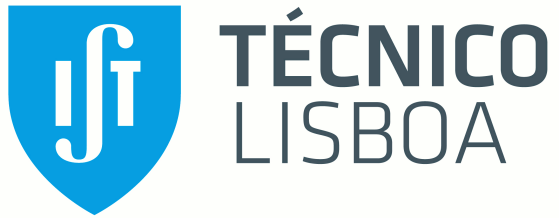
Lecture 12: Deep Generative Models

André Martins, Francisco Melo, Mário Figueiredo



Deep Learning Course, Winter 2023-2024

Announcements

- Thursday (January 4): guest lecture by Chrysoula Zerva.

  Grande Auditório, Centro de Congressos, 13:30

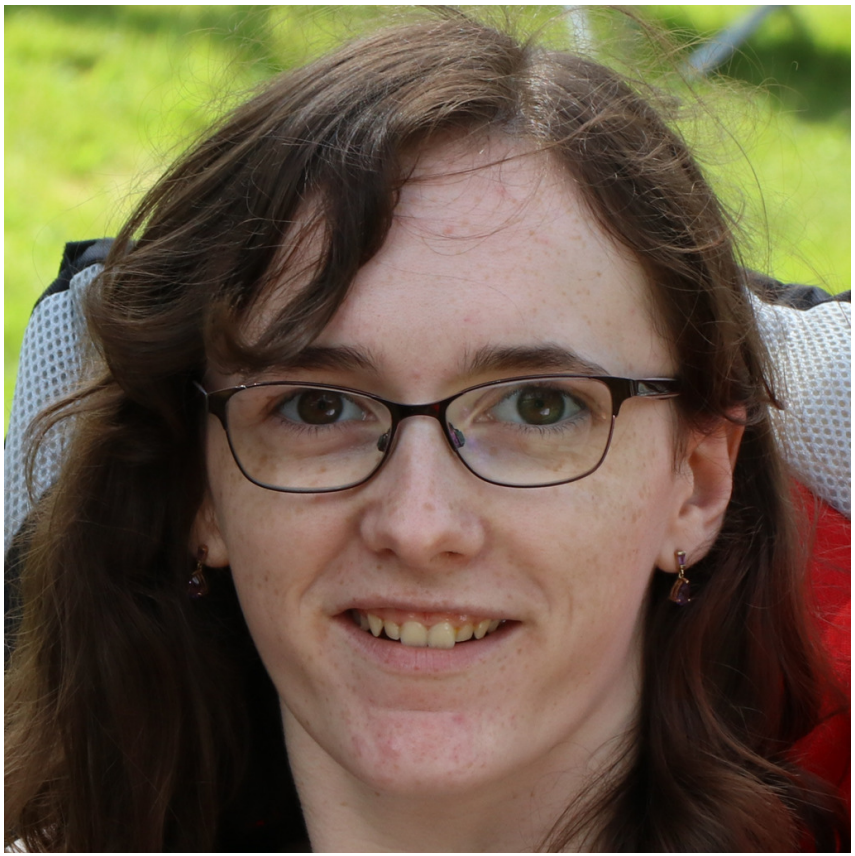
Today's Roadmap

Most of the course was about supervised learning.

Today we'll talk about deep generative models and unsupervised learning.

- Deep auto-regressive models
- Evidence lower bound (ELBO) and variational inference
- Variational auto-encoders
- Generative adversarial networks

Which of these people is real?



