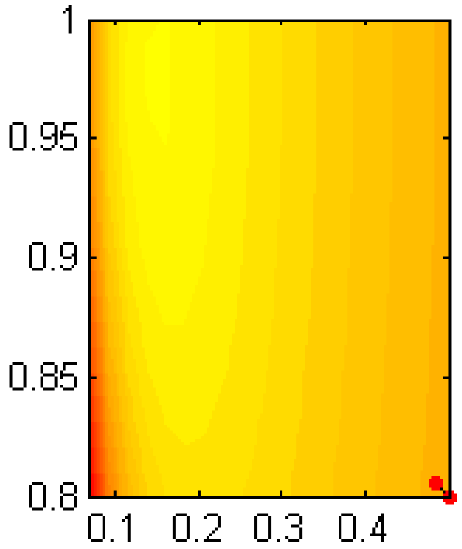
- Generative Models: Overview
- Plain Generative Models
    - Autoregressive Models
- Latent Variable Models
  - Deterministic Generative Models
    - Generative Adversarial Nets
    - Flow-Based Models
  - Probabilistic Graphical Models
    - Directed PGMs
      - **Bayesian Inference** (variational inference, **MCMC**)
      - Deep Bayesian Models (VAE)
    - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
    - Diffusion-Based Models

Bayesian Inference: MCMC

- Monte Carlo
  - Directly draw (i.i.d.) samples from $p(z|x)$.
  - Almost always impossible to directly do so (esp. w/ unnormalized $p(z|x)$).
- Markov Chain Monte Carlo (MCMC):

  Simulate a Markov chain whose stationary distribution is $p(z|x)$.
  - Easier to implement: only requires unnormalized $p(z|x)$ (*e.g.*, $p(z,x)$).
  - Asymptotically accurate.
  - Drawback/Challenge: sample auto-correlation.

    Less effective than i.i.d. samples.



[GC11]

Bayesian Inference: MCMC

A fantastic MCMC animation site: https://chi-feng.github.io/mcmc-demo/

The Markov-chain Monte Carlo Interactive Gallery

Click on an algorithm below to view interactive demo:

- Random Walk Metropolis Hastings
- Adaptive Metropolis Hastings [1]
- Hamiltonian Monte Carlo [2]
- No-U-Turn Sampler [2]
- Metropolis-adjusted Langevin Algorithm (MALA) [3]
- Hessian-Hamiltonian Monte Carlo (H2MC) [4]
- Stein Variational Gradient Descent (SVGD) [5]
- Nested Sampling with RadFriends (RadFriends-NS) [6]

View the source code on github: https://github.com/chi-feng/mcmc-demo.

Bayesian Inference: MCMC

Classical MCMC

- Metropolis-Hastings framework [MRR+53, Has70]:

  Draw $z^* \sim q\left(z^* | z^{(k)}\right)$ and take $z^{(k+1)}$ as z^* with probability
  $$\min\left\{1, \frac{q\left(z^{(k)} \middle| z^*\right) p(z^* | x)}{q\left(z^* \middle| z^{(k)}\right) p\left(z^{(k)} \middle| x\right)}\right\},$$
  else take $z^{(k+1)}$ as $z^{(k)}$.

  - Note that $\frac{p(z^* | x)}{p\left(z^{(k)} \middle| x\right)} = \frac{p(z^*, x)}{p\left(z^{(k)}, x\right)}$ can be evaluated.
  - Proposal distribution $q(z^* | z)$: e.g., taken as $\mathcal{N}(z^* | z, \sigma^2)$.

Bayesian Inference: MCMC

Classical MCMC

- Gibbs sampling [GG87]:

  Iteratively sample from conditional distributions, which are easier to draw:

$$
\begin{aligned}
&z_1^{(1)} \sim p\left(z_1 \,\middle|\, \phantom{z_1^{(1)},} z_2^{(0)}, z_3^{(0)}, \ldots, z_d^{(0)}, x\right), \\
&z_2^{(1)} \sim p\left(z_2 \,\middle|\, z_1^{(1)}, \phantom{z_2^{(0)},} z_3^{(0)}, \ldots, z_d^{(0)}, x\right), \\
&z_3^{(1)} \sim p\left(z_3 \,\middle|\, z_1^{(1)}, z_2^{(1)}, \phantom{z_3^{(0)},} \ldots, z_d^{(0)}, x\right), \\
&\ldots, \\
&z_i^{(k+1)} \sim p\left(z_i \,\middle|\, z_1^{(k+1)}, \ldots, z_{i-1}^{(k+1)}, \phantom{z_i^{(k)},} z_{i+1}^{(k)}, \ldots, z_d^{(k)}, x\right).
\end{aligned}
$$

Bayesian Inference: MCMC

Dynamics-based MCMC

- Simulates a jump-free continuous-time Markov process (dynamics):

$$\mathrm{d}z = \underbrace{f(z)\,\mathrm{d}t}_{\text{drift}} + \underbrace{\sqrt{2D(z)}\,\mathrm{d}B_t(z)}_{\text{diffusion}},$$

Pos. semi-def. matrix

Brownian motion

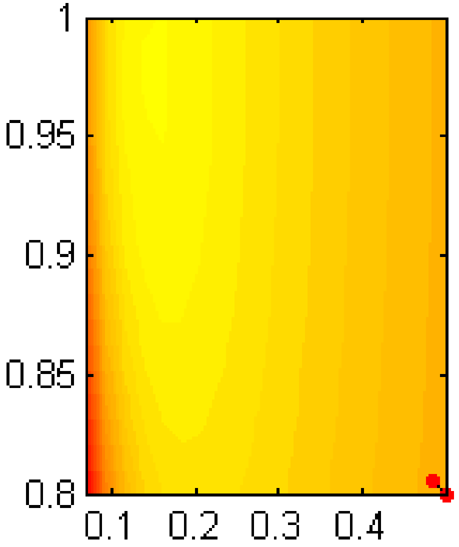
$$\Delta z = f(z)\varepsilon + \mathcal{N}(0, 2D(z)\varepsilon) + o(\varepsilon),$$

with appropriate $f(z)$ and $D(z)$ so that $p(z|x)$ is kept stationary/invariant.

- Informative transition using gradient $\nabla_z \log p(z|x)$.
- Some are compatible with *stochastic gradient* (SG): more efficient.

$$\nabla_z \log p(z|x) = \nabla_z \log p(z) + \sum_{n\in\mathcal{D}} \nabla_z \log p\left(x^{(n)} \middle| z\right),$$

$$\tilde{\nabla}_z \log p(z|x) = \nabla_z \log p(z) + \frac{|\mathcal{D}|}{|\mathcal{S}|} \sum_{n\in\mathcal{S}} \nabla_z \log p\left(x^{(n)} \middle| z\right), \mathcal{S} \subset \mathcal{D}.$$



[GC11]

Bayesian Inference: MCMC

Dynamics-based MCMC

- Langevin Dynamics [RS02] (compatible with SG [WT11, CDC15, TTV16]):
$$z^{(k+1)} = z^{(k)} + \varepsilon \nabla \log p\left(z^{(k)} \middle| x\right) + \mathcal{N}(0,2\varepsilon).$$
- Hamiltonian Monte Carlo [DKPR87, Nea11, Bet17]

  (*incompatible* with SG [CFG14, Bet15]; leap-frog integrator [CDC15]):
$$r^{(0)} \sim \mathcal{N}(0,\Sigma), \qquad \begin{cases} r^{(k+1/2)} = r^{(k)} + (\varepsilon/2)\nabla \log p\left(z^{(k)} \middle| x\right), \\ z^{(k+1)} = z^{(k)} + \varepsilon \Sigma^{-1} r^{(k+1/2)}, \\ r^{(k+1)} = r^{(k+1/2)} + (\varepsilon/2)\nabla \log p\left(z^{(k+1)} \middle| x\right). \end{cases}$$
- Stochastic Gradient Hamiltonian Monte Carlo [CFG14] (compatible with SG):
$$\begin{cases} z^{(k+1)} = z^{(k)} + \varepsilon \Sigma^{-1} r^{(k)}, \\ r^{(k+1)} = r^{(k)} + \varepsilon \nabla \log p\left(z^{(k)} \middle| x\right) - \varepsilon C \Sigma^{-1} r^{(k)} + \mathcal{N}(0,2C\varepsilon). \end{cases}$$
- …

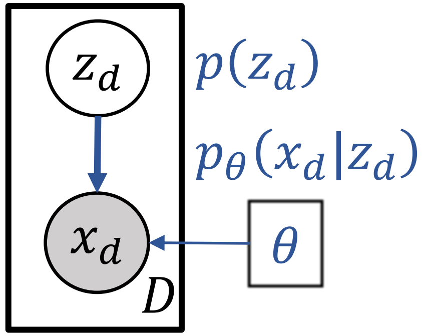
Bayesian Inference: Comparison

	Parametric VI	Particle-Based VI	MCMC
Asymptotic Accuracy	No	Yes	Yes
Approximation Flexibility	Limited	Unlimited	Unlimited
Empirical Convergence Speed	High	High	Low
Particle Efficiency	(Do not apply)	High	Low
High-Dimensional Efficiency	High	Low	High

Outline

- Generative Models: Overview
- Plain Generative Models
    - Autoregressive Models
- Latent Variable Models
  - Deterministic Generative Models
    - Generative Adversarial Nets
    - Flow-Based Models
  - Probabilistic Graphical Models
    - Directed PGMs
      - Bayesian Inference (variational inference, MCMC)
      - **Deep Bayesian Models (VAE)**
    - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
    - Diffusion-Based Models

Variational Auto-Encoder



More *flexible* Bayesian model using *deep learning* tools.

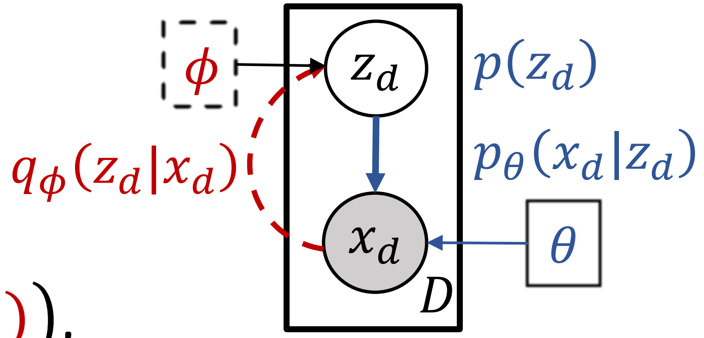
- Model structure (decoder) [KW14]:

  $z_d \sim p(z_d) = \mathcal{N}(z_d|0, I)$,

  $x_d \sim p_\theta(x_d|z_d) = \mathcal{N}\big(x_d|\mu_\theta(z_d), \Sigma_\theta(z_d)\big)$,

  where $\mu_\theta(z_d)$ and $\Sigma_\theta(z_d)$ are modeled by neural networks.

Variational Auto-Encoder



- Variational inference (encoder) [KW14]:

  $$q_\phi(z|x) \coloneqq \prod_{d=1}^{D} q_\phi(z_d|x_d) = \prod_{d=1}^{D} \mathcal{N}\big(z_d \big| \nu_\phi(x_d), \Gamma_\phi(x_d)\big),$$

  where $\nu_\phi(x_d), \Gamma_\phi(x_d)$ are also NNs.

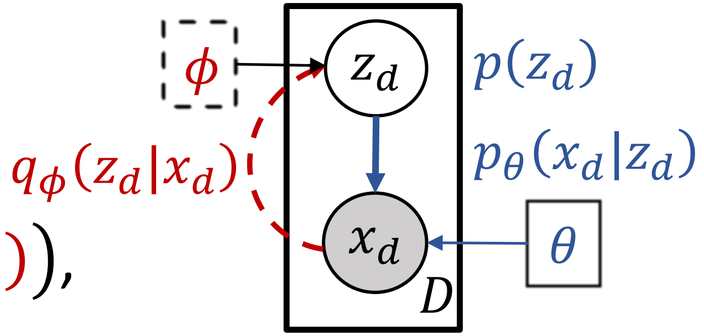
  $$\mathrm{ELBO}(x_d) = \mathbb{E}_{q_\phi(z_d|x_d)}[\log p_\theta(z_d) p_\theta(x_d|z_d) - \log q_\phi(z_d|x_d)].$$

  - Gradient estimation with the *reparameterization trick*:

    $$z_d \sim q_\phi(z_d|x_d) \iff z_d = g_\phi(x_d, \epsilon) \coloneqq \nu_\phi(x_d) + \epsilon\sqrt{\Gamma_\phi(x_d)}, \epsilon \sim q(\epsilon) \coloneqq \mathcal{N}(\epsilon|0, I).$$

    - Gradient estimation: $\nabla_{\phi,\theta}\mathrm{ELBO}(x_d) =$
      $\mathbb{E}_{q(\epsilon)}\left[\nabla_{\phi,\theta}\left(\log p_\theta\left(g_\phi(x_d,\epsilon)\right) p_\theta\left(x_d | g_\phi(x_d,\epsilon)\right) - \log q_\phi\big(g_\phi(x_d,\epsilon)|x_d\big)\right)\right].$
    - Smaller variance than REINFORCE-like estimator [Wil92]:
      $\nabla_\phi \mathbb{E}_{q_\phi}[f_\phi] = \mathbb{E}_{q_\phi}[\nabla_\phi f_\phi + f_\phi \nabla_\phi \log q_\phi].$

Variational Auto-Encoder

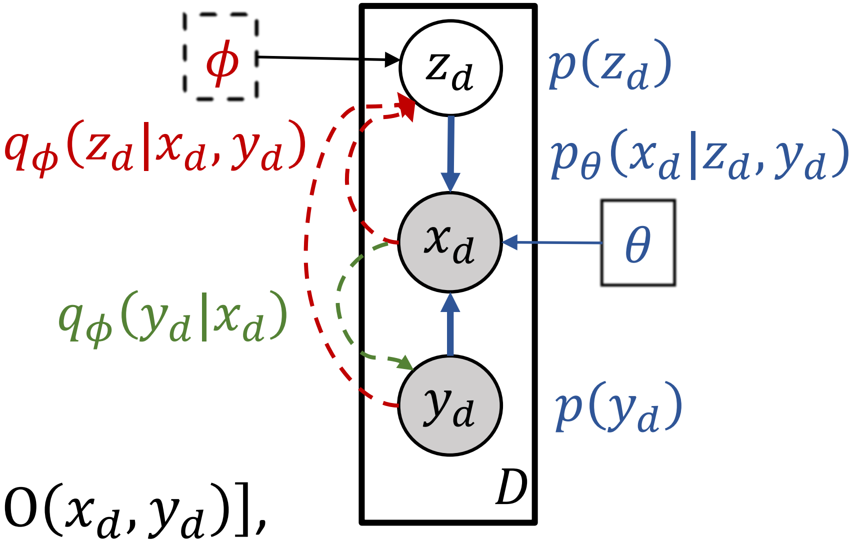


- Variational inference (encoder) [KW14]:

  $$q_\phi(z|x) := \prod_{d=1}^{D} q_\phi(z_d|x_d) = \prod_{d=1}^{D} \mathcal{N}\big(z_d \big| \nu_\phi(x_d), \Gamma_\phi(x_d)\big),$$

  where $\nu_\phi(x_d), \Gamma_\phi(x_d)$ are also NNs.
  - Amortized inference: to approximate local posteriors $\{p(z_d|x_d)\}_{d=1}^{D}$,
    - instead of using $q_{\phi_d}(z_d)$ for each $p(z_d|x_d)$ and learning *local* parameters $\{\phi_d\}$ (like LDA),
    - use $q_\phi(z_d|x_d)$ and learn the *global* parameter ϕ (**fast inference for unseen x_d**).

