Deep Generative Models

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Deep Learning For Science School
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@adityagrover_

Age of Big **Unlabeled** Data

Opportunity: High-throughput data and computation

Particle Accelerators

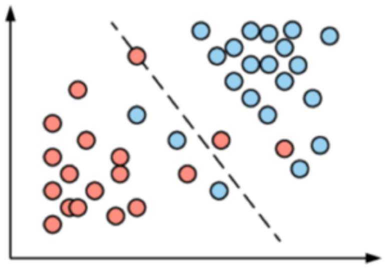
Materials Project

GenBank

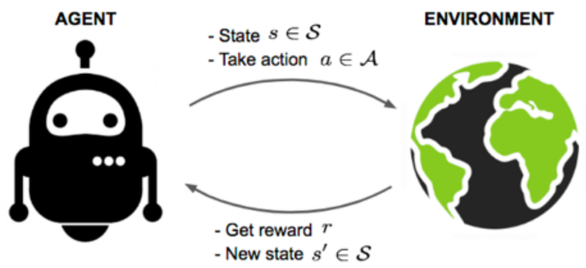
Challenge: Supervision signals such as labels are *expensive*

e.g., time, money, expertise, safety costs

Learning With Limited Supervision

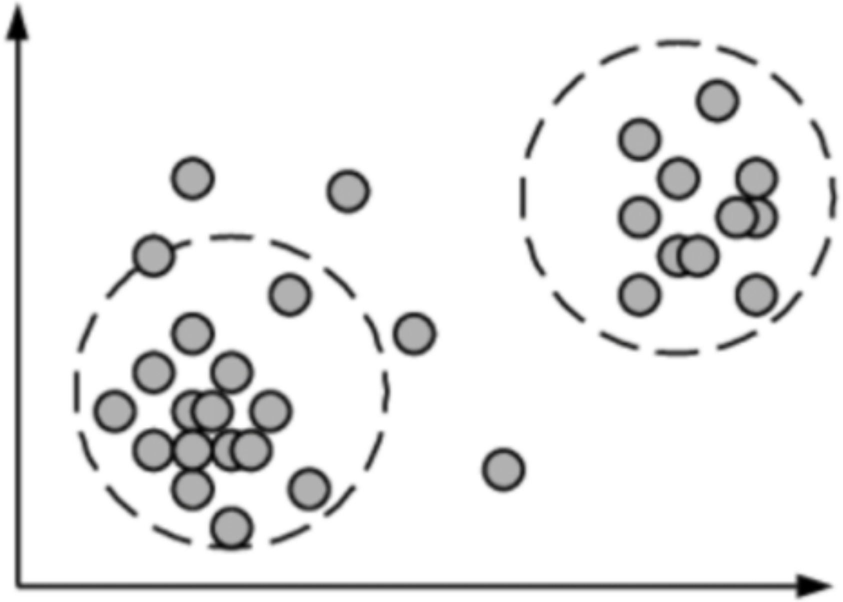


Classification
w/ active querying



Reinforcement Learning
w/ sparse rewards

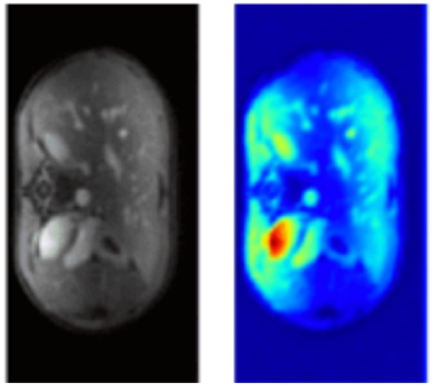
Can we learn with *no* supervision?



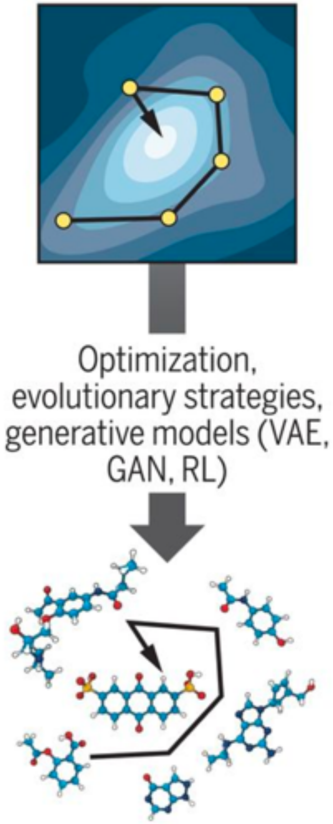
Recent Advances in Unsupervised Learning

Karras et al.

Huang et al.

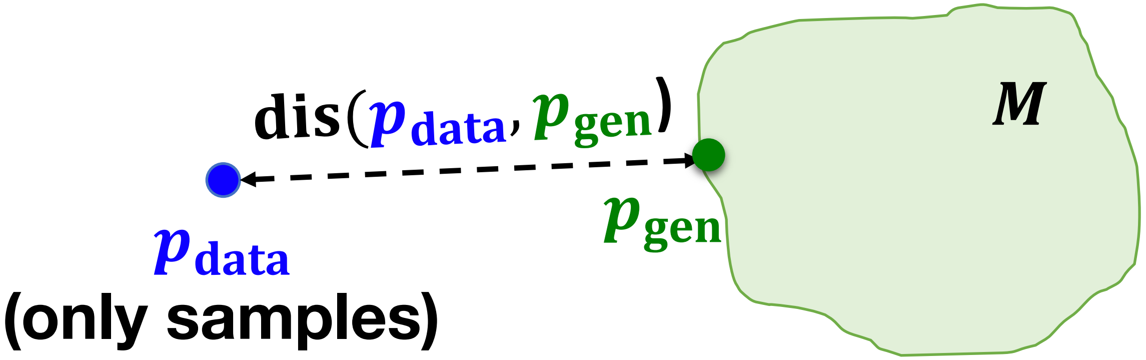


Mardani et al.



Sanchez-Lengelin et al.

Generative Models: Fit Data Distributions



$$\boxed{\min_{p_{\mathrm{gen}} \in M} \mathrm{dis}(p_{\mathrm{data}}, p_{\mathrm{gen}})}$$

Example

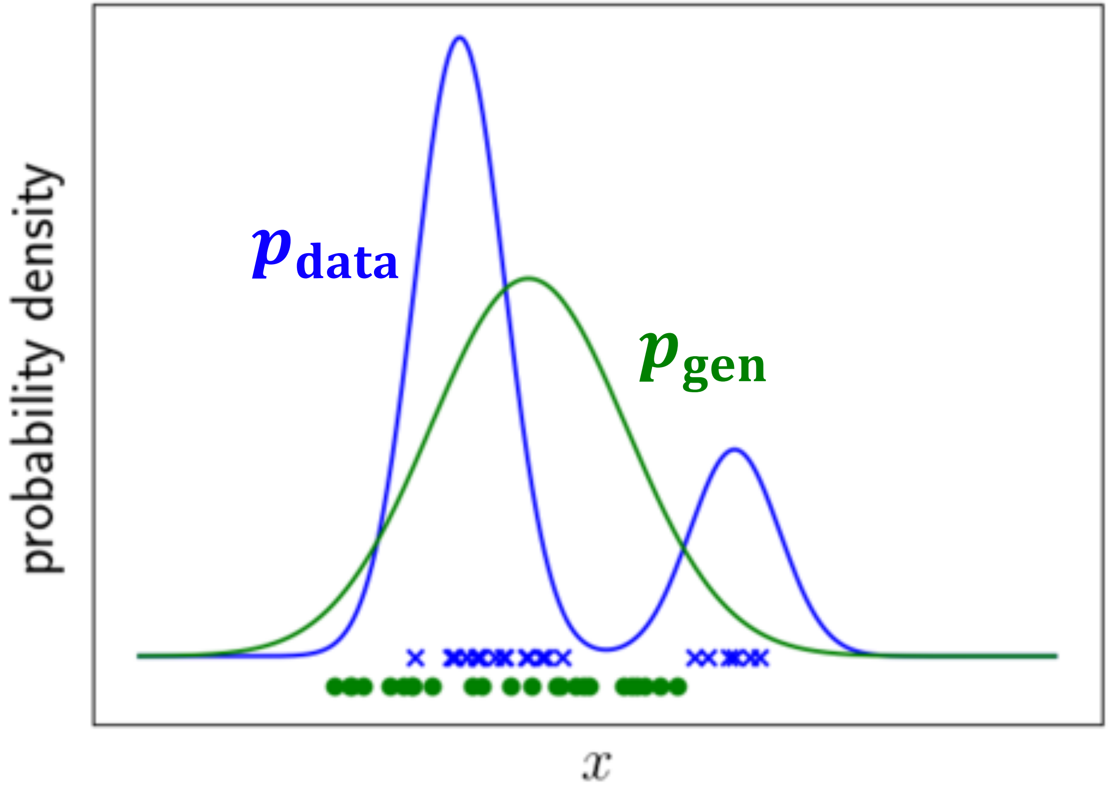
p_{data} data distribution (unknown)