(http://www.whichfaceisreal.com)

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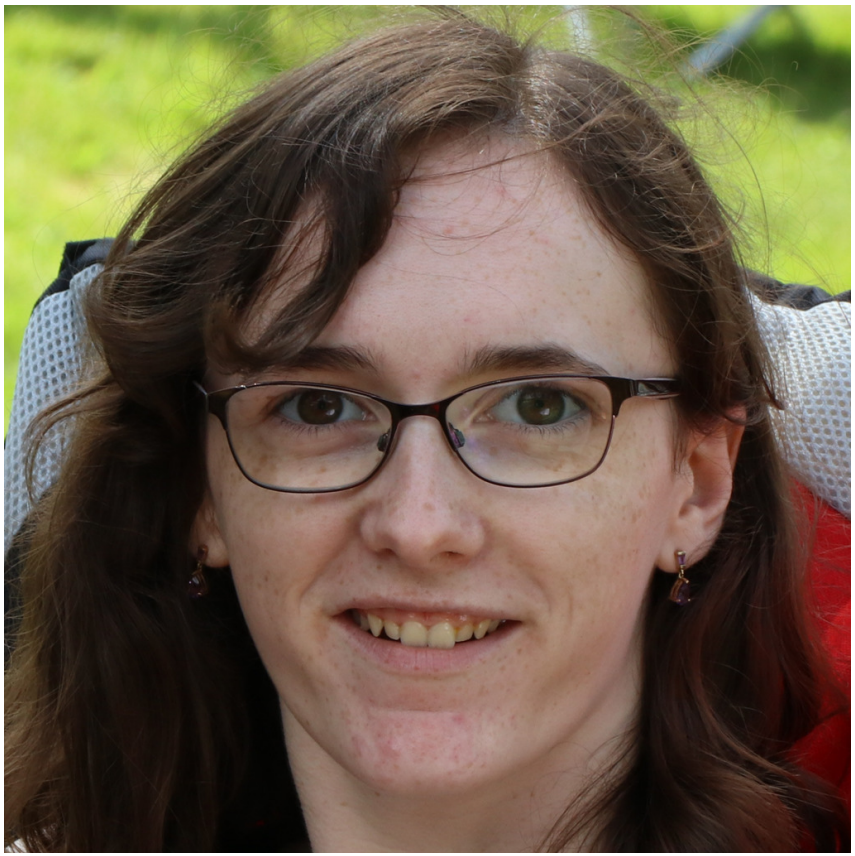

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- Deep generative models are currently making remarkable progress.
- Unsupervised learning: modelling $\mathbb{P}(\boldsymbol{x})$.
- Supervised learning: modelling $\mathbb{P}(\boldsymbol{x}, \boldsymbol{y})$.
- Often, generative models use latent variables $\boldsymbol{h}$, such that

$$\mathbb{P}(\boldsymbol{x}) = \sum_{\boldsymbol{h}} \mathbb{P}(\boldsymbol{x}, \boldsymbol{h}) \quad \text{or} \quad \mathbb{P}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\boldsymbol{h}} \mathbb{P}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{h})$$

  where $\mathbb{P}(\boldsymbol{x}, \boldsymbol{h})$ and $\mathbb{P}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{h})$ are "simple".

Examples of Deep Generative Models

- Auto-regressive networks
- Restricted Boltzmann machines
- Deep belief networks
- Deep Boltzmann machines
- Gaussian-Bernoulli RBMs
- Convolutional Boltzmann machines
- Variational auto-encoders (VAE)
- Generative adversarial networks (GAN)
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Outline

Energy Based Models

- A probability distribution (mixing observed and latent variables) via an energy function $E(\boldsymbol{x}, \boldsymbol{h}; \boldsymbol{\theta})$:

$$\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) = \frac{\exp(-E(\boldsymbol{x}, \boldsymbol{h}; \boldsymbol{\theta}))}{Z(\boldsymbol{\theta})}, \quad \text{where } Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}, \boldsymbol{h}} \exp(-E(\boldsymbol{x}, \boldsymbol{h}; \boldsymbol{\theta}))$$