Variational Auto-Encoder



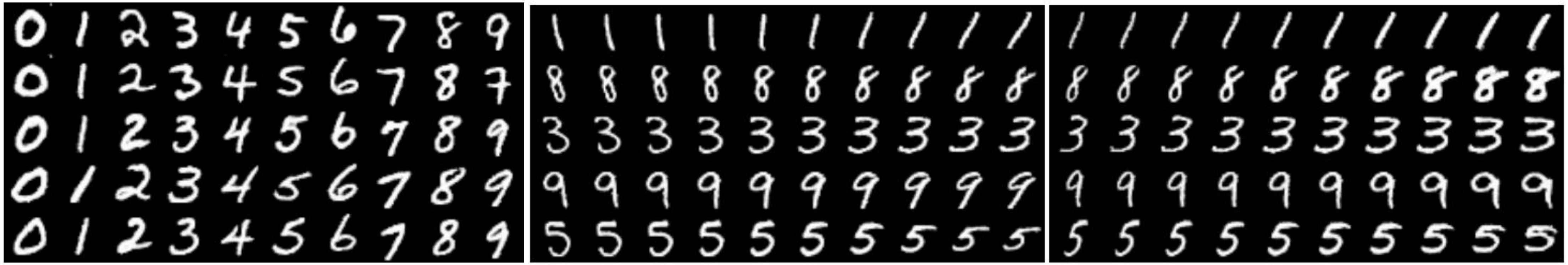
- Semi-supervised VAE [KMRW14, M2]
  - For labeled data:
    - Required encoder: $q_\phi(z_d|x_d, y_d)$.
    - Objective: $\mathbb{E}_{\hat{p}(x_d,y_d)}[\log p_\theta(x_d, y_d)] \geq \mathbb{E}_{\hat{p}(x_d,y_d)}[\mathrm{ELBO}(x_d, y_d)]$,

    $$\mathrm{ELBO}(x_d, y_d) = \mathbb{E}_{q_\phi(z_d|x_d,y_d)}\left[\log p_\theta(z_d) p_\theta(y_d) p_\theta(x_d|z_d, y_d) - \log q_\phi(z_d|x_d, y_d)\right].$$
  - For unlabeled data:
    - Required encoder: $q_\phi(y_d, z_d|x_d) = q_\phi(y_d|x_d) q_\phi(z_d|x_d, y_d)$.
    - Objective: $\mathbb{E}_{\hat{p}(x_d)}[\log p_\theta(x_d)] \geq \mathbb{E}_{\hat{p}(x_d)}[\mathrm{ELBO}(x_d)]$,

    $$\begin{aligned}\mathrm{ELBO}(x_d) &= \mathbb{E}_{q_\phi(y_d, z_d|x_d)}\left[\log p_\theta(z_d) p_\theta(y_d) p_\theta(x_d|z_d, y_d) - \log q_\phi(y_d, z_d|x_d)\right] \\ &= \mathbb{E}_{q_\phi(y_d|x_d)}\left[\mathrm{ELBO}(x_d, y_d) - \log q_\phi(y_d|x_d)\right].\end{aligned}$$
  - For prediction: use $q_\phi(y_d|x_d)$.

Variational Auto-Encoder

- Learning disentangled representation
  - InfoGAN [CDH+16]: max mutual_info(part_of_z, generated_x).
  - β-VAE [HLP+17]: upscale the KL term ($q(z|x)$ to factorized prior $p(z)$) in ELBO.
  - Total Correlation VAE [CLG+18]: upscale the total-correlation term in a finer decomposition of ELBO.



(a) Varying c_1 on InfoGAN (Digit type) (c) Varying c_2 from -2 to 2 on InfoGAN (Rotation) (d) Varying c_3 from -2 to 2 on InfoGAN (Width)

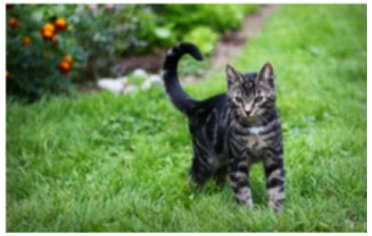
Variational Auto-Encoder

- Learning disentangled representation
  - Formal definition [HAP+18] (roughly): a class of transformations on x (holding some semantics) changes only one dimension of the representation.
  - Impossibility theorem [LBL+19]:

Theorem 1. *For $d > 1$, let $\mathbf{z} \sim P$ denote any distribution which admits a density $p(\mathbf{z}) = \prod_{i=1}^{d} p(\mathbf{z}_i)$. Then, there exists an infinite family of bijective functions $f : \operatorname{supp}(\mathbf{z}) \to \operatorname{supp}(\mathbf{z})$ such that $\frac{\partial f_i(\boldsymbol{u})}{\partial u_j} \neq 0$ almost everywhere for all i and j (i.e., $\mathbf{z}$ and $f(\mathbf{z})$ are completely entangled) and $P(\mathbf{z} \leq \boldsymbol{u}) = P(f(\mathbf{z}) \leq \boldsymbol{u})$ for all $\boldsymbol{u} \in \operatorname{supp}(\mathbf{z})$ (i.e., they have the same marginal distribution).*

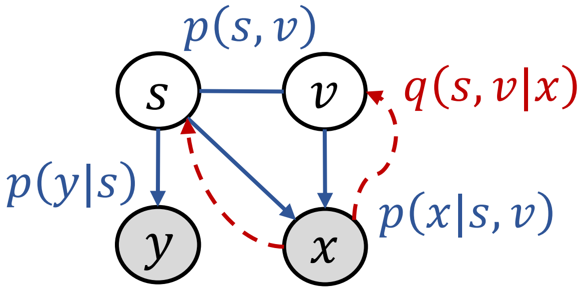
  - Works afterwards:
    - Weak supervision: a few labels [LTB+19], pairwise similarity [CB20], paired unsupervised data [LPR+20], rank pairing [SCK+20].
    - If the cause of z is observed, z's suff. stat. can be **identified** up to a permutation [KKM+20].

Variational Auto-Encoder

Train: 

Test: 

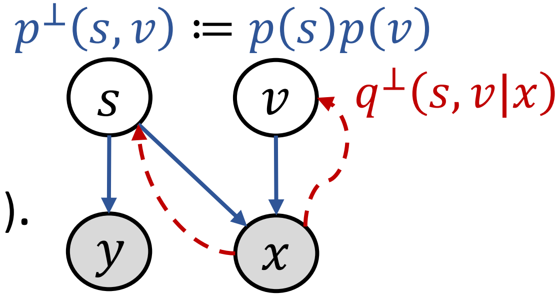
- Learning causal representation.
  - Causal relations tend to hold across domains [SJP+12, PJS17, Sch19].
  - Causal generative model [LSW+21] (single training domain; [SWZ+21] for multiple tr. dom.):

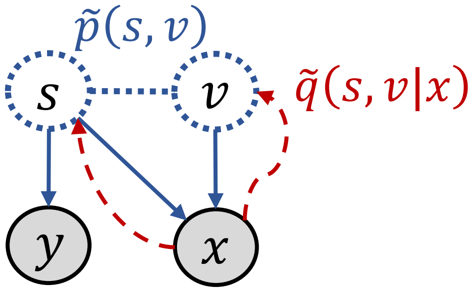


Model:

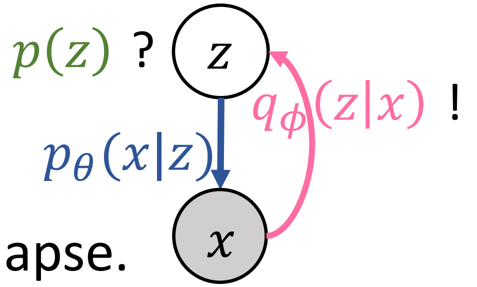
- Not all representation *causes* y ➔ the $s$emantic-$v$ariation split.
- Generative process is more likely causal/invariant than inference process.
- Domain shift comes from the change of **prior** (repr. distr.).

- **Prediction**: use an *independent prior* (if no test data) or a *newly learned prior* (unlabeled test data).
- **Learning**: using the test-domain inf. model $q^{\perp}(s,v|x)$ or $\tilde{q}(s,v|x)$ suffices.
- **Theory**: under certain conditions,
  a well-learned model **identifies** the semantics s,
  and the test-domain/out-of-distr. prediction error
  is bounded (no test data) or vanishes (unlabeled test data).





Cyclic Generative Models [LTQ+21]



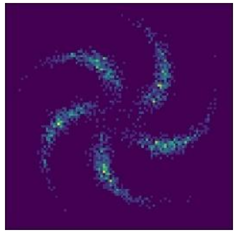
- VAE problem: modeling $p(x, z)$ by specifying a prior $p(z)$:

(1) Hard inference.

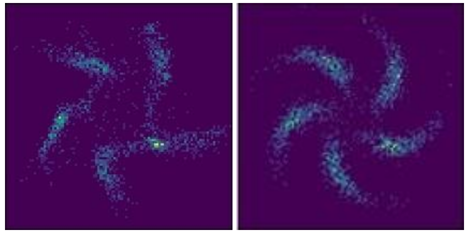
Need inference model $q_\phi(z|x)$ anyway.

(2) Manifold mismatch.

true data distr.



learned data distr.



(3) Posterior collapse.

class-wise posterior samples

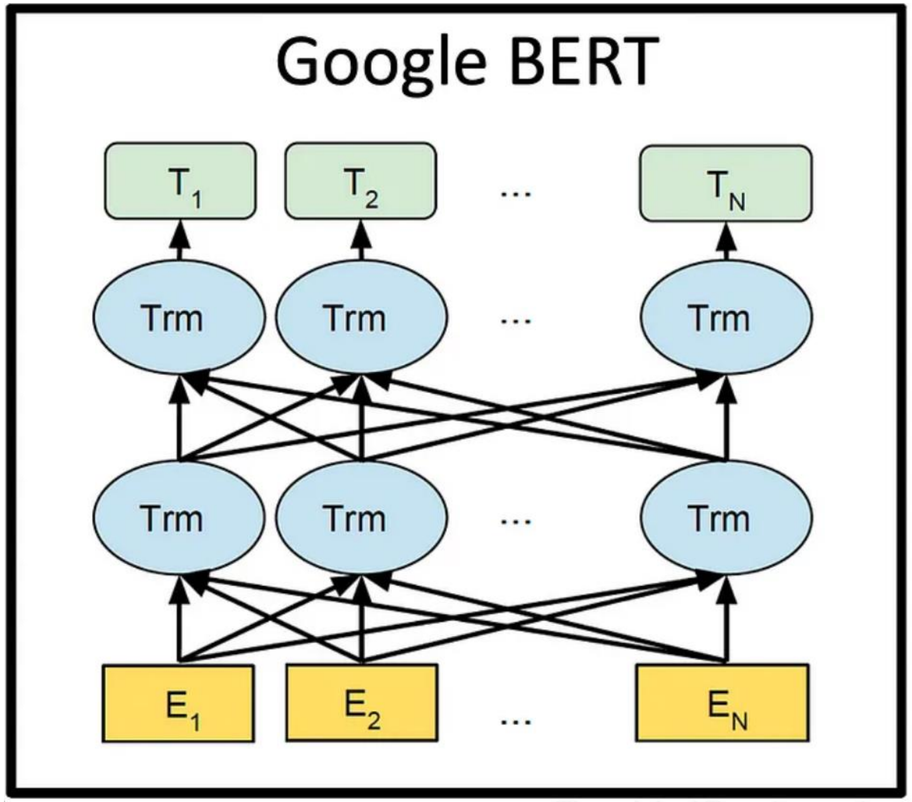
Use $q_\phi(z|x)$ in place of $p(z)$ to define $p(x, z)$:

- Thm (informal): Conditional densities $p(x|z)$, $q(z|x)$ come from a common joint $p(x, z)$ (*compatible*), **iff.** $\frac{p(x|z)}{q(z|x)}$ factorizes as $a(x)b(z)$ on *a certain region that they determine*.