× data samples (known)

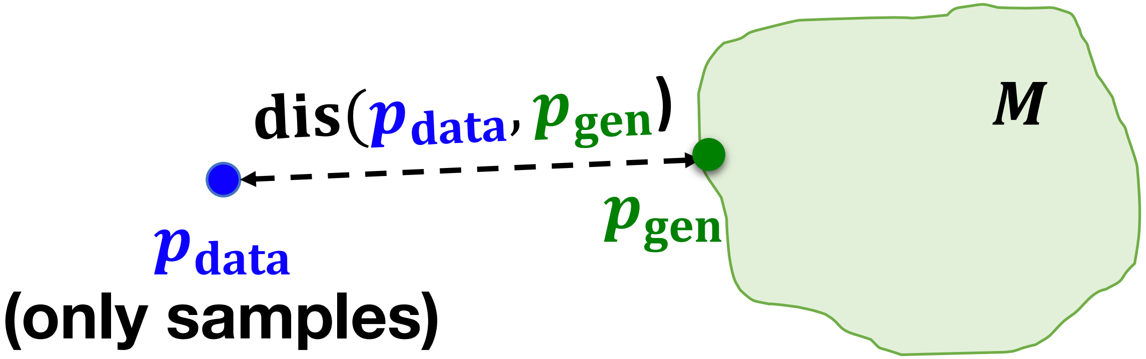
M mixture of 1d Gaussians

p_{gen} generative model

● generated samples



Key Challenge: Curse of Dimensionality

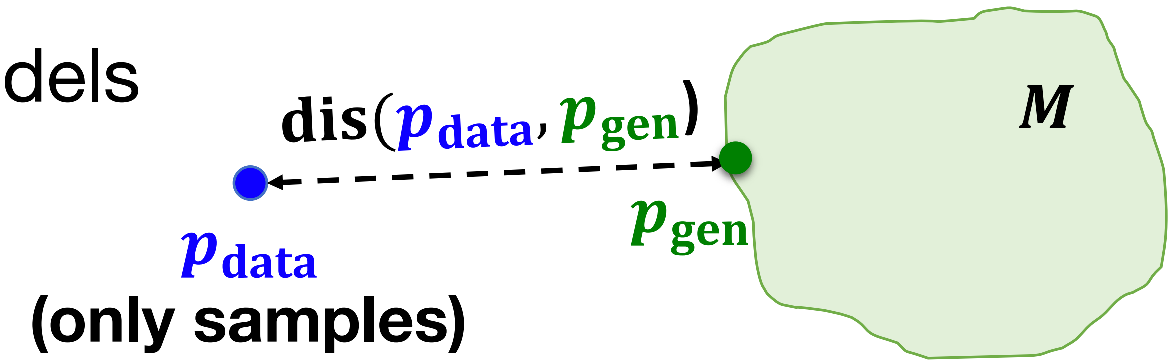


$$\boxed{\min_{p_{\text{gen}} \in M} \mathbf{dis}(p_{\text{data}}, p_{\text{gen}})}$$

In high dimensions:
(a) p_{data} can contain many modes
(b) Training samples cover very small region of true support

Roadmap

- Introduction
- Likelihood-based Generative Models
  - Autoregressive Models
  - Variational Autoencoders
  - Normalizing Flow Models
- Likelihood-free Generative Models
  - Generative Adversarial Networks
- Applications In Scientific Discovery



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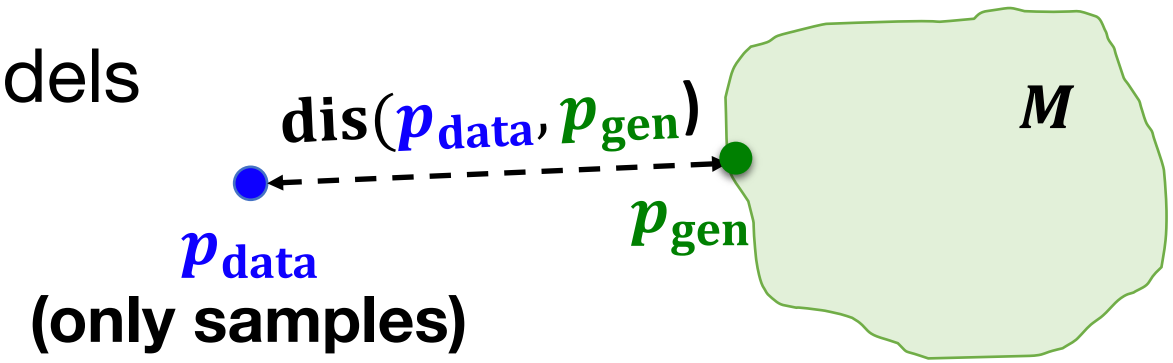


Autoregressive Generative Models

- Directed, fully-observed graphical models

- **Key idea:** Decompose the joint distribution as a **product of tractable conditionals**

$$p_\theta(\mathbf{x}) = \prod_{i=1}^{n} p_\theta(x_i | x_1, x_2, \ldots, x_{i-1}) = \prod_{i=1}^{n} p_\theta(x_i | x_{<i})$$

Learning and Inference

- **Learning** maximizes the model log-likelihood over the dataset $\mathcal{D}$

$$\max_{\theta} \log p_{\theta}(\mathcal{D}) = \sum_{\mathbf{x} \in \mathcal{D}} \log p_{\theta}(\mathbf{x}) = \sum_{\mathbf{x} \in \mathcal{D}} \sum_{i=1}^{n} \log p_{\theta}(x_i | x_{<i}))$$

- Tractable conditionals allow for **exact likelihood evaluation**
  - Conditional evaluated in parallel during training

- Directed model permits **ancestral sampling**, one variable at a time

$$x_1 \sim p_{\theta}(x_1), x_2 \sim p_{\theta}(x_2|x_1), \ldots, x_n \sim p_{\theta}(x_n|x_{<n})$$