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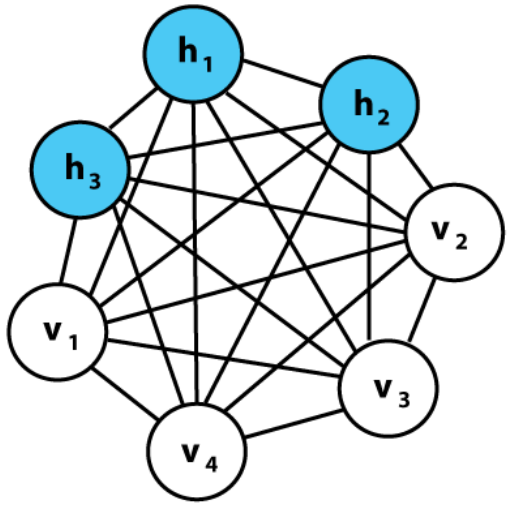
- Maximizing probability corresponds to minimizing the energy.

- Challenges:
  - Computing the partition function $Z(\boldsymbol{\theta})$
  - Computing the evidence $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{\boldsymbol{h}} \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h})$
  - Computing the posterior $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h} \mid \boldsymbol{x}) = \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) / \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})$
  - Sampling from $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h})$ or from $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})$

Boltzmann Machine (Ackley et al., 1985)

- Energy-based model over binary vectors

- Some variables are observed ($\boldsymbol{v}$), others are latent/hidden ($\boldsymbol{h}$)



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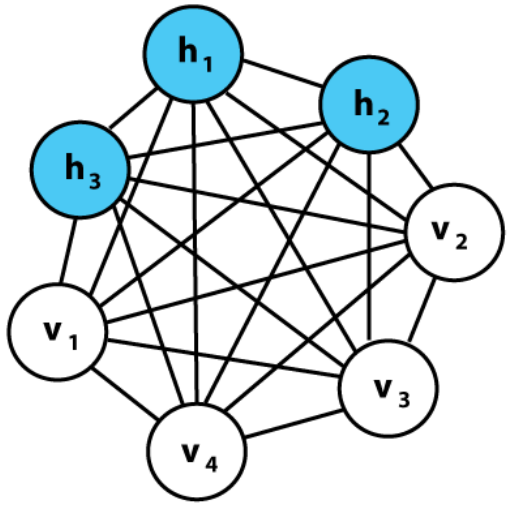

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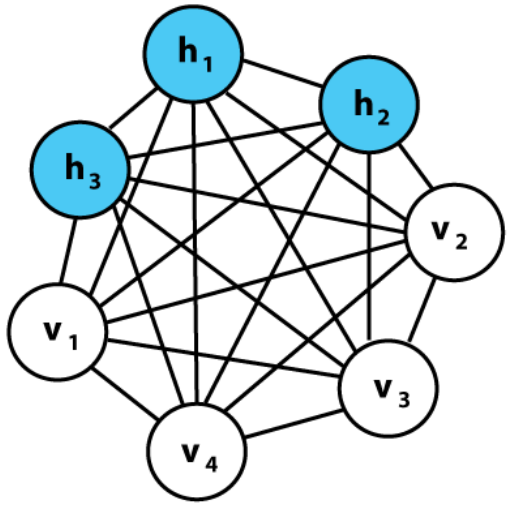

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- Energy function, with $\boldsymbol{\theta} = (\boldsymbol{R}, \boldsymbol{W}, \boldsymbol{S}, b, \boldsymbol{c})$,

$$E(\boldsymbol{v}, \boldsymbol{h}; \boldsymbol{\theta}) = -\boldsymbol{v}^\top \boldsymbol{R} \boldsymbol{v} - \boldsymbol{v}^\top \boldsymbol{W} \boldsymbol{h} - \boldsymbol{h}^\top \boldsymbol{S} \boldsymbol{h} - b^\top \boldsymbol{v} - \boldsymbol{c}^\top \boldsymbol{h}$$