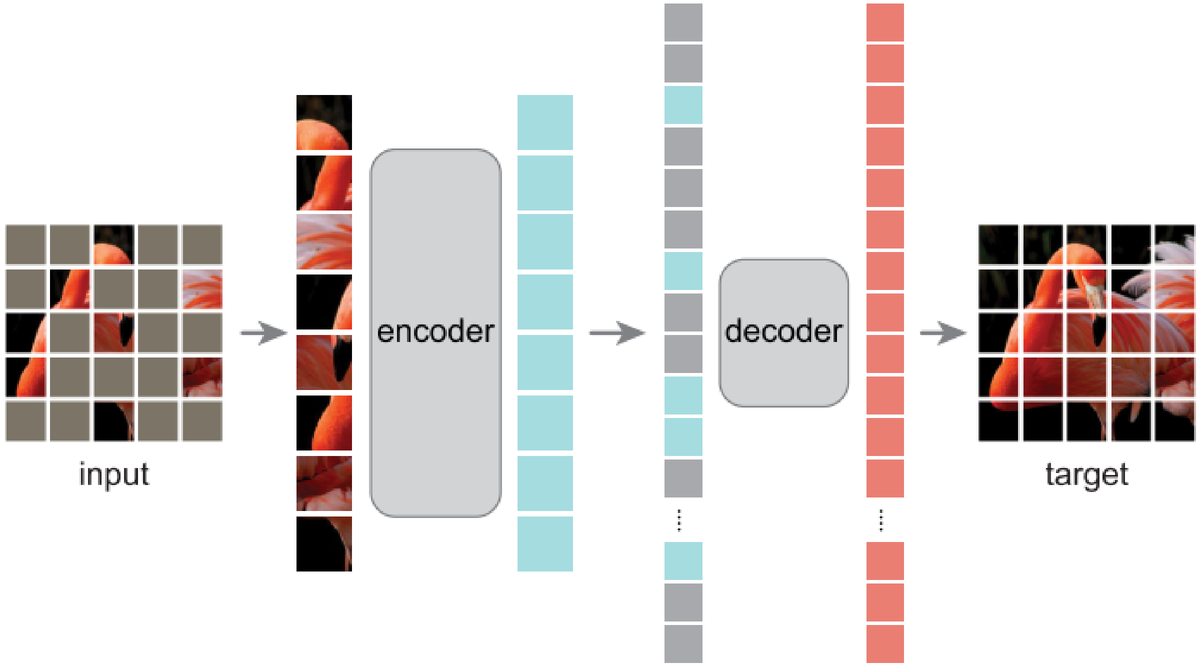
  Such $p(x, z)$ is unique on each of such regions (*determinacy*).
  - For $p(x|z) = \delta_{f(z)}(x)$: Compatibility $\Leftrightarrow \exists x_0$ s.t. $q(f^{-1}(\{x_0\})|x_0) = 1$;
    Trivial determinacy: each region is a $(f(z_0), z_0)$ point, so $p(x, z) = \delta_{(f(z_0), z_0)}(x, z)$.
- Algorithms are possible!
  - Enforcing compatibility: min $\mathbb{E}_{p^*(x) q_\phi(z|x)} \left\| \nabla_x \nabla_z^\top \log \left(p_\theta(x|z) / q_\phi(z|x) \right) \right\|_F^2$.
  - Data-fitting: MLE: $\mathbb{E}_{p^*(x)}[\log p_{\theta,\phi}(x)] = \mathbb{E}_{p^*(x)} \left[-\log \mathbb{E}_{q_\phi(z'|x)}[1/p_\theta(x|z')] \right]$.
  - Data gen.: MCMC: $\Delta x^{(t)} = \varepsilon \nabla_{x^{(t)}} \log \frac{p_\theta(x^{(t)}|z^{(t)})}{q_\phi(z^{(t)}|x^{(t)})} + \sqrt{2\varepsilon}\, \eta^{(t)}$, where $z^{(t)} \sim q_\phi(z|x^{(t)})$, $\eta^{(t)} \sim \mathcal{N}(0, I)$.

Cyclic Generative Models [LTQ+21]

- Masked language/vision models are Cyclic Generative Models!
  - BERT / Masked Auto-Encoder: learns $p(x_i|x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_N)$ for each i.
  - They are almost generative models.



[DCLT18]

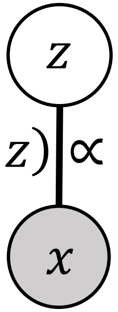


[HCX+21]

Outline

- Generative Models: Overview
- Plain Generative Models
    - Autoregressive Models
- Latent Variable Models
  - Deterministic Generative Models
    - Generative Adversarial Nets
    - Flow-Based Models
  - Probabilistic Graphical Models
    - Directed PGMs
      - Bayesian Inference (variational inference, MCMC)
      - Deep Bayesian Models (VAE)
    - **Undirected PGMs (Boltzmann machines, energy-based models, score-based models)**
    - Diffusion-Based Models

Undirected PGMs



$p_\theta(x,z) \propto \exp(-E_\theta(x,z))$

Specify $p_\theta(x,z)$ by an energy function $E_\theta(x,z)$:

$$p_\theta(x,z) = \frac{1}{Z_\theta} \exp(-E_\theta(x,z)), Z_\theta = \int \exp(-E_\theta(x',z')) \, \mathrm{d}x' \mathrm{d}z'.$$

- Only correlation and no causality: $p(x,z)$ is either $p(z)p(x|z)$ or $p(x)p(z|x)$.

\+ Flexible and simple in modeling dependency.

\- Harder to learn and generate than directed PGMs.

- Learning: even $p_\theta(x,z)$ is unavailable.

$$\nabla_\theta \mathbb{E}_{\hat{p}(x)}[\log p_\theta(x)] = -\underbrace{\mathbb{E}_{\hat{p}(x) p_\theta(z|x)}}_{\substack{\text{(augmented) data distribution} \\ \text{(Bayesian inference)}}}[\nabla_\theta E_\theta(x,z)] + \underbrace{\mathbb{E}_{p_\theta(x,z)}}_{\substack{\text{model distribution} \\ \text{(generation)}}}[\nabla_\theta E_\theta(x,z)].$$

=0 if $E = \log p$.

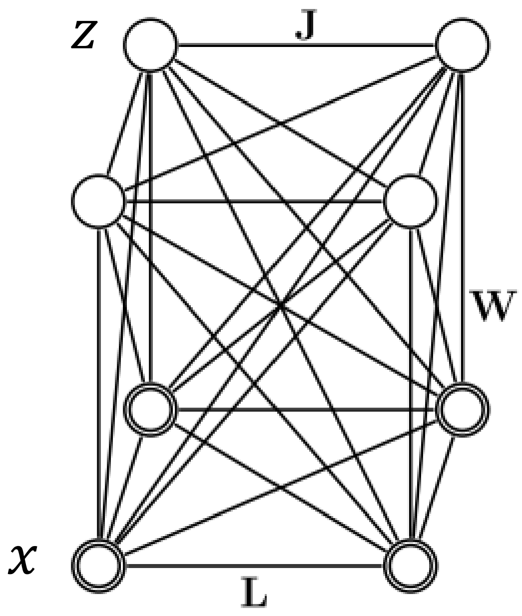
- Bayesian inference: generally same as directed PGMs.
- Generation: rely on MCMC or training a generator.

Undirected PGMs

- Learning: $\nabla_\theta \mathbb{E}_{\hat{p}(x)}[\log p_\theta(x)] = -\mathbb{E}_{\hat{p}(x) p_\theta(z|x)}[\nabla_\theta E_\theta(x,z)] + \mathbb{E}_{p_\theta(x,z)}[\nabla_\theta E_\theta(x,z)]$.

  Bayesian Inference　　Generation

  - Boltzmann Machine: Gibbs sampling for both inference and generation [HS83].



$$E_\theta(x,z) = -x^\top W z - \frac{1}{2} x^\top L x - \frac{1}{2} z^\top J z.$$

$$\Longrightarrow$$

$$p_\theta(z_j | x, z_{-j}) = \mathrm{Bern}\left(\sigma\left(\textstyle\sum_{i=1}^{D} W_{ij} x_i + \sum_{m \neq j}^{P} J_{jm} z_j\right)\right),$$

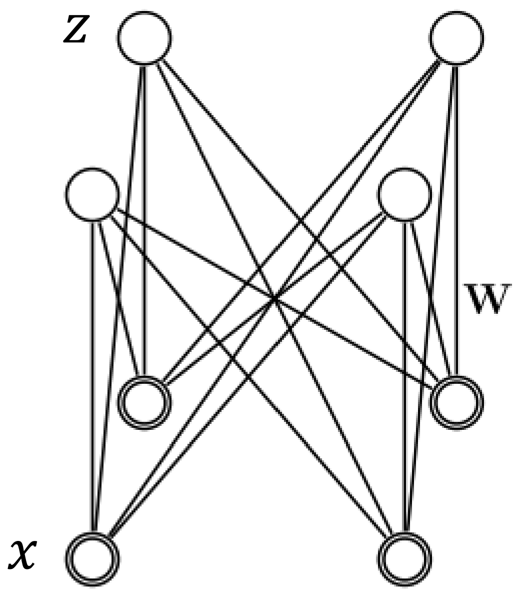
$$p_\theta(x_i | z, x_{-i}) = \mathrm{Bern}\left(\sigma\left(\textstyle\sum_{j=1}^{P} W_{ij} z_j + \sum_{k \neq i}^{D} L_{ik} x_k\right)\right).$$

Undirected PGMs

- Learning: $\nabla_\theta \mathbb{E}_{\hat{p}(x)}[\log p_\theta(x)] = -\mathbb{E}_{\hat{p}(x)p_\theta(z|x)}[\nabla_\theta E_\theta(x,z)] + \mathbb{E}_{p_\theta(x,z)}[\nabla_\theta E_\theta(x,z)]$.

  Bayesian Inference Generation

  - Restricted Boltzmann Machine [Smo86]:



$$E_\theta(x,z) = -x^\top W z + {b^{(x)}}^\top x + {b^{(z)}}^\top z.$$

- Bayesian Inference is exact:
  $$p_\theta(z_k|x) = \mathrm{Bern}\left(\sigma\left(x^\top W_{:k} + b_k^{(z)}\right)\right).$$
- Generation: Gibbs sampling.
  Iterate:
  $$p_\theta(z_k|x) = \mathrm{Bern}\left(\sigma\left(x^\top W_{:k} + b_k^{(z)}\right)\right),$$
  $$p_\theta(x_k|z) = \mathrm{Bern}\left(\sigma\left(W_{k:} z + b_k^{(x)}\right)\right).$$

Undirected PGMs

Deep Energy-Based Models:

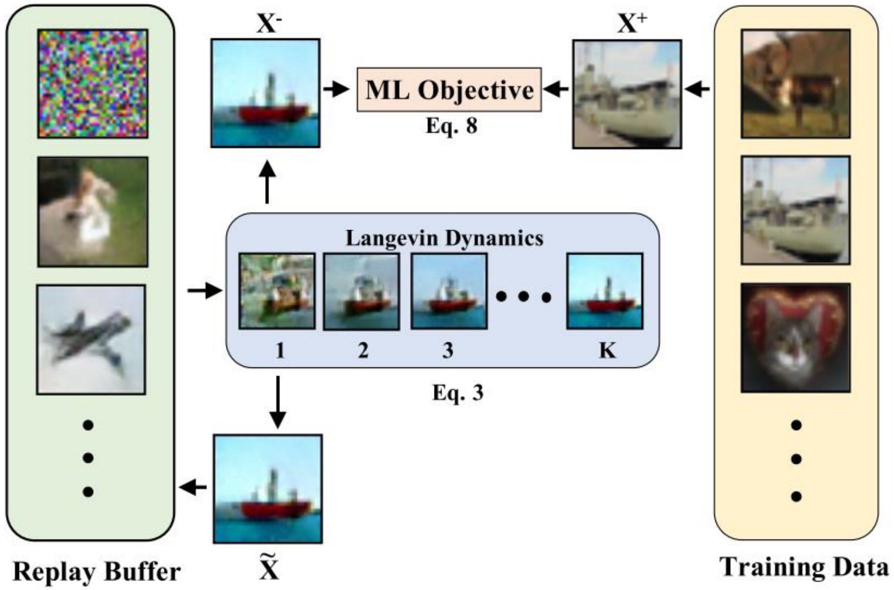
No latent variable; $E_\theta(x)$ is modeled by a neural network.

$$\nabla_\theta \mathbb{E}_{\hat{p}(x)}[\log p_\theta(x)] = -\mathbb{E}_{\hat{p}(x)}[\nabla_\theta E_\theta(x)] + \mathbb{E}_{p_\theta(x')}[\nabla_\theta E_\theta(x')].$$

- [DM19]: estimate $\mathbb{E}_{p_\theta(x')}[\cdot]$ by samples drawn by the Langevin Dynamics

$$x^{(k+1)} = x^{(k)} - \varepsilon \nabla_x E_\theta\left(x^{(k)}\right) + \mathcal{N}(0, 2\varepsilon).$$

  - Same as the generation process.
  - Replay buffer for initializing the LD chain.
  - L_2-regularization on the energy function.



Score-Based Generative Models

- Score-based methods [Hyv05]:
  - Learn $\mathbf{s}_\theta(\mathbf{x})$ (represents $\nabla_\mathbf{x} \log p_\theta(\mathbf{x}) = -\nabla_\mathbf{x} E_\theta(\mathbf{x})$) to approx $\nabla_\mathbf{x} \log p_{\text{data}}(\mathbf{x})$.
  - Data generation: run MCMC, e.g., Langevin dynamics with $\mathbf{s}_\theta(\mathbf{x})$.

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \varepsilon \mathbf{s}_\theta\left(\mathbf{x}^{(k)}\right) + \mathcal{N}(0, 2\varepsilon).$$

Score-Based Generative Models

- Training with **Score Matching (SM)**: Recall $\mathbf{s}_\theta(\mathbf{x}) \coloneqq \nabla_{\mathbf{x}} \log p_\theta(\mathbf{x})$, so:

$$\operatorname*{argmin}_\theta \mathbb{E}_{q(\mathbf{x})} \|\mathbf{s}_\theta(\mathbf{x}) - \nabla \log q(\mathbf{x})\|^2 \quad = \operatorname*{argmin}_\theta \mathbb{E}_{q(\mathbf{x})} [\|\mathbf{s}_\theta(\mathbf{x})\|^2 + 2\nabla \cdot \mathbf{s}_\theta(\mathbf{x})] \text{ [Hyv05].}$$

$\nabla \log q(\mathbf{x})$ is unknown...

Only requires data from $q(\mathbf{x})$!