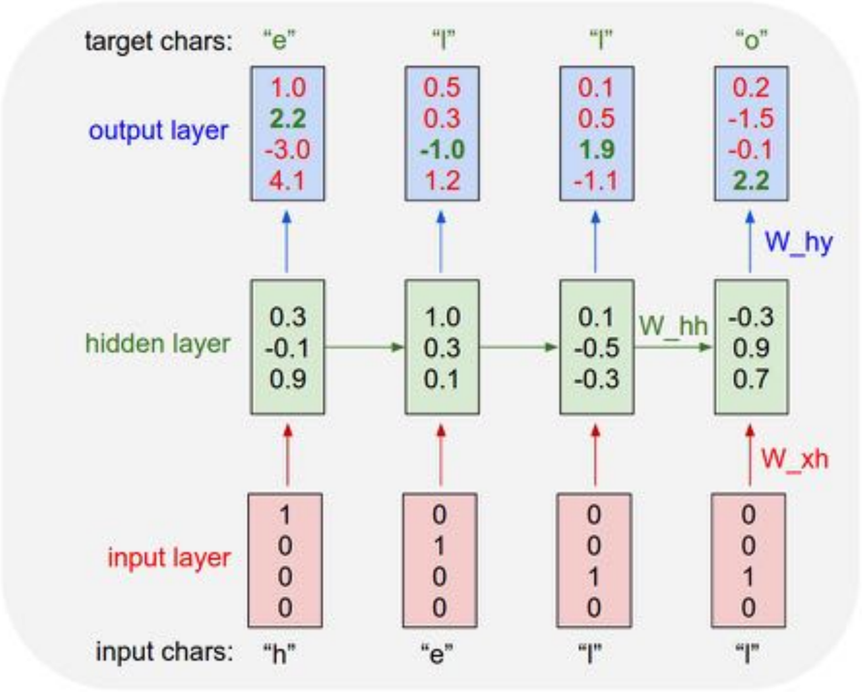
Parameterizing AGMs

Linear/multi-layer NN based parameterizations

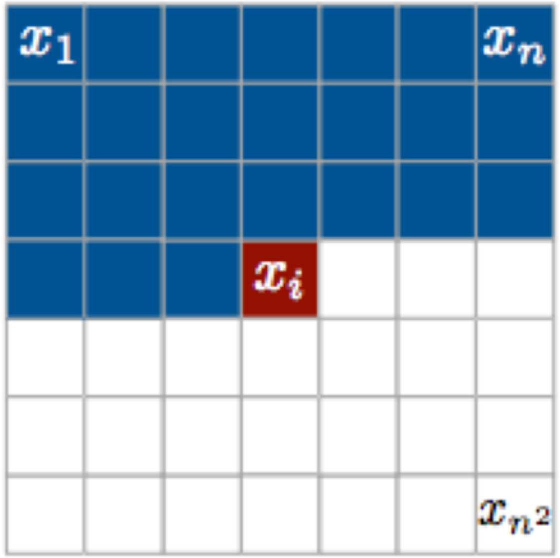
- Fully-visible sigmoid belief networks (FVSBN)
- Neural autoregressive density estimator (NADE): 1 hidden layer NN
- Masked autoencoder distribution estimation (MADE): multilayer NN

Neal, 1992, Larochelle & Murray, 2011, Germain et al., 2015

RNN-based parameterizations



Char-RNN

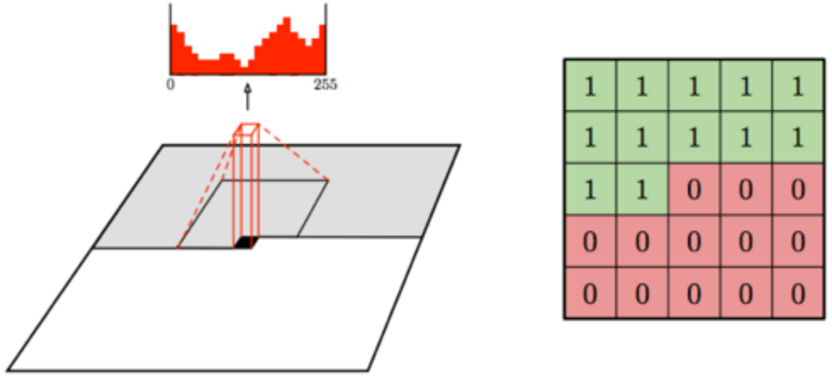


Pixel-RNN

Sutskevar et al., 2011, Karpathy, 2015, Theis & Bethge, 2015, van den Oord, 2016a

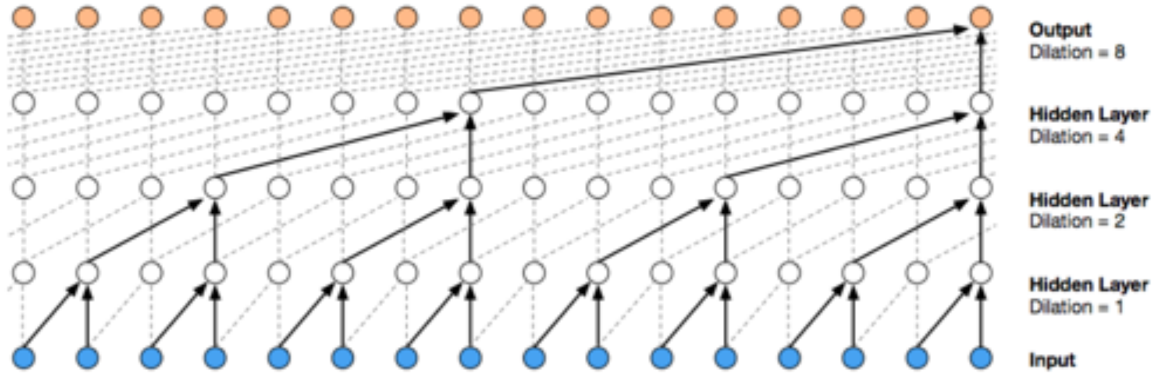
CNN-based parameterizations

Masked convolutions preserve raster scan order



PixelCNN

Dilated convolutions increase the receptive field



WaveNet

van den Oord et al., 2016b, c

Recent: Transformer-based parameterizations
[Radford et al., 2018, 2019 Brown et al., 2020, Chen et al., 2020]

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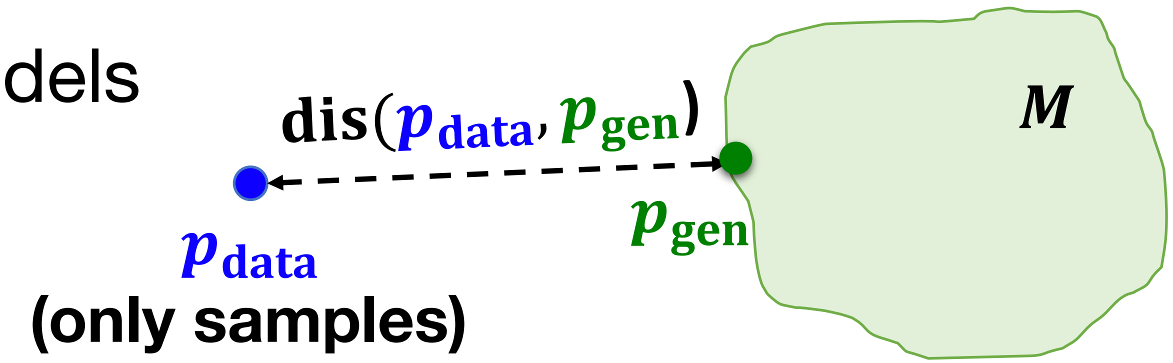
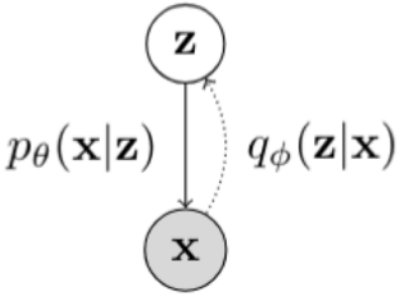


Variational Autoencoders

- Directed, latent-variable models, **with an inference network**



- **Goal:** Maximize the marginal log-likelihood of the dataset

$$\max_{\theta} \Sigma_{x \in \mathcal{D}} \log p_\theta(\mathbf{x})$$

Variational Autoencoders

- **Challenge:** Marginal log-likelihood of any data point $\mathbf{x}$ is intractable