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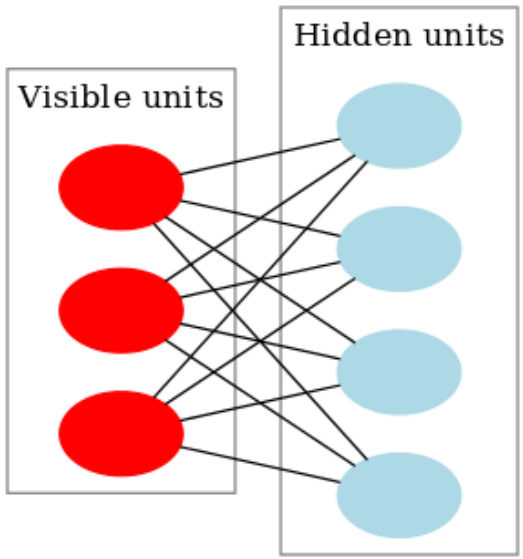
- In summary: learning a general BM is usually very challenging, so we typically use a particular version.
- Not covered here, but check Goodfellow et al. (2016, Chapter 18).

Particular Case: Restricted Boltzmann Machines

- Also called harmonium (Smolensky, 1986)
- A layer of observable variables
- A single layer of latent variables.



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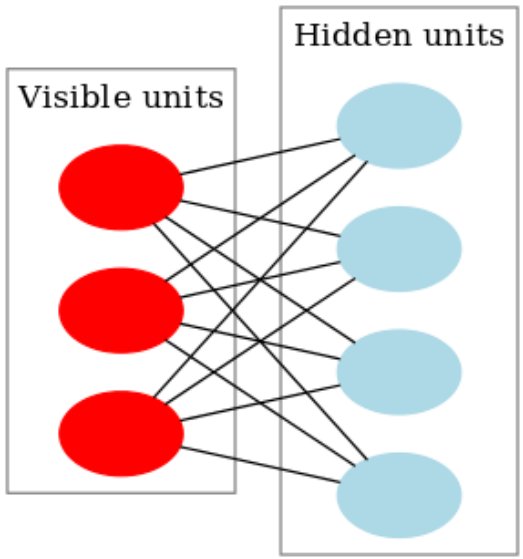

- Bipartite graph, no intra-layer connections: $\boldsymbol{R} = 0$; $\boldsymbol{S} = 0$.
- The energy function becomes:

$$E(\boldsymbol{v}, \boldsymbol{h}; \boldsymbol{\theta}) = -\boldsymbol{v}^\top \boldsymbol{W}\boldsymbol{h} - \boldsymbol{b}^\top \boldsymbol{v} - \boldsymbol{c}^\top \boldsymbol{h}$$

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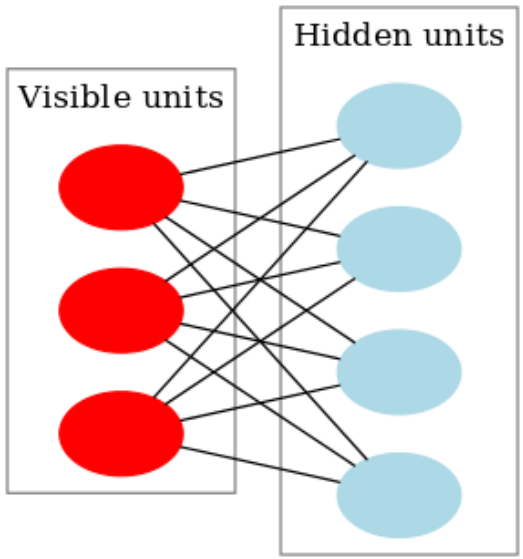

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- What is the advantage?