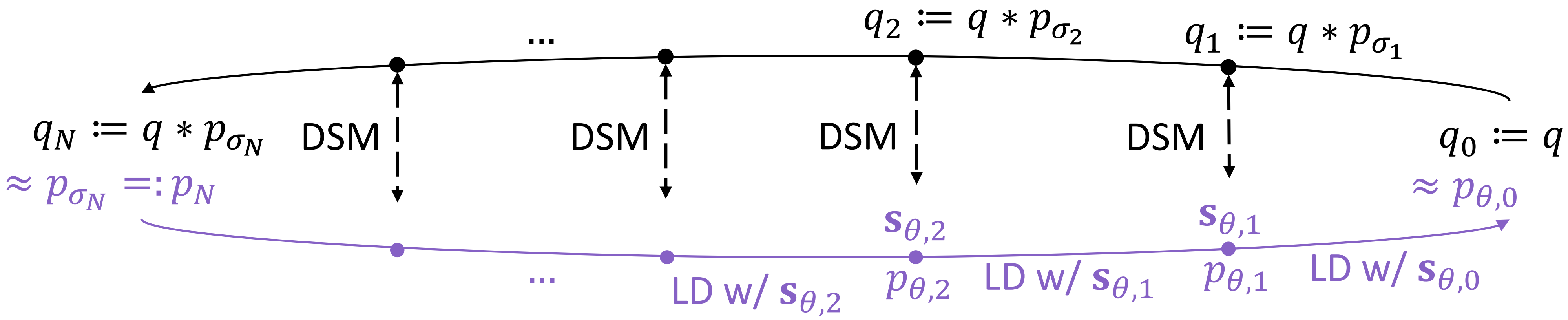
- **Denoising Score Matching (DSM)** [Vin11]:
  - When data distributes on a low-dimensional manifold, $\nabla \log q(\mathbf{x})$ is ill-defined.
    ➔ Learn the score of $q_\sigma(\tilde{\mathbf{x}}) \coloneqq (q * p_\sigma)(\tilde{\mathbf{x}}) = \int q(\mathbf{x}) q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) \, \mathrm{d}\mathbf{x}, \quad q_\sigma(\tilde{\mathbf{x}}|\mathbf{x}) \coloneqq \mathcal{N}(\tilde{\mathbf{x}}|\mathbf{x}, \sigma^2 \mathbf{I}_D)$.
  - SM to perturbed: $\operatorname*{argmin}_\theta \mathbb{E}_{q_\sigma(\tilde{\mathbf{x}})} [\|\mathbf{s}_\theta(\tilde{\mathbf{x}})\|^2 + 2\nabla \cdot \mathbf{s}_\theta(\tilde{\mathbf{x}})]$

    DSM: $= \operatorname*{argmin}_\theta \mathbb{E}_{q(\mathbf{x})} \mathbb{E}_{p_\sigma(\boldsymbol{\epsilon})} \left\| \mathbf{s}_\theta(\mathbf{x} + \sigma\boldsymbol{\epsilon}) + \frac{\boldsymbol{\epsilon}}{\sigma} \right\|^2$:

    drives $\mathbf{s}_\theta(\tilde{\mathbf{x}}) \to \nabla \log q_\sigma(\tilde{\mathbf{x}}) = \nabla \log(q * p_\sigma)(\tilde{\mathbf{x}})$.

Score-Based Generative Models

- Noise-Conditioned Score Network (NCSN) [SE19]:



$$\mathcal{L}_{\text{DSM}} \coloneqq \mathbb{E}_{\text{U}(i|\{0,\dots,N\})} \lambda_i \mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{q_{\sigma_i}(\tilde{\mathbf{x}}|\mathbf{x})} \left\| \mathbf{s}_{\theta,i}(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_{\sigma_i}(\tilde{\mathbf{x}}|\mathbf{x}) \right\|^2.$$

Outline

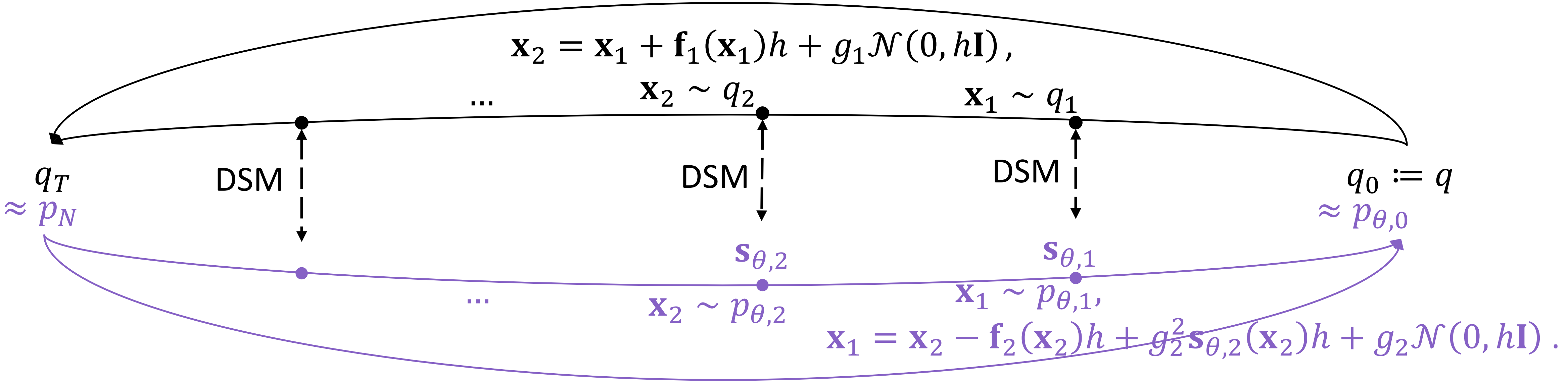
- Generative Models: Overview
- Plain Generative Models
    - Autoregressive Models
- Latent Variable Models
  - Deterministic Generative Models
    - Generative Adversarial Nets
    - Flow-Based Models
  - Probabilistic Graphical Models
    - Directed PGMs
      - Bayesian Inference (variational inference, MCMC)
      - Deep Bayesian Models (VAE)
    - Undirected PGMs (Boltzmann machines, energy-based models, score-based models)
    - **Diffusion-Based Models [More detailed introduction]**

Score-Based and Diffusion-Based Generative Models

- Diffusion-based generative model (cont. time form [SSK+21]):

$$\Leftrightarrow \mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t - g_t^2 \nabla \log q_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\overline{\mathbf{B}}_t$$ (equiv. in path distr. $q(\mathbf{x}_{1:T})$).

$$\mathbf{x}_t \sim q_t\text{:}\;\; \mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\mathbf{B}_t$$



$$\mathbf{x}_{\bar{t}} \sim q_{\bar{t}}\text{:}\;\; \mathrm{d}\mathbf{x}_{\bar{t}} = -\mathbf{f}_{\bar{t}}(\mathbf{x}_{\bar{t}})\,\mathrm{d}\bar{t} + g_{\bar{t}}^2 \nabla \log q_{\bar{t}}(\mathbf{x}_{\bar{t}})\,\mathrm{d}\bar{t} + g_{\bar{t}}\,\mathrm{d}\mathbf{B}_{\bar{t}}$$

Only needs the score!

$$\mathcal{L}_{\mathrm{DSM}} \coloneqq \mathbb{E}_{\mathrm{U}(i|\{0,\dots,N\})}\lambda_i \mathbb{E}_{q_0(\mathbf{x})}\mathbb{E}_{q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x})}\left\|\mathbf{s}_{\theta,i}(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x})\right\|^2$$ [SSK+21].

(Real continuous-time training available.)

Diffusion-Based Generative Models

- Specification of diffusion-based generative model:
  - To make $q_T \approx p_N$ where p_N is tractable,
    ➔ LD targeting $p_N := \mathcal{N}(0, \mathbf{I})$ with time dilation β_t [WWJ16],
    $$\mathrm{d}\mathbf{x}_t = \frac{\beta_t}{2} \nabla \log p_N(\mathbf{x}_t)\, \mathrm{d}t + \sqrt{\beta_t}\, \mathrm{d}\mathbf{B}_t = -\frac{\beta_t}{2} \mathbf{x}_t\, \mathrm{d}t + \sqrt{\beta_t}\, \mathrm{d}\mathbf{B}_t.$$
    [SWMG15, HJA20: DDPM; SSK+21: VP SDE]
  - For $\mathcal{L}_{\mathrm{DSM}}(\theta) := \mathbb{E}_{\mathrm{U}(i|\{0,\ldots,N\})} \lambda_i \mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x})} \left\| \mathbf{s}_{\theta,i}(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x}) \right\|^2$ [SSK+21]:
    $$q_{t|0}(\tilde{\mathbf{x}}|\mathbf{x}) = \mathcal{N}(\varsigma_t \mathbf{x}, (1 - \varsigma_t^2)\mathbf{I}),\ \varsigma_t := e^{\int_0^t -\frac{\beta_s}{2} \mathrm{d}s}\ \left(\varsigma_i = \prod_{j=1}^{i} \sqrt{1 - \beta_j} + o(h)\right),$$
    ➔ $$\mathcal{L}_{\mathrm{DSM}}(\theta) = \mathbb{E}_i \lambda_i \mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x})} \left\| \mathbf{s}_{\theta,i}(\tilde{\mathbf{x}}) + \frac{\tilde{\mathbf{x}} - \varsigma_i \mathbf{x}}{1 - \varsigma_i^2} \right\|^2$$
    $$= \mathbb{E}_i \lambda_i \mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{p(\epsilon_i)} \left\| \mathbf{s}_{\theta,i}\left(\varsigma_i \mathbf{x} + \sqrt{1 - \varsigma_i^2}\, \boldsymbol{\epsilon}_i\right) + \frac{\boldsymbol{\epsilon}_i}{\sqrt{1 - \varsigma_i^2}} \right\|^2$$
    [SSK+21]

Diffusion-Based Generative Models

- Different forms of model:

Under $\mathrm{d}\mathbf{x}_t = \frac{\beta_t}{2} \nabla \log p_N(\mathbf{x}_t)\, \mathrm{d}t + \sqrt{\beta_t}\, \mathrm{d}\mathbf{B}_t = -\frac{\beta_t}{2} \mathbf{x}_t\, \mathrm{d}t + \sqrt{\beta_t}\, \mathrm{d}\mathbf{B}_t$ [SWMG15, HJA20]:

- $\mathcal{L}_{\mathrm{DSM}}(\theta) = \mathbb{E}_i \lambda_i \mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{p(\boldsymbol{\epsilon}_i)} \left\| \mathbf{s}_{\theta,i}\left(\varsigma_i \mathbf{x} + \sqrt{1-\varsigma_i^2}\boldsymbol{\epsilon}_i\right) + \frac{\boldsymbol{\epsilon}_i}{\sqrt{1-\varsigma_i^2}} \right\|^2$ [SSK+21]

Let $\boldsymbol{\epsilon}_{\theta,i}(\mathbf{x}_i) \coloneqq -\sqrt{1-\varsigma_i^2}\, \mathbf{s}_{\theta,i}(\mathbf{x}_i)$:

$$= \mathbb{E}_i \frac{\lambda_i}{1-\varsigma_i^2} \mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{p(\boldsymbol{\epsilon}_i)} \left\| \boldsymbol{\epsilon}_{\theta,i}\left(\varsigma_i \mathbf{x} + \sqrt{1-\varsigma_i^2}\boldsymbol{\epsilon}_i\right) - \boldsymbol{\epsilon}_i \right\|^2.$$

[HJA20: DDPM simple loss]

Let $\mathbf{x}_{0\theta,i}(\mathbf{x}_i) \coloneqq \frac{\mathbf{x}_i - \sqrt{1-\varsigma_i^2}\, \boldsymbol{\epsilon}_{\theta,i}(\mathbf{x}_i)}{\varsigma_i} = \frac{\mathbf{x}_i + (1-\varsigma_i^2)\mathbf{s}_{\theta,i}(\mathbf{x}_i)}{\varsigma_i}$: [SME21, KSPH21, KAAL22, SDCS23, WMH+23]

$$= \mathbb{E}_i \frac{\lambda_i \varsigma_i^2}{(1-\varsigma_i^2)^2} \mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{p(\boldsymbol{\epsilon}_i)} \left\| \mathbf{x}_{0\theta,i}\left(\varsigma_i \mathbf{x} + \sqrt{1-\varsigma_i^2}\boldsymbol{\epsilon}_i\right) - \mathbf{x} \right\|^2.$$

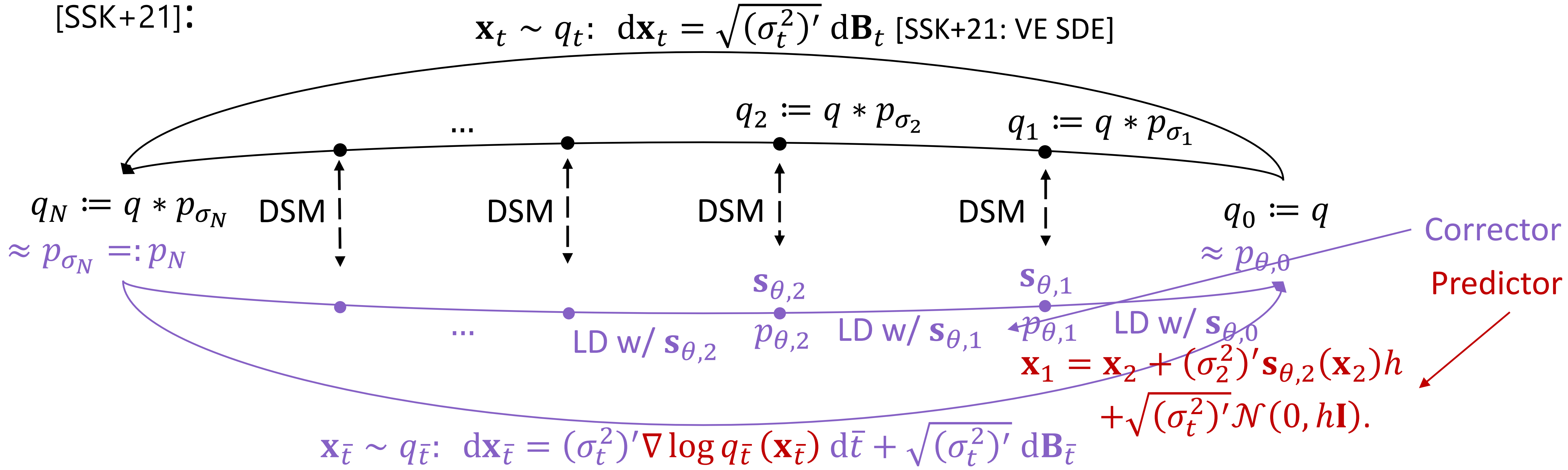
== Denoising model $\mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{q(\tilde{\mathbf{x}}|\mathbf{x})} \|\mathbf{x}_{0\theta}(\tilde{\mathbf{x}}) - \mathbf{x}\|^2$!
[VLBM08: Denoising AutoEncoder; Vin11, AB14: connection to (D)SM].

Does not (and impossible!) to recover the exact $\boldsymbol{\epsilon}_i$ or $\mathbf{x}_0$ used to produce $\tilde{\mathbf{x}}$!

Understand as a statistics or a score parameterization.

Diffusion-Based Generative Models

- Noise-Conditioned Score Network (NCSN) [SE19] as a diffusion model [SSK+21]:



$$\mathcal{L}_{\mathrm{DSM}} := \mathbb{E}_{\mathrm{U}(i|\{0,\dots,N\})}\lambda_i \mathbb{E}_{q_0(\mathbf{x})}\mathbb{E}_{q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x})}\left\|\mathbf{s}_{\theta,i}(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}}\log q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x})\right\|^2$$ [SSK+21].