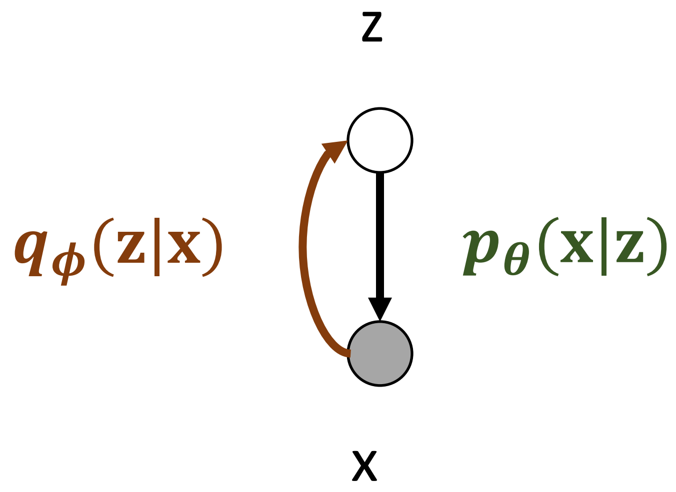
$$\log p_\theta(\mathbf{x}) = \log \int p_\theta(\mathbf{x}, \mathbf{z}) \mathrm{d}\mathbf{z}$$

- **Key ideas**
  - Approximate the posterior $p_\theta(\mathbf{z}|\mathbf{x})$ with a simpler, tractable distribution $q_\phi(\mathbf{z}|\mathbf{x})$
  - Cast **inference as optimization** over θ and ϕ

Inference as Optimization

- Goal: Maximize the marginal log-likelihood of the data is **intractable!**

$$\log \int_{\mathbf{z}} p_\theta(\mathbf{x}, \mathbf{z}) = \log \int_{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x}) \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$



Inference as Optimization

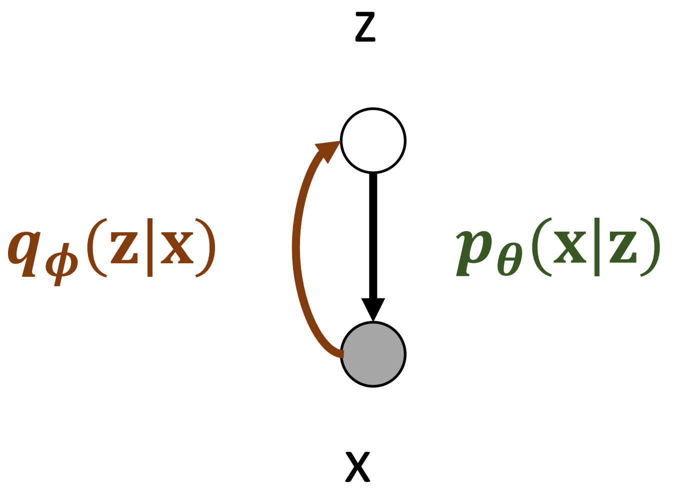
- **New** Goal: Maximize **lower bound** to the marginal log-likelihood of the data is **tractable!**

$$\log \int_{\mathbf{z}} p_\theta(\mathbf{x}, \mathbf{z}) = \log \int_{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x}) \frac{p_\theta(\mathbf{x}, \mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}$$

$$\geq \underbrace{\int_{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x}) \log \frac{p_\theta(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}}_{\mathrm{ELBO}(\mathbf{x};\theta,\phi)}$$

Tightness Condition

$$q_\phi(\mathbf{z}|\mathbf{x}) = p_\theta(\mathbf{z}|\mathbf{x})$$

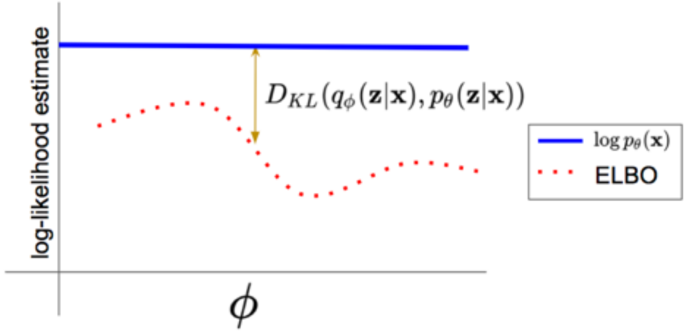


Variational Bayes

- Evidence lower bound (ELBO) for the marginal log-likelihood of $\mathbf{x}$

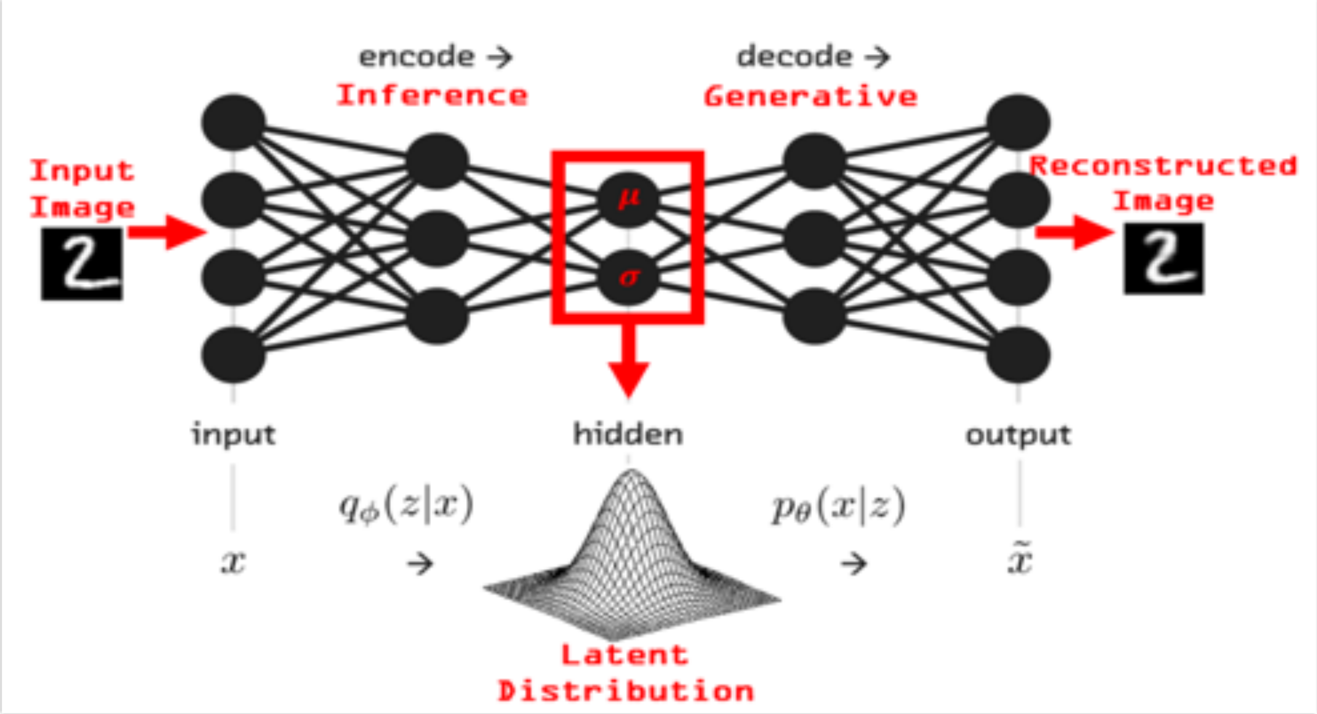
$$\log p_\theta(\mathbf{x}) = \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log\left(\frac{p_\theta(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right)\right]}_{\mathrm{ELBO}(\mathbf{x};\theta,\phi)} + \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})\|p_\theta(\mathbf{z}|\mathbf{x}))$$

- KL gap depends on the quality of the variational approximation



The Autoencoder Perspective

$$\mathrm{ELBO}(\mathbf{x};\theta,\phi) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log\left(\frac{p_\theta(\mathbf{x},\mathbf{z})}{q_\phi(\mathbf{z}|\mathbf{x})}\right)\right] = \underbrace{\mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}\left[\log p_\theta(\mathbf{x}|\mathbf{z})\right]}_{\text{neg. reconstruction error}} - \underbrace{\mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x}), p_\theta(\mathbf{z}))}_{\text{regularization penalty}}$$