- A corrector is also available for DDPM (VP SDE) [SSK+21].
- $\sigma_t \propto \sqrt{t}$ in NCSN equivalent [SE19, SSK+21]. $\sigma_t \propto t$ is recommended in [KAAL22].

Diffusion-Based Generative Models

- Probability flow (PF) ODE [SSK+21]:

$$\Leftrightarrow \mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t - g_t^2 \nabla \log q_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\bar{\mathbf{B}}_t \text{ (equiv. in path distr. } q(\mathbf{x}_{1:T})\text{).}$$

$$\mathbf{x}_t \sim q_t\text{:}\;\; \mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t + g_t\,\mathrm{d}\mathbf{B}_t$$

$$\Leftrightarrow \mathrm{d}\mathbf{x}_t = \mathbf{f}_t(\mathbf{x}_t)\,\mathrm{d}t - \frac{g_t^2}{2} \nabla \log q_t(\mathbf{x}_t)\,\mathrm{d}t \text{ (equiv. in marginal distr. } q_t(\mathbf{x}_t), \forall t\text{).}$$

$$q_T \qquad\qquad q_0 \coloneqq q$$

$$\Leftrightarrow \mathrm{d}\mathbf{x}_{\bar{t}} = -\mathbf{f}_{\bar{t}}(\mathbf{x}_{\bar{t}})\,\mathrm{d}\bar{t} + \frac{g_{\bar{t}}^2}{2} \nabla \log q_{\bar{t}}(\mathbf{x}_{\bar{t}})\,\mathrm{d}\bar{t} \text{ (equiv. in marginal distr. } q_{\bar{t}}(\mathbf{x}_{\bar{t}}), \forall \bar{t}\text{).}$$

$$\mathbf{x}_{\bar{t}} \sim q_{\bar{t}}\text{:}\;\; \mathrm{d}\mathbf{x}_{\bar{t}} = -\mathbf{f}_{\bar{t}}(\mathbf{x}_{\bar{t}})\,\mathrm{d}\bar{t} + g_{\bar{t}}^2 \nabla \log q_{\bar{t}}(\mathbf{x}_{\bar{t}})\,\mathrm{d}\bar{t} + g_{\bar{t}}\,\mathrm{d}\mathbf{B}_{\bar{t}}$$

Still only needs the score!

- Deterministic equivalent: $\mathbf{x}_T$ holds all information about $\mathbf{x}_0$
  ➔ representation, interpolation, ...
- Likelihood/density evaluation (same way as cont.-time flow models).
- Continuous-time rev. proc. simulation using ODE solver for generation:
  - More accurate vs. discrete-time.
  - Enable techniques for faster generation (larger step size, DPM-Solver(++), ...).

Diffusion-Based Generative Models

- Probability flow (PF) ODE:
  - The [KAAL22] diffusion process:
    Different diffusion processes (VE, VP, sub-VP, ...) parameterize the same PF ODE:
    - For $\mathbf{f}_t(\mathbf{x}_t) = a_t \mathbf{x}_t$, PF ODE is:
      $$\frac{\mathrm{d}\mathbf{x}_t}{\mathrm{d}t} = a_t \mathbf{x}_t - \frac{g_t^2}{2} \nabla \log q_t(\mathbf{x}_t) = \frac{\varsigma_t'}{\varsigma_t} \mathbf{x}_t - \frac{\varsigma_t^2 (v_t^2)'}{2} \nabla \log q_t(\mathbf{x}_t),$$
      where $\varsigma_t := e^{\int_0^t a_s \,\mathrm{d}s}$, $v_t^2 := \int_0^t \frac{g_s^2}{\varsigma_s^2} \,\mathrm{d}s$ which directly parametrizes $q(\mathbf{x}_t | \mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t | \varsigma_t \mathbf{x}_0, \varsigma_t^2 v_t^2 \mathbf{I})$,
    - This is equivalent to: $\mathrm{d}\hat{\mathbf{x}}_t = -\frac{1}{2} \nabla \log \hat{q}_t(\hat{\mathbf{x}}_t) \,\mathrm{d}v_t^2$ by reparametrizing $\hat{\mathbf{x}}_t := \frac{\mathbf{x}_t}{\varsigma_t}$.

		VP [42]	VE [42]	iDDPM [33] + DDIM [40]	Ours
Sampling (Section 3)					
Schedule	v_t	$\sqrt{e^{\frac{1}{2}\beta_{\mathrm{d}} t^2 + \beta_{\min} t} - 1}$	$\sqrt{t}$	t	t
Scaling	ς_t	$1/\sqrt{e^{\frac{1}{2}\beta_{\mathrm{d}} t^2 + \beta_{\min} t}}$	1	1	1

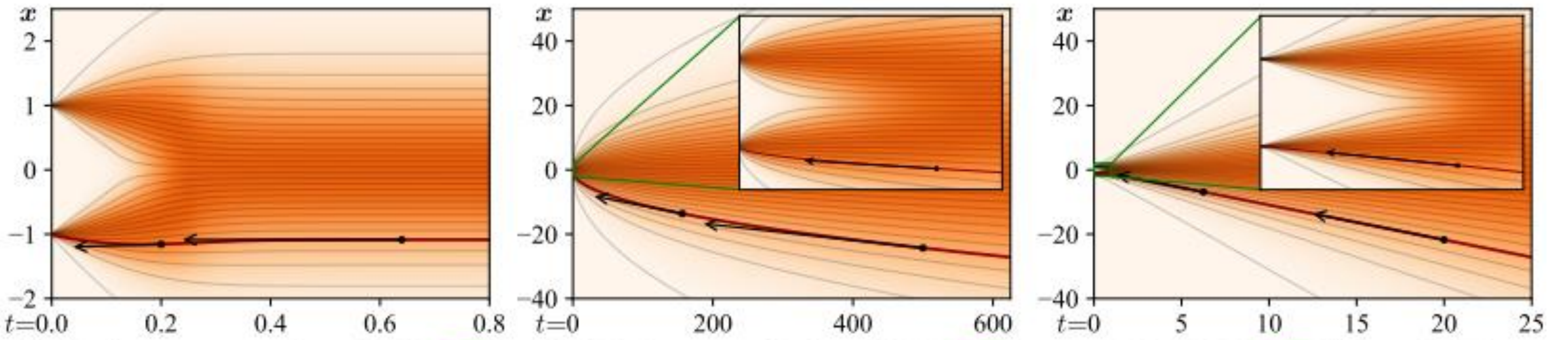
Diffusion-Based Generative Models

- Probability flow (PF) ODE:
  - The [KAAL22] diffusion process:
    - Taking $\varsigma_t \equiv 1$, $\upsilon_t = t$: $\mathrm{d}\mathbf{x}_t = \sqrt{2t}\,\mathrm{d}\mathbf{B}_t$ ➔ PF ODE is $\frac{\mathrm{d}\mathbf{x}_t}{\mathrm{d}t} = \frac{\mathbf{x}_t - \mathbf{x}_{0\theta,t}(\mathbf{x}_t)}{t}$

    ➔ A single Euler step to $t = 0$ is the output of the $\mathbf{x}_{0\theta,t}$ model:
    $\mathbf{x}_0 = \mathbf{x}_t - t\,\frac{\mathbf{x}_t - \mathbf{x}_{0\theta,t}(\mathbf{x}_t)}{t} = \mathbf{x}_{0\theta,t}(\mathbf{x}_t)$.

    ➔ Integral curves of the PF ODE are *nearly linear*: $\mathbf{x}_{0\theta,t}(\mathbf{x}_t)$ *approximately* points to the $\mathbf{x}_0$ on the same PF ODE curve as $\mathbf{x}_t$.

$q_t(\mathbf{x})$ plot,
with $q_0 = \frac{1}{2}(\delta_1 + \delta_{-1})$



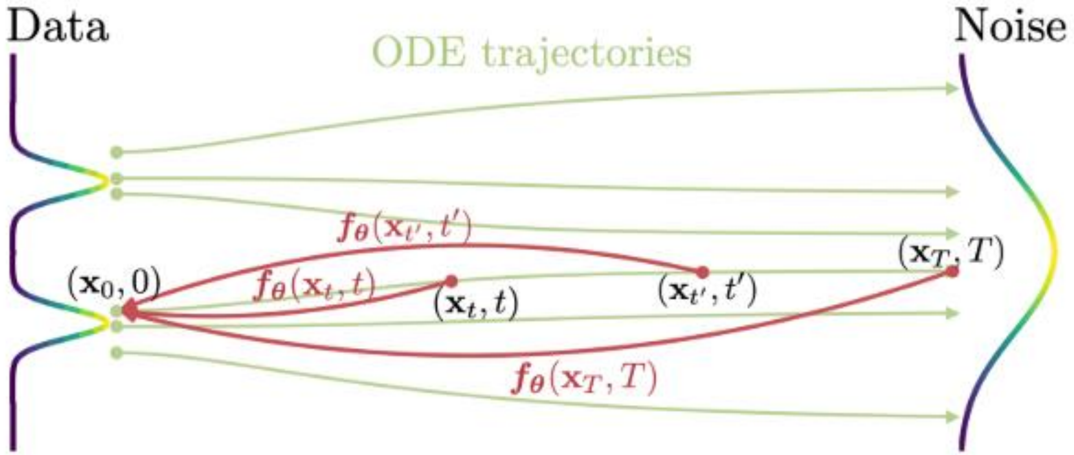
(a) Variance preserving ODE [42] (b) Variance exploding ODE [42] (c) DDIM [40] / Our ODE

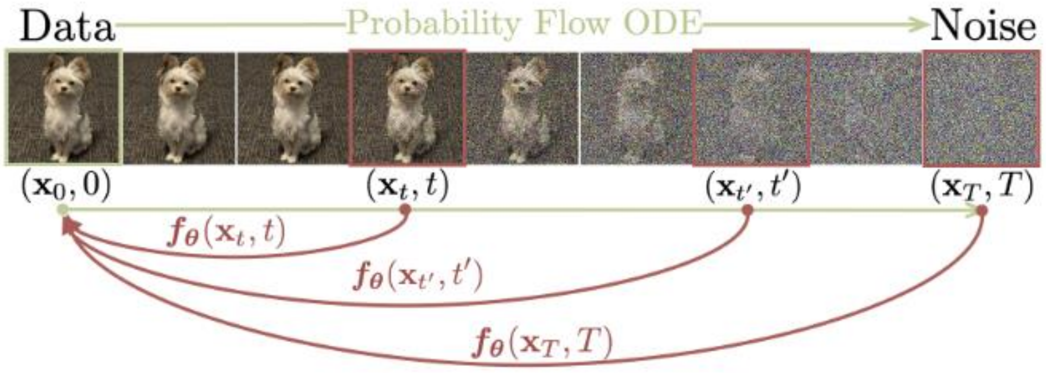
Diffusion-Based Generative Models

- Summary
  - vs. VAE/GAN/NF:
    - Guidance to the generator from a given distribution-transformation process.
    - Losses at different steps are decoupled: effective training (vs. cont.-time normalizing flow training).

$$\mathcal{L}_{\mathrm{DSM}} \coloneqq \mathbb{E}_{\mathrm{U}(i|\{0,\ldots,N\})} \lambda_i \mathbb{E}_{q_0(\mathbf{x})} \mathbb{E}_{q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x})} \left\| \mathbf{s}_{\theta,i}(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_{i|0}(\tilde{\mathbf{x}}|\mathbf{x}) \right\|^2.$$

Consistency Model [SDCS23]





- Generative modeling by learning the solution to reverse PF ODE:
  - $\mathbf{c}_{\theta,t}(\mathbf{x}_t)$ inverts the forward PF ODE to find the clean data point $\mathbf{x}_0$ of a "noised" input $\mathbf{x}_t$.
  - $\mathbf{c}_{\theta,t}(\mathbf{x}_t) = \mathbf{x}_{\bar{0}}$ solves the reverse PF ODE: $\mathrm{d}\mathbf{x}_{\bar{t}} = -\mathbf{f}_{\bar{t}}(\mathbf{x}_{\bar{t}})\,\mathrm{d}\bar{t} + \frac{g_{\bar{t}}^2}{2}\nabla \log q_{\bar{t}}(\mathbf{x}_{\bar{t}})\,\mathrm{d}\bar{t}$, given $\mathbf{x}_{\bar{t}} = \mathbf{x}_t$.
- Benefits of the $\mathbf{c}_{\theta,t}(\mathbf{x}_t)$ model:
  - Generation in **one evaluation**: $\mathbf{x}_T \sim p_T, \mathbf{x}_0 = \mathbf{c}_{\theta,T}(\mathbf{x}_T)$ (same mode as VAE/GAN/NF!).
  - Can also be used iteratively: Enable trade-off b/t quality and cost!

$\mathbf{x}_T \sim p_T, \mathbf{x}_0 = \mathbf{c}_{\theta,T}(\mathbf{x}_T)$; $\qquad$ $\mathbf{x}_{T-1} \sim q_{T-1|0}(\mathbf{x}_{T-1}|\mathbf{x}_0), \mathbf{x}_0 = \mathbf{c}_{\theta,T-1}(\mathbf{x}_{T-1})$; ...