Learning and Inference

- Learning maximizes the ELBO for the observed data $\mathcal{D}$
- ELBO gives **lower bounds** on true, intractable log-likelihood
- Directed model permits **ancestral sampling**

$$\mathbf{z} \sim p(\mathbf{z}), \mathbf{x} \sim p_\theta(\mathbf{x} \,|\mathbf{z})$$

- **Latent representations** for any $\mathbf{x}$ can be inferred via $q_\phi(\mathbf{z} \,|\mathbf{x})$

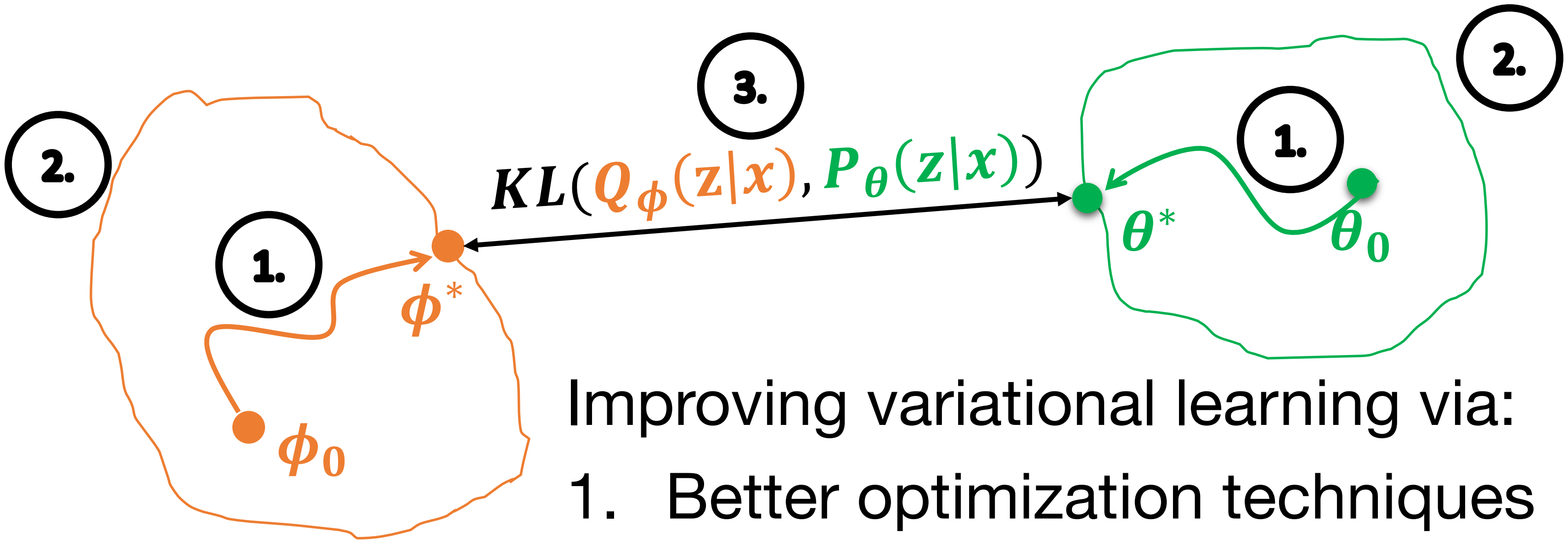
Neal, 1998

NVAE

- Deep hierarchical VAEs with spectral regularization (and other tricks)

Vahdat & Kautz, 2020

Research avenues in a nutshell



Improving variational learning via:

1. Better optimization techniques
2. More expressive approximating families
3. Alternate loss functions

Figure inspired from David Blei's keynote at AISTATS 2018

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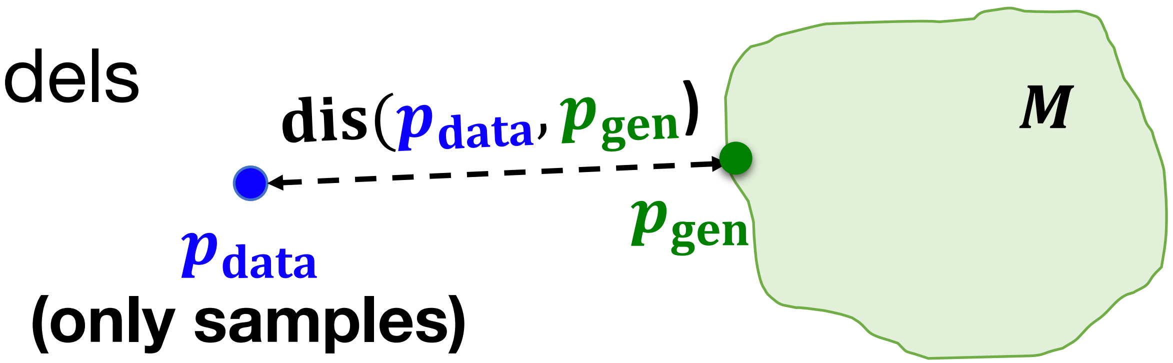
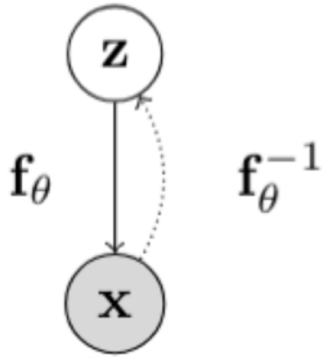


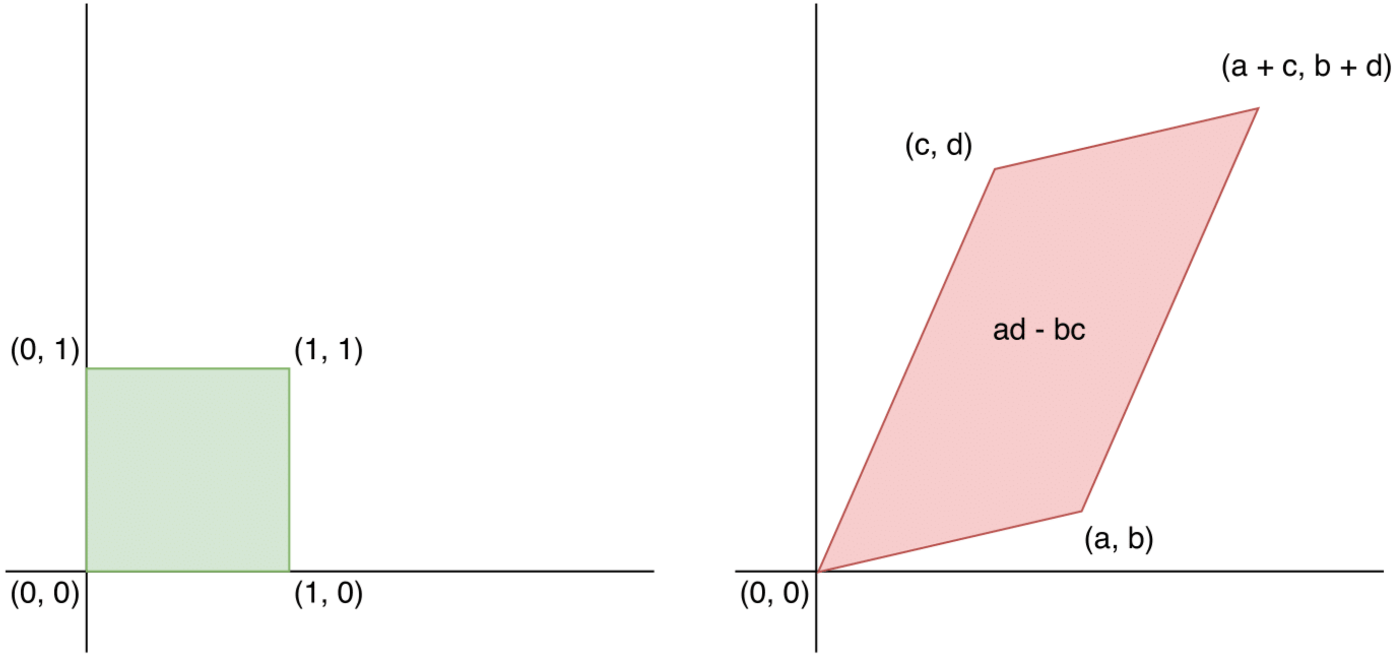
Normalizing flow models

Directed, latent-variable **invertible** models



Key idea: The mapping between $\mathbf{z}$ and $\mathbf{x}$, given by $\mathbf{f}_\theta: \mathbb{R}^n \rightarrow \mathbb{R}^n$, is **deterministic and invertible** such that $\mathbf{x} = \mathbf{f}_\theta(\mathbf{z})$ and $\mathbf{z} = \mathbf{f}_\theta^{-1}(\mathbf{x})$.