Consistency Model [SDCS23]

- Consistency training: $\mathbf{c}_{\theta,t}(\mathbf{x}_t) = \mathbf{c}_{\theta,t'}(\mathbf{x}_{t'})$ for $\mathbf{x}_{t\in[0,T]}$ on the same PF ODE curve.
  - **Distillation**: learn from a pre-trained diffusion model $\mathbf{s}_{\phi,t}(\mathbf{x}_t)$.

    $$\mathbb{E}_i \mathbb{E}_{q(\mathbf{x}_i)}\left[\lambda_i d\left(\mathbf{c}_{\theta,i}(\mathbf{x}_i), \mathbf{c}_{\theta^-,i-1}\left(\hat{\mathbf{x}}_{\phi,i-1}(\mathbf{x}_i)\right)\right)\right],$$

    - $\hat{\mathbf{x}}_{\phi,i-1}(\mathbf{x}_i)$ is one-step reverse PF ODE simulation using $\mathbf{s}_\phi$ from $\mathbf{x}_i$, s.t. $\left(\hat{\mathbf{x}}_{\phi,i-1}(\mathbf{x}_i), \mathbf{x}_i\right)$ are on the same PF curve.
    - θ^-: exponential moving avg. and stopped-grad.
    - Drawing $q(\mathbf{x}_i)$: draw a sample $\mathbf{x}_0$ from dataset, and draw from $q(\mathbf{x}_i|\mathbf{x}_0)$ stochastically.
  - **Train from scratch**: use a stochastic est. of score in place of $\mathbf{s}_{\phi,t}(\mathbf{x}_t)$:

    $$\mathbb{E}_i \mathbb{E}_{q(\mathbf{x}_i)}\left[\lambda_i d\left(\mathbf{c}_{\theta,i}(\mathbf{x}_i), \mathbf{c}_{\theta^-,i-1}(\hat{\mathbf{x}}_{i-1}(\mathbf{x}_i, \nabla \log q_i(\mathbf{x}_i)))\right)\right]$$

    $$=^{\text{Fisher id.}} \mathbb{E}_i \mathbb{E}_{q(\mathbf{x}_i)}\left[\lambda_i d\left(\mathbf{c}_{\theta,i}(\mathbf{x}_i), \mathbf{c}_{\theta^-,i-1}\left(\hat{\mathbf{x}}_{i-1}\left(\mathbf{x}_i, \mathbb{E}_{q(\mathbf{x}_0|\mathbf{x}_i)}\left[\nabla_{\mathbf{x}_i} \log q(\mathbf{x}_i|\mathbf{x}_0)\right]\right)\right)\right)\right] \text{ intractable}$$

    $$\leq \mathbb{E}_i \mathbb{E}_{q(\mathbf{x}_i)} \mathbb{E}_{q(\mathbf{x}_0|\mathbf{x}_i)}\left[\lambda_i d\left(\mathbf{c}_{\theta,i}(\mathbf{x}_i), \mathbf{c}_{\theta^-,i-1}\left(\hat{\mathbf{x}}_{i-1}\left(\mathbf{x}_i, \nabla_{\mathbf{x}_i} \log q(\mathbf{x}_i|\mathbf{x}_0)\right)\right)\right)\right]$$

    $$= \mathbb{E}_i \mathbb{E}_{q(\mathbf{x}_0)} \mathbb{E}_{q(\mathbf{x}_i|\mathbf{x}_0)}\left[\lambda_i d\left(\mathbf{c}_{\theta,i}(\mathbf{x}_i), \mathbf{c}_{\theta^-,i-1}\left(\hat{\mathbf{x}}_{i-1}\left(\mathbf{x}_i, \nabla_{\mathbf{x}_i} \log q(\mathbf{x}_i|\mathbf{x}_0)\right)\right)\right)\right] \text{ tractable.}$$

    - But the bound cannot be made tight, so the final objective may bias the optimality.

Consistency Model [SDCS23]

- Consistency training: $\mathbf{c}_{\theta,t}(\mathbf{x}_t) = \mathbf{c}_{\theta,t'}(\mathbf{x}_{t'})$ for $\mathbf{x}_{t\in[0,T]}$ on the same PF ODE curve.

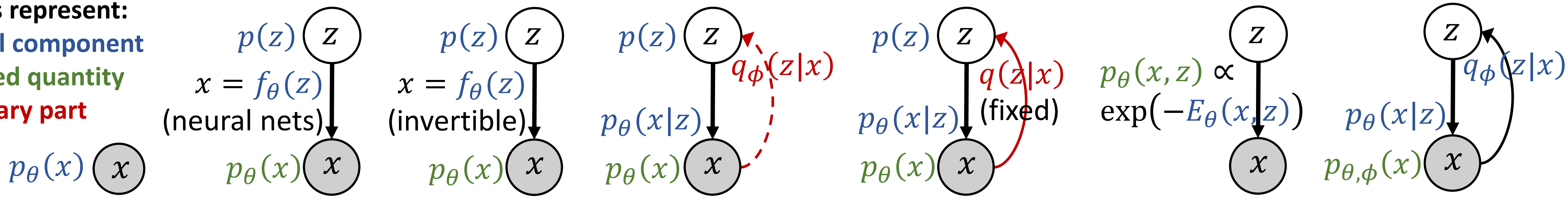
  $$\mathbb{E}_i \mathbb{E}_{q(\mathbf{x}_i)} \left[\lambda_i d \left(\mathbf{c}_{\theta,i}(\mathbf{x}_i), \mathbf{c}_{\theta^-,i-1} \left(\hat{\mathbf{x}}_{\phi,i-1}(\mathbf{x}_i) \right) \right) \right].$$

  Comments:
  - A version of PINN loss:
    - Same spirit: The evolution of the model should match the evolution from the ODE.
    - This version: Discretize the time derivative of the model.
    - Formally, the PDE for $\mathbf{c}_{\theta,t}$ is $\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{c}_{\theta,t}(\mathbf{x}_t) = 0 = \frac{\partial}{\partial t}\mathbf{c}_{\theta,t}(\mathbf{x}_t) + \nabla\mathbf{c}_{\theta,t}(\mathbf{x}_t) \cdot \frac{\mathrm{d}\mathbf{x}_t}{\mathrm{d}t}$ with initial condition $\mathbf{c}_{\theta,0}(\mathbf{x}) = \mathbf{x}$, where $\frac{\mathrm{d}\mathbf{x}_t}{\mathrm{d}t}$ is given through the PF ODE.
      - What about directly using the conventional PINN loss for this PDE?
  - The consistency model $\mathbf{c}_{\theta,t}(\mathbf{x}_t)$ minimizing the consistency loss is **not** the $\mathbf{x}_{0\theta,t}(\mathbf{x}_t)$ model (as a score-model parameterization) that minimizes the DSM loss!

Generative Model: Summary

Plain Gen.	Latent Variable Models					
Autoregressive Models	Deterministic Generative		Probabilistic Graphical Models			
	GANs	Flow-Based	Directed	Dir.: Diffusion	Undirected	Bidirectional
+ Easy generation + Explicit llh (easy learning) - No natural repr. - Slow/seq. generation	+ Easy generation				- Hard generation (use MCMC)	
	- No llh (hard learning) - Hard repr. + Flexible model	+ Explicit llh (easy learning) + Easy repr. - High-dim. repr. - Hard model design	Unnormalized llh: + stable learning, - need expectation est.			
			+ Moderate repr. + Prior knowledge + Small-data robust + Describe causality	+ Easy repr. + Allow big model - High-dim. repr.	- Hard repr. - MCMC in learning + Simple dependency modeling	+ Easy & flexible repr. + Flexible distribution

Colors represent:
Model component
Derived quantity
Auxiliary part



Questions?

References

References

- Plain Generative Models
  - Autoregressive Models

    - [Fre98] Frey, Brendan J. (1998). *Graphical models for machine learning and digital communication*. MIT press.
    - [LM11] Larochelle, H. and Murray, I. The neural autoregressive distribution estimator. In *Proceedings of the International Conference on Artificial Intelligence and Statistics*, 2011.
    - [UML14] Uria, B., Murray, I., & Larochelle, H. (2014). A deep and tractable density estimator. In *International Conference on Machine Learning* (pp. 467-475).
    - [GGML15] Germain, M., Gregor, K., Murray, I., & Larochelle, H. (2015). MADE: Masked autoencoder for distribution estimation. In *International Conference on Machine Learning* (pp. 881-889).
    - [OKK16] Oord, A. V. D., Kalchbrenner, N., & Kavukcuoglu, K. (2016). Pixel recurrent neural networks. *arXiv preprint arXiv:1601.06759*.
    - [ODZ+16] Oord, A. V. D., Dieleman, S., Zen, H., Simonyan, K., Vinyals, O., Graves, A., Kalchbrenner, N., Senior, A., & Kavukcuoglu, K. (2016). WaveNet: A generative model for raw audio. *arXiv preprint arXiv:1609.03499*.

References

- Deterministic Generative Models
  - Generative Adversarial Networks

    - [GPM+14] Goodfellow, I., Pouget-Abadie, J., Mirza, M., Xu, B., Warde-Farley, D., Ozair, S., Courville, A., & Bengio, Y. (2014). Generative adversarial nets. In *Advances in neural information processing systems* (pp. 2672-2680).
    - [ACB17] Arjovsky, M., Chintala, S., & Bottou, L. (2017). Wasserstein generative adversarial networks. In *International Conference on Machine Learning* (pp. 214-223).

  - Flow-Based Models

    - [DKB15] Dinh, L., Krueger, D., & Bengio, Y. (2015). NICE: Non-linear independent components estimation. *ICLR workshop*.
    - [DSB17] Dinh, L., Sohl-Dickstein, J., & Bengio, S. (2017). Density estimation using real NVP. In *Proceedings of the International Conference on Learning Representations*.
    - [PPM17] Papamakarios, G., Pavlakou, T., & Murray, I. (2017). Masked autoregressive flow for density estimation. In *Advances in Neural Information Processing Systems*.
    - [KD18] Kingma, D. P., & Dhariwal, P. (2018). Glow: Generative flow with invertible 1x1 convolutions. In *Advances in Neural Information Processing Systems*.

References

- Deterministic Generative Models
  - Flow-Based Models
    - [KSJ+16] Kingma, D. P., Salimans, T., Jozefowicz, R., Chen, X., Sutskever, I., & Welling, M. (2016). Improved Variational Inference with Inverse Autoregressive Flow. In *Advances in Neural Information Processing Systems*.
    - [GCB+18] Grathwohl, W., Chen, R. T., Bettencourt, J., Sutskever, I., & Duvenaud, D. (2018). FFJORD: Free-form continuous dynamics for scalable reversible generative models. In *Proceedings of International Conference on Learning Representations*.
    - [BGC19] Behrmann, J., Grathwohl, W., Chen, R. T., Duvenaud, D., & Jacobsen, J. H. (2019). Invertible residual networks. In *International Conference on Machine Learning*.
    - [CBD19] Chen, R. T., Behrmann, J., Duvenaud, D., & Jacobsen, J. H. (2019). Residual Flows for Invertible Generative Modeling. In *Advances in Neural Information Processing Systems*.
    - [KC20] Kong, Z., & Chaudhuri, K. (2020). The expressive power of a class of normalizing flow models. In *International Conference on Artificial Intelligence and Statistics*.
    - [TIT+20] Teshima, T., Ishikawa, I., Tojo, K., Oono, K., Ikeda, M., & Sugiyama, M. (2020). Coupling-based invertible neural networks are universal diffeomorphism approximators. *arXiv preprint arXiv:2006.11469*.

References

- Bayesian Inference: Variational Inference
  - Explicit Parametric VI:

    - [SJJ96] Saul, L. K., Jaakkola, T., & Jordan, M. I. (1996). Mean field theory for sigmoid belief networks. *Journal of artificial intelligence research*, 4, 61-76.
    - [BNJ03] Blei, D. M., Ng, A. Y., & Jordan, M. I. (2003). Latent Dirichlet Allocation. *Journal of Machine Learning Research*, 3(Jan), pp.993-1022.
    - [GHB12] Gershman, S., Hoffman, M., & Blei, D. (2012). Nonparametric variational inference. arXiv preprint arXiv:1206.4665.
    - [HBWP13] Hoffman, M. D., Blei, D. M., Wang, C., & Paisley, J. (2013). Stochastic variational inference. *The Journal of Machine Learning Research*, *14*(1), 1303-1347.
    - [RGB14] Ranganath, R., Gerrish, S., & Blei, D. (2014). Black box variational inference. In *Artificial Intelligence and Statistics* (pp. 814-822).
    - [RM15] Rezende, D.J., & Mohamed, S. (2015). Variational inference with normalizing flows. In *Proceedings of the International Conference on Machine Learning* (pp. 1530-1538).
    - [KSJ+16] Kingma, D.P., Salimans, T., Jozefowicz, R., Chen, X., Sutskever, I., & Welling, M. (2016). Improved variational inference with inverse autoregressive flow. In *Advances in neural information processing systems* (pp. 4743-4751).

References

- Bayesian Inference: Variational Inference
  - Implicit Parametric VI: density ratio estimation

    - [MSJ+15] Makhzani, A., Shlens, J., Jaitly, N., Goodfellow, I., & Frey, B. (2016). Adversarial Autoencoders. In *Proceedings of the International Conference on Learning Representations*.
    - [MNG17] Mescheder, L., Nowozin, S., & Geiger, A. (2017). Adversarial variational Bayes: Unifying variational autoencoders and generative adversarial networks. In *Proceedings of the International Conference on Machine Learning* (pp. 2391-2400).
    - [Hus17] Huszár, F. (2017). Variational inference using implicit distributions. *arXiv preprint* arXiv:1702.08235.
    - [TRB17] Tran, D., Ranganath, R., & Blei, D. (2017). Hierarchical implicit models and likelihood-free variational inference. In *Advances in Neural Information Processing Systems* (pp. 5523-5533).
    - [SSZ18a] Shi, J., Sun, S., & Zhu, J. (2018). Kernel Implicit Variational Inference. In *Proceedings of the International Conference on Learning Representations*.

  - Implicit Parametric VI: gradient estimation

    - [VLBM08] Vincent, P., Larochelle, H., Bengio, Y., & Manzagol, P. A. (2008). Extracting and composing robust features with denoising autoencoders. In *Proceedings of the 25th international conference on Machine learning* (pp. 1096-1103). ACM.
    - [LT18] Li, Y., & Turner, R. E. (2018). Gradient estimators for implicit models. In *Proceedings of the International Conference on Learning Representations*.
    - [SSZ18b] Shi, J., Sun, S., & Zhu, J. (2018). A spectral approach to gradient estimation for implicit distributions. In *Proceedings of the 35th International Conference on Machine Learning* (pp. 4651-4660).

References

- Bayesian Inference: Variational Inference
  - Particle-Based VI

    - [LW16] Liu, Q., & Wang, D. (2016). Stein variational gradient descent: A general purpose Bayesian inference algorithm. In *Advances In Neural Information Processing Systems* (pp. 2378-2386).
    - [Liu17] Liu, Q. (2017). Stein variational gradient descent as gradient flow. In *Advances in neural information processing systems* (pp. 3115-3123).
    - [CZ17] Chen, C., & Zhang, R. (2017). Particle optimization in stochastic gradient MCMC. *arXiv preprint arXiv:1711.10927*.
    - [FWL17] Feng, Y., Wang, D., & Liu, Q. (2017). Learning to Draw Samples with Amortized Stein Variational Gradient Descent. In *Proceedings of the Conference on Uncertainty in Artificial Intelligence*.
    - [PGH+17] Pu, Y., Gan, Z., Henao, R., Li, C., Han, S., & Carin, L. (2017). VAE learning via Stein variational gradient descent. In *Advances in Neural Information Processing Systems* (pp. 4236-4245).
    - [LZ18] Liu, C., & Zhu, J. (2018). Riemannian Stein Variational Gradient Descent for Bayesian Inference. In *Proceedings of the 32nd AAAI Conference on Artificial Intelligence* (pp. 3627-3634).

References

- Bayesian Inference: Variational Inference
  - Particle-Based VI

    - [CMG+18] Chen, W. Y., Mackey, L., Gorham, J., Briol, F. X., & Oates, C. J. (2018). Stein points. *arXiv preprint arXiv:1803.10161*.
    - [FCSS18] Futami, F., Cui, Z., Sato, I., & Sugiyama, M. (2018). Frank-Wolfe Stein sampling. *arXiv preprint arXiv:1805.07912*.
    - [CZW+18] Chen, C., Zhang, R., Wang, W., Li, B., & Chen, L. (2018). A unified particle-optimization framework for scalable Bayesian sampling. In *Proceedings of the Conference on Uncertainty in Artificial Intelligence*.
    - [ZZC18] Zhang, J., Zhang, R., & Chen, C. (2018). Stochastic particle-optimization sampling and the non-asymptotic convergence theory. *arXiv preprint arXiv:1809.01293*.
    - [LZC+19] Liu, C., Zhuo, J., Cheng, P., Zhang, R., Zhu, J., & Carin, L. (2019). Understanding and Accelerating Particle-Based Variational Inference. In *Proceedings of the 36th International Conference on Machine Learning* (pp. 4082-4092).

References

- Bayesian Inference: MCMC
  - Classical MCMC
    - [MRR+53] Metropolis, N., Rosenbluth, A. W., Rosenbluth, M.N., Teller, A.H., & Teller, E. (1953). Equation of state calculations by fast computing machines. *The Journal of Chemical Physics*, 21(6), pp.1087-1092.
    - [Has70] Hastings, W. (1970). Monte Carlo sampling methods using Markov chains and their applications. *Biometrika*, 57(1), pp.97-109.
    - [GG87] Geman, S., & Geman, D. (1987). Stochastic relaxation, Gibbs distributions, and the Bayesian restoration of images. In *Readings in computer vision* (pp. 564-584).
    - [ADDJ03] Andrieu, C., De Freitas, N., Doucet, A., & Jordan, M. I. (2003). An introduction to MCMC for machine learning. *Machine learning*, *50*(1-2), 5-43.

References

- Bayesian Inference: MCMC
  - Dynamics-Based MCMC: full-batch

    - [Lan08] Langevin, P. (1908). Sur la théorie du mouvement Brownien. *Compt. Rendus*, *146*, 530-533.
    - [DKPR87] Duane, S., Kennedy, A.D., Pendleton, B.J., Roweth, D. (1987). Hybrid Monte Carlo. *Physics letters B*, 195(2), pp.216-222.
    - [RT96] Roberts, G. O., & Tweedie, R. L. (1996). Exponential convergence of Langevin distributions and their discrete approximations. *Bernoulli*, *2*(4), 341-363.
    - [RS02] Roberts, G.O., & Stramer, O. (2002). Langevin diffusions and Metropolis-Hastings algorithms. *Methodology and computing in applied probability*, 4(4), pp.337-357.
    - [Nea11] Neal, R.M. (2011). MCMC using Hamiltonian dynamics. Handbook of Markov chain Monte Carlo, 2(11), p.2.
    - [ZWC+16] Zhang, Y., Wang, X., Chen, C., Henao, R., Fan, K., & Carin, L. (2016). Towards unifying Hamiltonian Monte Carlo and slice sampling. In *Advances in Neural Information Processing Systems* (pp. 1741-1749).
    - [TRGT17] Tripuraneni, N., Rowland, M., Ghahramani, Z., & Turner, R. (2017, August). Magnetic Hamiltonian Monte Carlo. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70* (pp. 3453-3461).
    - [Bet17] Betancourt, M. (2017). A conceptual introduction to Hamiltonian Monte Carlo. *arXiv preprint arXiv:1701.02434*.

References

- Bayesian Inference: MCMC
  - Dynamics-Based MCMC: full-batch (manifold support)

    - [GC11] Girolami, M., & Calderhead, B. (2011). Riemann manifold Langevin and Hamiltonian Monte Carlo methods. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, *73*(2), 123-214.
    - [BSU12] Brubaker, M., Salzmann, M., & Urtasun, R. (2012, March). A family of MCMC methods on implicitly defined manifolds. In *Artificial intelligence and statistics* (pp. 161-172).
    - [BG13] Byrne, S., & Girolami, M. (2013). Geodesic Monte Carlo on embedded manifolds. *Scandinavian Journal of Statistics*, *40*(4), 825-845.
    - [LSSG15] Lan, S., Stathopoulos, V., Shahbaba, B., & Girolami, M. (2015). Markov chain Monte Carlo from Lagrangian dynamics. *Journal of Computational and Graphical Statistics*, *24*(2), 357-378.

References

- Bayesian Inference: MCMC
  - Dynamics-Based MCMC: stochastic gradient

    - [WT11] Welling, M., & Teh, Y. W. (2011). Bayesian learning via stochastic gradient Langevin dynamics. In *Proceedings of the International Conference on Machine Learning* (pp. 681-688).
    - [CFG14] Chen, T., Fox, E., & Guestrin, C. (2014). Stochastic gradient Hamiltonian Monte Carlo. In *Proceedings of the International conference on machine learning* (pp. 1683-1691).
    - [DFB+14] Ding, N., Fang, Y., Babbush, R., Chen, C., Skeel, R. D., & Neven, H. (2014). Bayesian sampling using stochastic gradient thermostats. In *Advances in neural information processing systems* (pp. 3203-3211).
    - [Bet15] Betancourt, M. (2015). The fundamental incompatibility of scalable Hamiltonian Monte Carlo and naive data subsampling. In *International Conference on Machine Learning* (pp. 533-540).
    - [TTV16] Teh, Y. W., Thiery, A. H., & Vollmer, S. J. (2016). Consistency and fluctuations for stochastic gradient Langevin dynamics. *The Journal of Machine Learning Research*, *17*(1), 193-225.
    - [LPH+16] Lu, X., Perrone, V., Hasenclever, L., Teh, Y. W., & Vollmer, S. J. (2016). Relativistic Monte Carlo. *arXiv preprint arXiv:1609.04388*.
    - [ZCG+17] Zhang, Y., Chen, C., Gan, Z., Henao, R., & Carin, L. (2017, August). Stochastic gradient monomial Gamma sampler. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70* (pp. 3996-4005).
    - [LTL17] Li, Y., Turner, R.E., & Liu, Q. (2017). Approximate inference with amortised MCMC. *arXiv preprint arXiv:1702.08343*.

References

- Bayesian Inference: MCMC
  - Dynamics-Based MCMC: stochastic gradient (manifold support)
    - [PT13] Patterson, S., & Teh, Y.W. (2013). Stochastic gradient Riemannian Langevin dynamics on the probability simplex. In *Advances in neural information processing system*s (pp. 3102-3110).
    - [MCF15] Ma, Y. A., Chen, T., & Fox, E. (2015). A complete recipe for stochastic gradient MCMC. In *Advances in Neural Information Processing Systems* (pp. 2917-2925).
    - [LZS16] Liu, C., Zhu, J., & Song, Y. (2016). Stochastic Gradient Geodesic MCMC Methods. In *Advances in Neural Information Processing Systems* (pp. 3009-3017).
  - Dynamics-Based MCMC: general theory
    - [JKO98] Jordan, R., Kinderlehrer, D., & Otto, F. (1998). The variational formulation of the Fokker-Planck equation. *SIAM journal on mathematical analysis*, *29*(1), 1-17.
    - [MCF15] Ma, Y. A., Chen, T., & Fox, E. (2015). A complete recipe for stochastic gradient MCMC. In *Advances in Neural Information Processing Systems* (pp. 2917-2925).
    - [CDC15] Chen, C., Ding, N., & Carin, L. (2015). On the convergence of stochastic gradient MCMC algorithms with high-order integrators. In *Advances in Neural Information Processing Systems* (pp. 2278-2286).
    - [LZZ19] Liu, C., Zhuo, J., & Zhu, J. (2019). Understanding MCMC Dynamics as Flows on the Wasserstein Space. In *Proceedings of the 36th International Conference on Machine Learning* (pp. 4093-4103).

References

- Probabilistic Graphical Models
  - Directed PGM: Causality

    - [SG91] Spirtes, P., Glymour, C. (1991). An algorithm for fast recovery of sparse causal graphs. *Social Science Computer Review*. 9 (1): 62–72.
    - [Pearl09] Pearl, J. (2009). *Causality*. Cambridge university press.
    - [PJS17] Peters, J., Janzing, D., & Schölkopf, B. (2017). *Elements of causal inference: foundations and learning algorithms*. The MIT Press.
    - [IW09] Imbens, G. W. & Wooldridge, J. M. Recent developments in the econometrics of program evaluation. *Journal of economic literature*, 47(1):5–86, 2009.
    - [Pearl15] Pearl, J. Detecting latent heterogeneity. *Sociological Methods & Research*, pp. 0049124115600597, 2015.
    - [SJP+12] Schölkopf, B., Janzing, D., Peters, J., Sgouritsa, E., Zhang, K., & Mooij, J. (2012). On causal and anticausal learning. In *International Conference on Machine Learning*.

References

- Probabilistic Graphical Models
  - Directed PGM: Causality
    - [Sch19] Schölkopf, B. (2019). Causality for machine learning. *arXiv preprint arXiv:1911.10500*.
    - [YGL+20] Yu, K., Guo, X., Liu, L., Li, J., Wang, H., Ling, Z., & Wu, X. (2020). Causality-based feature selection: Methods and evaluations. *ACM Computing Surveys (CSUR)*, 53(5), 1-36.
    - [LSW+21] Liu, C., Sun, X., Wang, J., Tang, H., Li, T., Qin, T., Chen, W., & Liu, T. Y. (2021). Learning Causal Semantic Representation for Out-of-Distribution Prediction. In *Advances in Neural Information Processing Systems*.
    - [SWZ+21] Sun, X., Wu, B., Zheng, X., Liu, C., Chen, W., Qin, T., & Liu, T. Y. (2021). Recovering Latent Causal Factor for Generalization to Distributional Shifts. In *Advances in Neural Information Processing Systems*.
  - Related:
    - [ABGL19] Arjovsky, M., Bottou, L., Gulrajani, I., & Lopez-Paz, D. (2019). Invariant risk minimization. *arXiv preprint arXiv:1907.02893*.

References

- Probabilistic Graphical Models
  - Directed PGM: Topic Models

    - [BNJ03] Blei, D. M., Ng, A. Y., & Jordan, M. I. (2003). Latent Dirichlet Allocation. *Journal of Machine Learning Research*, 3(Jan), pp.993-1022.
    - [GS04] Griffiths, T.L., & Steyvers, M. (2004). Finding scientific topics. *Proceedings of the National academy of Sciences*, 101 (suppl 1), pp.5228-5235.
    - [SG07] Steyvers, M., & Griffiths, T. (2007). Probabilistic topic models. *Handbook of latent semantic analysis*, *427*(7), 424-440.
    - [MB08] Mcauliffe, J.D., & Blei, D.M. (2008). Supervised topic models. In *Advances in neural information processing systems* (pp. 121-128).
    - [ZAX12] Zhu, J., Ahmed, A., & Xing, E. P. (2012). MedLDA: maximum margin supervised topic models. *Journal of Machine Learning Research*, *13*(Aug), 2237-2278.
    - [PT13] Patterson, S., & Teh, Y.W. (2013). Stochastic gradient Riemannian Langevin dynamics on the probability simplex. In *Advances in neural information processing systems* (pp. 3102-3110).
    - [ZCX14] Zhu, J., Chen, N., & Xing, E. P. (2014). Bayesian inference with posterior regularization and applications to infinite latent SVMs. *The Journal of Machine Learning Research*, *15*(1), 1799-1847.

References

- Probabilistic Graphical Models
  - Directed PGM: Topic Models

    - [LARS14] Li, A.Q., Ahmed, A., Ravi, S., & Smola, A.J. (2014). Reducing the sampling complexity of topic models. In *Proceedings of the ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 891-900).
    - [YGH+15] Yuan, J., Gao, F., Ho, Q., Dai, W., Wei, J., Zheng, X., Xing, E.P., Liu, T.Y., & Ma, W.Y. (2015). LightLDA: Big topic models on modest computer clusters. In *Proceedings of the 24th International Conference on World Wide Web* (pp. 1351-1361).
    - [CLZC16] Chen, J., Li, K., Zhu, J., & Chen, W. (2016). WarpLDA: a cache efficient o(1) algorithm for latent Dirichlet allocation. *Proceedings of the VLDB Endowment*, 9(10), pp.744-755.

References

- Probabilistic Graphical Models
  - Directed PGM: Variational Auto-Encoders

    - [KW14] Kingma, D.P., & Welling, M. (2014). Auto-encoding variational Bayes. In *Proceedings of the International Conference on Learning Representations*.
    - [KMRW14] Kingma, D. P., Mohamed, S., Rezende, D. J., & Welling, M. (2014). Semi-supervised learning with deep generative models. In *Advances in neural information processing systems* (pp. 3581-3589).
    - [SLY15] Sohn, K., Lee, H., & Yan, X. (2015). Learning structured output representation using deep conditional generative models. In *Advances in Neural Information Processing Systems*, 28, 3483-3491.
    - [GDG+15] Gregor, K., Danihelka, I., Graves, A., Rezende, D. J., & Wierstra, D. (2015). DRAW: A recurrent neural network for image generation. In *Proceedings of the 32nd International Conference on Machine Learning*.
    - [BGS15] Burda, Y., Grosse, R., & Salakhutdinov, R. (2015). Importance weighted autoencoders. *arXiv preprint arXiv:1509.00519*.