Example: Linear Transformation



Normalizing flow models

- Use **change-of-variables** to relate densities in the spaces defined by $\mathbf{z}$ and $\mathbf{x}$:

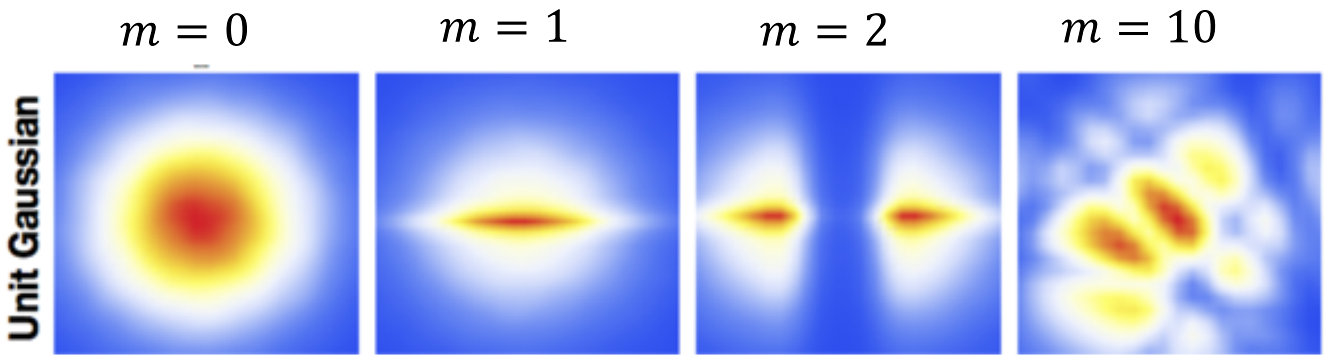
$$p_X(\mathbf{x};\theta) = p_Z(\mathbf{z}) \left| \det \frac{\partial (\mathbf{f}_\theta)^{-1}}{\partial X} \right|_{X=\mathbf{x}}$$

- Transformations shape densities via **volume expansions and contractions**
- Jacobian determinant quantifies the per-unit change in volume

A flow of transformations

Invertible transformations can be composed with each other

$$\mathbf{z}^M \triangleq \mathbf{x} = \mathbf{f}_\theta^M \circ \cdots \circ \mathbf{f}_\theta^1(\mathbf{z}^0); \qquad p_X(\mathbf{x};\theta) = p_{Z^0}(\mathbf{z}^0) \prod_{m=1}^{M} \left| \det \frac{\partial (\mathbf{f}_\theta^m)^{-1}}{\partial Z^m} \right|_{Z^m = \mathbf{z}^m}$$



Rezende & Mohamed, 2016

Learning and inference

- **Learning** maximizes the model likelihood over the dataset $\mathcal{D}$

$$\max_{\theta} \log p_X(\mathcal{D};\theta) = \sum_{\mathbf{x}\in\mathcal{D}} \left(\log p_Z(\mathbf{z}) - \log \left| \det \frac{\partial (\mathbf{f}_\theta)^{-1}}{\partial X} \right|_{X=\mathbf{x}} \right)$$

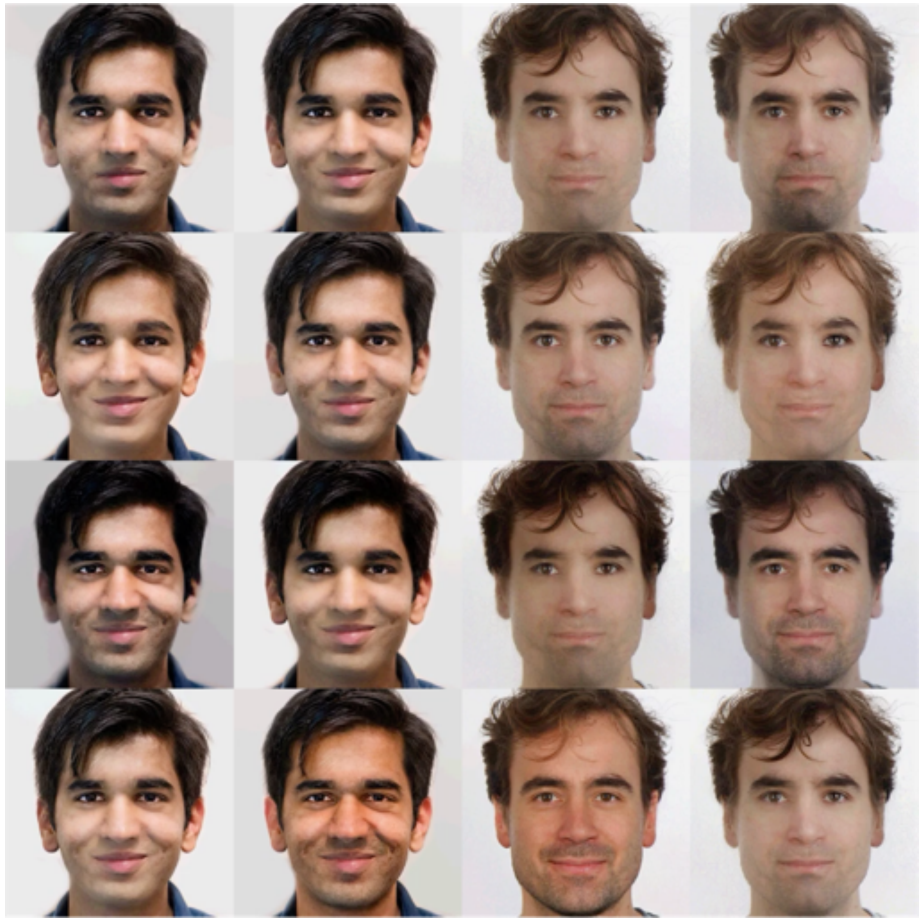
- **Exact likelihood evaluation** via inverse transformations
- **Ancestral sampling** via forward transformations

$$\mathbf{z} \sim p_Z(\mathbf{z}), \quad \mathbf{x} = \mathbf{f}_\theta(\mathbf{z})$$