References

- Probabilistic Graphical Models
  - Directed PGM: Variational Auto-Encoders

    - [DFD+18] Davidson, T.R., Falorsi, L., De Cao, N., Kipf, T., & Tomczak, J.M. (2018). Hyperspherical variational auto-encoders. In *Proceedings of the Conference on Uncertainty in Artificial Intelligence*.
    - [MSJ+15] Makhzani, A., Shlens, J., Jaitly, N., Goodfellow, I., & Frey, B. (2016). Adversarial Autoencoders. In *Proceedings of the International Conference on Learning Representations*.
    - [CDH+16] Chen, X., Duan, Y., Houthooft, R., Schulman, J., Sutskever, I., & Abbeel, P. (2016). InfoGAN: Interpretable representation learning by information maximizing generative adversarial nets. In *Advances in neural information processing systems* (pp. 2172-2180).
    - [MNG17] Mescheder, L., Nowozin, S., & Geiger, A. (2017). Adversarial variational Bayes: Unifying variational autoencoders and generative adversarial networks. In *Proceedings of the International Conference on Machine Learning* (pp. 2391-2400).
    - [TBGS17] Tolstikhin, I., Bousquet, O., Gelly, S., & Schoelkopf, B. (2017). Wasserstein Auto-Encoders. *arXiv preprint arXiv:1711.01558*.

References

- Probabilistic Graphical Models
  - Directed PGM: Variational Auto-Encoders

    - [FWL17] Feng, Y., Wang, D., & Liu, Q. (2017). Learning to Draw Samples with Amortized Stein Variational Gradient Descent. In *Proceedings of the Conference on Uncertainty in Artificial Intelligence*.
    - [PGH+17] Pu, Y., Gan, Z., Henao, R., Li, C., Han, S., & Carin, L. (2017). VAE learning via Stein variational gradient descent. In *Advances in Neural Information Processing Systems* (pp. 4236-4245).
    - [KSDV18] Kocaoglu, M., Snyder, C., Dimakis, A. G., & Vishwanath, S. (2018). CausalGAN: Learning causal implicit generative models with adversarial training. In *Proceedings of the International Conference on Learning Representations*.
    - [LWZZ18] Li, C., Welling, M., Zhu, J., & Zhang, B. (2018). Graphical generative adversarial networks. In *Advances in Neural Information Processing Systems* (pp. 6069-6080).
    - [DW19] Dai, B., & Wipf, D. (2019). Diagnosing and Enhancing Gaussian VAE Models. In *International Conference on Learning Representations*.

References

- Probabilistic Graphical Models
  - Directed PGM: Variational Auto-Encoders

    - [LBN+19] Luo, Y., Beatson, A., Norouzi, M., Zhu, J., Duvenaud, D., Adams, R. P., & Chen, R. T. (2019). SUMO: Unbiased Estimation of Log Marginal Probability for Latent Variable Models. In *International Conference on Learning Representations*.
    - [PHN+20] Pang, B., Han, T., Nijkamp, E., Zhu, S. C., & Wu, Y. N. (2020). Learning Latent Space Energy-Based Prior Model. In *Advances in Neural Information Processing Systems*.
    - [LTQ+21] Liu, C., Tang, H., Qin, T., Wang, J., & Liu, T. Y. (2021). On the Generative Utility of Cyclic Conditionals. In *Advances in Neural Information Processing Systems*.

References

- Probabilistic Graphical Models
  - Directed PGM: Disentanglement

    - [CDH+16] Chen, X., Duan, Y., Houthooft, R., Schulman, J., Sutskever, I., & Abbeel, P. (2016). InfoGAN: interpretable representation learning by information maximizing Generative Adversarial Nets. In *Neural Information Processing Systems*.
    - [HMP+17] Higgins, I., Matthey, L., Pal, A., Burgess, C., Glorot, X., Botvinick, M., Mohamed, S., & Lerchner, A. (2017). Beta-VAE: Learning basic visual concepts with a constrained variational framework. In *Proceedings of the International Conference on Learning Representations*.
    - [CLG+18] Chen, R. T., Li, X., Grosse, R., & Duvenaud, D. (2018). Isolating sources of disentanglement in VAEs. In *Neural Information Processing Systems*.
    - [HAP+18] Higgins, I., Amos, D., Pfau, D., Racaniere, S., Matthey, L., Rezende, D., & Lerchner, A. (2018). Towards a definition of disentangled representations. *arXiv preprint arXiv:1812.02230*.
    - [LBL+19] Locatello, F., Bauer, S., Lucic, M., Raetsch, G., Gelly, S., Schölkopf, B., & Bachem, O. (2019). Challenging common assumptions in the unsupervised learning of disentangled representations. In *International Conference on Machine Learning*.

References

- Probabilistic Graphical Models
  - Directed PGM: Disentanglement

    - [LTB+19] Locatello, F., Tschannen, M., Bauer, S., Rätsch, G., Schölkopf, B., & Bachem, O. (2019). Disentangling Factors of Variations Using Few Labels. In *International Conference on Learning Representations*.
    - [CB20] Chen, J., & Batmanghelich, K. (2020). Weakly supervised disentanglement by pairwise similarities. In *Proceedings of the AAAI Conference on Artificial Intelligence*.
    - [LPR+20] Locatello, F., Poole, B., Rätsch, G., Schölkopf, B., Bachem, O., & Tschannen, M. (2020). Weakly-supervised disentanglement without compromises. In *International Conference on Machine Learning*.
    - [SCK+20] Shu, R., Chen, Y., Kumar, A., Ermon, S., & Poole, B. (2020). Weakly Supervised Disentanglement with Guarantees. In *International Conference on Learning Representations*.
    - [KKM+20] Khemakhem, I., Kingma, D., Monti, R., & Hyvarinen, A. (2020). Variational autoencoders and nonlinear ICA: A unifying framework. In *International Conference on Artificial Intelligence and Statistics*.

References

- Probabilistic Graphical Models
  - Undirected PGM

    - [HS83] Hinton, G., & Sejnowski, T. (1983). Optimal perceptual inference. In *IEEE Conference on Computer Vision and Pattern Recognition*.
    - [Smo86] Smolensky, P. (1986). Information processing in dynamical systems: Foundations of harmony theory. In *Parallel Distributed Processing*, volume 1, chapter 6, pages 194-281. MIT Press.
    - [Hin02] Hinton, G. E. (2002). Training products of experts by minimizing contrastive divergence. *Neural computation*, 14(8), 1771-1800.
    - [LCH+06] LeCun, Y., Chopra, S., Hadsell, R., Ranzato, M., & Huang, F. (2006). A tutorial on energy-based learning. *Predicting structured data*, *1*(0).
    - [HOT06] Hinton, G. E., Osindero, S., & Teh, Y. W. (2006). A fast learning algorithm for deep belief nets. *Neural computation*, 18(7), 1527-1554.
    - [SH09] Salakhutdinov, R., & Hinton, G. (2009, April). Deep Boltzmann machines. *In AISTATS* (pp. 448-455).
    - [Sal15] Salakhutdinov, R. (2015). Learning deep generative models. *Annual Review of Statistics and Its Application*, 2, 361-385.
    - [KB16] Kim, T., & Bengio, Y. (2016). Deep directed generative models with energy-based probability estimation. *arXiv preprint arXiv:1606.03439*.
    - [DM19] Du, Y., & Mordatch, I. (2019). Implicit generation and generalization in energy-based models. In *Advances in Neural Information Processing Systems*.

References

- Probabilistic Graphical Models
  - Score-based methods

    - [Hyv05] Hyvärinen, A., & Dayan, P. (2005). Estimation of non-normalized statistical models by score matching. *Journal of Machine Learning Research*, 6(4).
    - [SE19] Song, Y., & Ermon, S. (2019). Generative Modeling by Estimating Gradients of the Data Distribution. In *Advances in Neural Information Processing Systems*.

References

- Probabilistic Graphical Models
  - Diffusion-based models

    - [SWMG15] Sohl-Dickstein, J., Weiss, E., Maheswaranathan, N., & Ganguli, S. (2015). Deep unsupervised learning using nonequilibrium thermodynamics. In *International Conference on Machine Learning* (pp. 2256-2265).
    - [HJA20] Ho, J., Jain, A., & Abbeel, P. (2020). Denoising diffusion probabilistic models. In *Advances in Neural Information Processing Systems*.
    - [SSK+21] Song, Y., Sohl-Dickstein, J., Kingma, D. P., Kumar, A., Ermon, S., & Poole, B. (2021). Score-Based Generative Modeling through Stochastic Differential Equations. In *International Conference on Learning Representations*.
    - [BTHD21] De Bortoli, V., Thornton, J., Heng, J., & Doucet, A. (2021). Diffusion Schrödinger bridge with applications to score-based generative modeling. In *Advances in Neural Information Processing Systems*.
    - [DVK22] Dockhorn, T., Vahdat, A., & Kreis, K. (2022). Score-Based Generative Modeling with Critically-Damped Langevin Diffusion. In *International Conference on Learning Representations*.

References

- Probabilistic Graphical Models
  - Diffusion-based models

    - [SWMG15] Sohl-Dickstein, J., Weiss, E., Maheswaranathan, N., & Ganguli, S. (2015). Deep unsupervised learning using nonequilibrium thermodynamics. In *International Conference on Machine Learning* (pp. 2256-2265).
    - [HJA20] Ho, J., Jain, A., & Abbeel, P. (2020). Denoising diffusion probabilistic models. In *Advances in Neural Information Processing Systems*.
    - [SSK+21] Song, Y., Sohl-Dickstein, J., Kingma, D. P., Kumar, A., Ermon, S., & Poole, B. (2021). Score-Based Generative Modeling through Stochastic Differential Equations. In *International Conference on Learning Representations*.
    - [SME21] Song, J., Meng, C., & Ermon, S. (2021). Denoising Diffusion Implicit Models. In *International Conference on Learning Representations*.
    - [ND21] Nichol, A. Q., & Dhariwal, P. (2021). Improved denoising diffusion probabilistic models. In *International Conference on Machine Learning* (pp. 8162-8171). PMLR.
    - [SDME21] Song, Y., Durkan, C., Murray, I., & Ermon, S. (2021). Maximum likelihood training of score-based diffusion models. In *Advances in Neural Information Processing Systems*, 34, 1415-1428.
    - [KSPH21] Kingma, D., Salimans, T., Poole, B., & Ho, J. (2021). Variational diffusion models. In *Advances in neural information processing systems*, 34, 21696-21707.
    - [DN21] Dhariwal, P., & Nichol, A. (2021). Diffusion models beat GANs on image synthesis. In *Advances in Neural Information Processing Systems*, 34, 8780-8794.

References

- Probabilistic Graphical Models
  - Diffusion-based models

    - [DTHD21] De Bortoli, V., Thornton, J., Heng, J., & Doucet, A. (2021). Diffusion Schrödinger bridge with applications to score-based generative modeling. In *Advances in Neural Information Processing Systems*, 34, 17695-17709.
    - [DVK22] Dockhorn, T., Vahdat, A., & Kreis, K. (2022). Score-Based Generative Modeling with Critically-Damped Langevin Diffusion. In *International Conference on Learning Representations*.
    - [BLZZ22] Bao, F., Li, C., Zhu, J., & Zhang, B. (2022). Analytic-DPM: an Analytic Estimate of the Optimal Reverse Variance in Diffusion Probabilistic Models. In *International Conference on Learning Representations*.
    - [BLS+22] Bao, F., Li, C., Sun, J., Zhu, J., & Zhang, B. (2022). Estimating the Optimal Covariance with Imperfect Mean in Diffusion Probabilistic Models. In *International Conference on Machine Learning*.
    - [LZB+22a] Lu, C., Zheng, K., Bao, F., Chen, J., Li, C., & Zhu, J. (2022). Maximum Likelihood Training for Score-Based Diffusion ODEs by High-Order Denoising Score Matching. In *International Conference on Machine Learning*.
    - [LZB+22b] Lu, C., Zhou, Y., Bao, F., Chen, J., Li, C., & Zhu, J. (2022). DPM-Solver: A Fast ODE Solver for Diffusion Probabilistic Model Sampling in Around 10 Steps. In *Advances in Neural Information Processing Systems*.
    - [KAAL22] Karras, T., Aittala, M., Aila, T., & Laine, S. (2022). Elucidating the Design Space of Diffusion-Based Generative Models. In *Advances in Neural Information Processing Systems*.
    - [ZBLZ22] Zhao, M., Bao, F., Li, C., & Zhu, J. (2022). EGSDE: Unpaired Image-to-Image Translation via Energy-Guided Stochastic Differential Equations. In *Advances in Neural Information Processing Systems*.

References

- Probabilistic Graphical Models
  - Diffusion-based models

    - [CLT22] Chen, T., Liu, G. H., & Theodorou, E. (2022). Likelihood Training of Schrödinger Bridge using Forward-Backward SDEs Theory. In *International Conference on Learning Representations*.
    - [SDCS23] Song, Y., Dhariwal, P., Chen, M., Sutskever, I. (2023). Consistency Models. In *International Conference on Machine Learning*.

References

- Probabilistic Graphical Models
  - Related
    - Sliced score matching: [SGSE19] Song, Y., Garg, S., Shi, J., & Ermon, S. (2019). Sliced score matching: A scalable approach to density and score estimation. In *Uncertainty in Artificial Intelligence* (pp. 574-584). PMLR.
    - Optimization: [WWJ16] Wibisono, A., Wilson, A. C., & Jordan, M. I. (2016). A variational perspective on accelerated methods in optimization. In *Proceedings of the National Academy of Sciences*, 113(47), E7351-E7358.

References

- Others
  - Probabilistic Graphical Models
    - [KYD+18] Kim, T., Yoon, J., Dia, O., Kim, S., Bengio, Y., & Ahn, S. (2018). Bayesian model-agnostic meta-learning. In *Advances in Neural Information Processing Systems* (pp. 7332-7342).
    - [LST15] Lake, B.M., Salakhutdinov, R., & Tenenbaum, J.B. (2015). Human-level concept learning through probabilistic program induction. *Science*, 350(6266), pp. 1332-1338.
  - Bayesian Neural Network
    - [LG17] Li, Y., & Gal, Y. (2017). Dropout inference in Bayesian neural networks with alpha-divergences. In *Proceedings of the International Conference on Machine Learning* (pp. 2052-2061).
  - Related References
    - [Wil92] Williams, R. J. (1992). Simple statistical gradient-following algorithms for connectionist reinforcement learning. *Machine learning*, *8*(3-4), 229-256.
    - [HV93] Hinton, G., & Van Camp, D. (1993). Keeping neural networks simple by minimizing the description length of the weights. In *in Proc. of the 6th Ann. ACM Conf. on Computational Learning Theory*.
    - [NJ01] Ng, A. Y., & Jordan, M. I. (2002). On discriminative vs. generative classifiers: A comparison of logistic regression and naive Bayes. In *Advances in neural information processing systems* (pp. 841-848).

The End