- **Latent representations** inferred via inverse transformations

$$\mathbf{z} = (\mathbf{f}_\theta)^{-1}(\mathbf{x})$$

Glow



Kingma & Dhariwal, 2018

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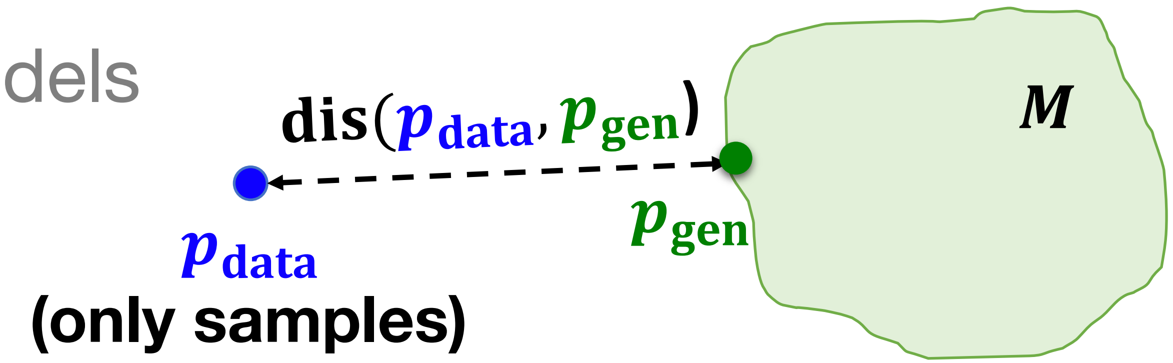


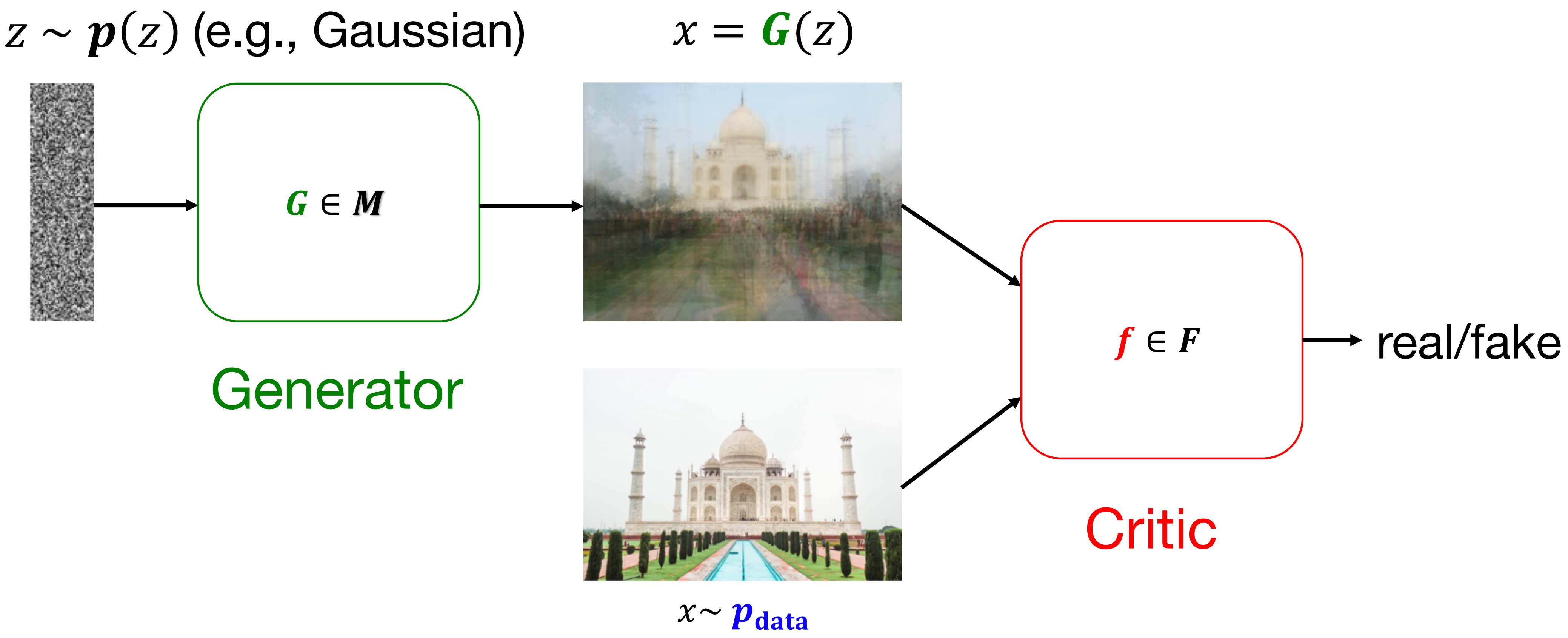
Two Sample Testing

- Compare samples from $\boldsymbol{p}_{\mathbf{data}}$ and $\boldsymbol{p}_{\mathbf{gen}}$ over set of real-valued functions $\boldsymbol{F}$

$$\min_{\boldsymbol{p}_{\mathbf{gen}} \in \boldsymbol{M}} \underbrace{\boxed{\max_{f \in \boldsymbol{F}} \mathbb{E}_{x \sim \boldsymbol{p}_{\mathbf{data}}}[f(x)] - \mathbb{E}_{x \sim \boldsymbol{p}_{\mathbf{gen}}}[f(x)]}}_{\mathbf{dis}(\boldsymbol{p}_{\mathbf{data}}, \boldsymbol{p}_{\mathbf{gen}})}$$

- Different choices of $\boldsymbol{F}$ lead to different discrepancy metrics, e.g., total-variation, Wasserstein, maximum mean discrepancy

Generative Adversarial Nets (GAN)



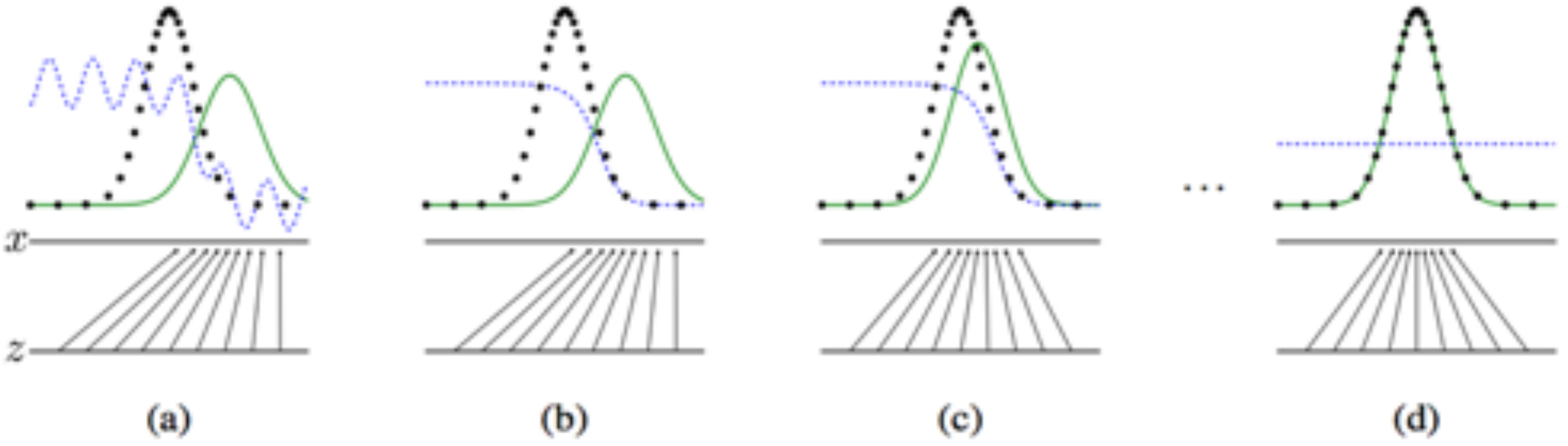
$$\min_{\boldsymbol{G} \in \boldsymbol{M}} \max_{\boldsymbol{f} \in \boldsymbol{F}} \mathbb{E}_{x \sim \boldsymbol{p}_{\mathbf{data}}}[f(x)] - \mathbb{E}_{z \sim \boldsymbol{p}(z)}[f(\boldsymbol{G}(z))]$$

A minimax learning objective

During learning, generator and critic are updated alternatively

$$\min_{G \in \boldsymbol{M}} \max_{f \in \boldsymbol{F}} \mathbb{E}_{x \sim \boldsymbol{p}_{\mathbf{data}}}[f(x)] - \mathbb{E}_{z \sim \boldsymbol{p}(z)}[f(\boldsymbol{G}(z))]$$

Data distribution
Discriminator
Generator



(a) Current state
(b) Update critic
(c) Update generator
(d) Convergence

Goodfellow et al., 2014

Inference

- **Likelihoods** may not be defined or tractable
  - Except when the generative model is invertible [Grover et al., 2018]

- Directed model permits **ancestral sampling**

$z \sim \boldsymbol{p}(z)$ (e.g., Gaussian)

$$x = \boldsymbol{G}(z)$$

GANs Over the Years

Pic credit: Ian Goodfellow

None of these individuals are real!

Have these models passed the ‘generation Turing test’?

Domain Translation & Adptation

- **Conditional GANs** for image translation

Pix2Pix (Isola et al., 2017), CycleGAN (Zhu et al., 2017)

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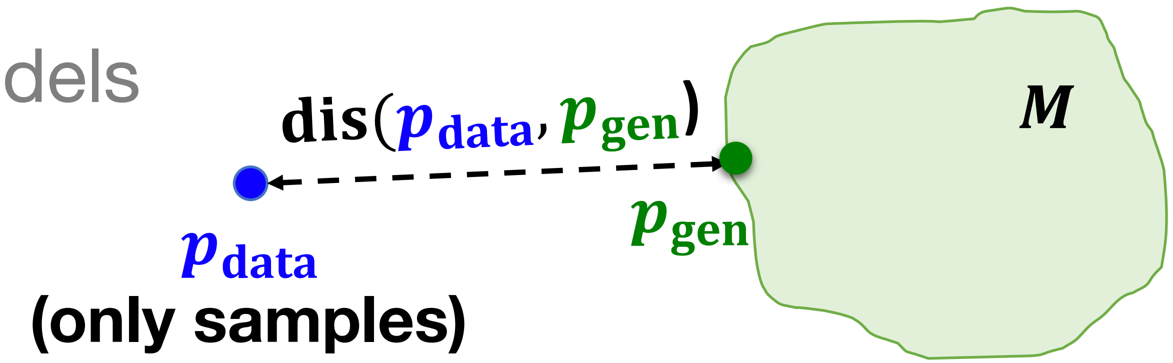


Many, many applications

Physics-aware Deep Generative Models for Creating Synthetic Microstructures

Automatic Chemical Design Using a Data-Driven Continuous Representation of Molecules

Deep Generative Adversarial Neural Networks for Compressive Sensing MRI

Generative deep fields: arbitrarily sized, random synthetic astronomical images through deep learning

Michael J. Smith★ & James E. Geach†

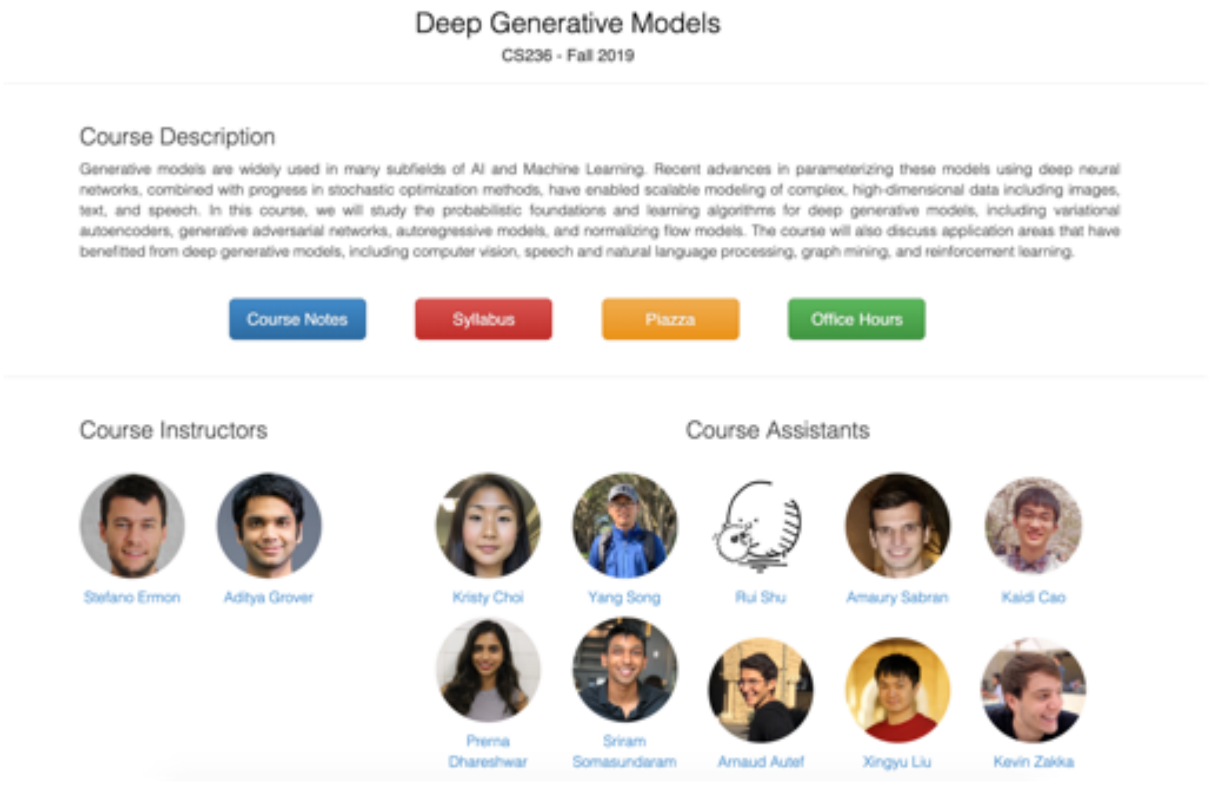
Centre for Astrophysics Research, School of Physics, Astronomy & Mathematics, University of Hertfordshire, Hatfield, AL10 9AB

Centre of Data Innovation Research, School of Physics, Astronomy & Mathematics, University of Hertfordshire, Hatfield, AL10 9AB

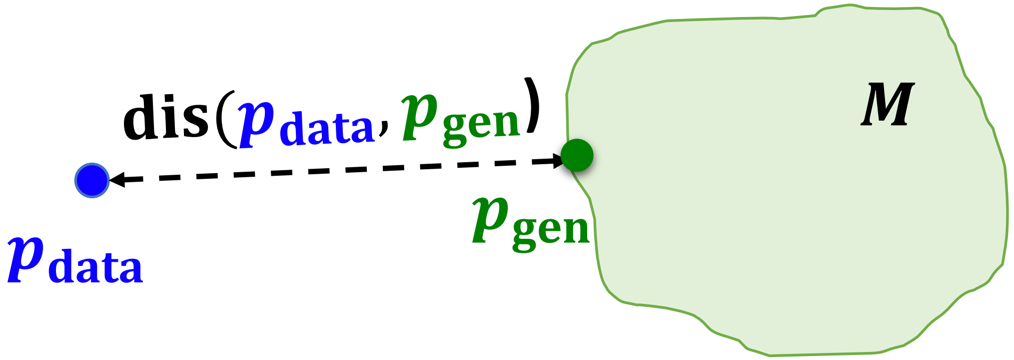
What’s Next for Deep Generative Models?

- Emerging classes of models
  - Energy-based models [Du et al., 2018], generalized generator-discriminator energy models [Grover et al. 2019, Arbel et al., 2020], score matching [Song et al., 2019], diffusion models [Ho et al., 2020]
- Evaluation metrics for sampling and representation learning
- Bias & fairness in generative modeling [Choi et al., 2020]
- Applications
  - Causal discovery and inference
  - Model-based reinforcement learning
  - Scientific discovery

Check out deepgenerativemodels.github.io for materials!



Thank You



"Imagination is the living power and prime agent of all human perception"

- Samuel Taylor Coleridge