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- Why are these easy? Conditional independence (next slide)

Restricted Boltzmann Machines

- Without intra-layer connections, $h_1, \ldots, h_N$ are conditionally independent given $\boldsymbol{v}$:

$$\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h} \mid \boldsymbol{v}) = \prod_{j=1}^{M} \mathbb{P}(h_j \mid \boldsymbol{v})$$

where

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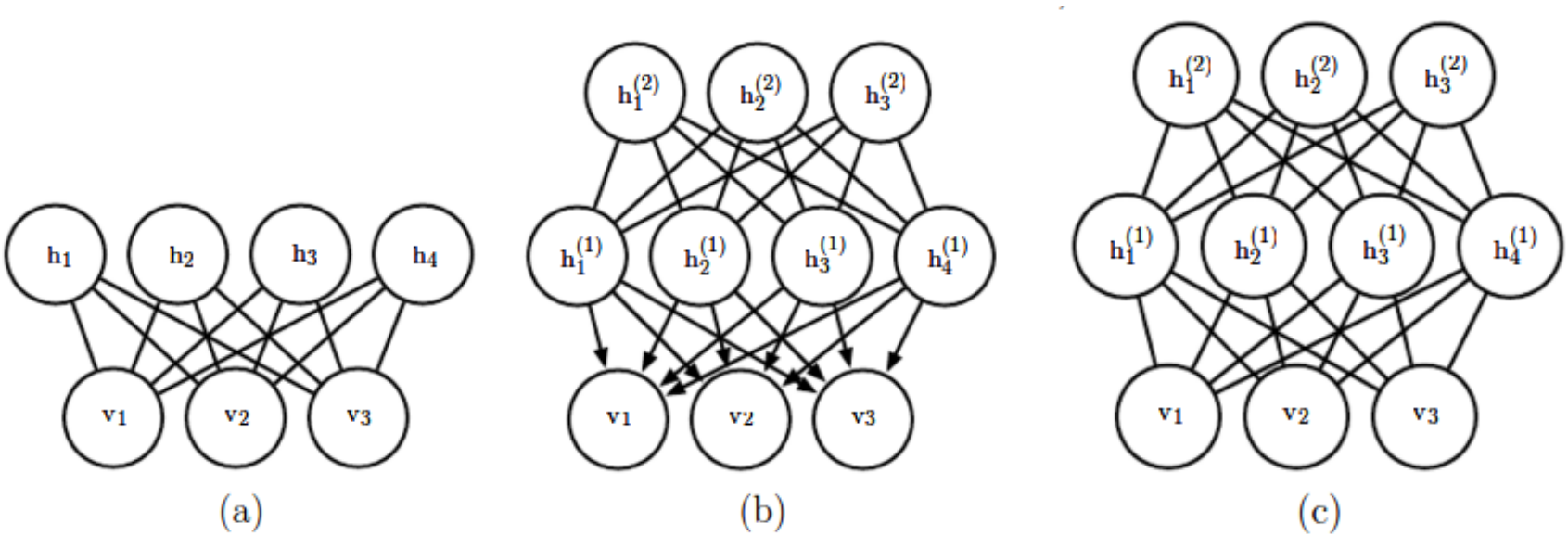
- RBMs may be stacked to form deeper models.

Some RBM's Friends



(Image from Goodfellow et al. (2016))

(a) Restricted Boltzmann machine (RBM)

(b) Deep belief network (DBN): hybrid directed/undirected GM with multiple latent layers

(c) Deep Boltzmann machine (DBM): undirected GM with several layers of latent variables.

Examples of Deep Generative Models

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- This idea underlies
  - Variational auto-encoders (VAE)
  - Generative adversarial networks (GAN)

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- Key idea: combine auto-encoders with variational inference.

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- Next: using variational inference to approximate these computations

Outline

Recap: Shannon's Entropy

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- Intuition: $H(\mathbb{P})$ measures how close to uniform the distribution is
- Coding perspective: expected number of bits (using $\log_2$) to optimally encode $\boldsymbol{x} \sim \mathbb{P}(\boldsymbol{x})$

Recap: Kullback-Leibler (KL) Divergence

- Let $\mathbb{P}$ and $\mathbb{Q}$ be two distributions over $\mathcal{X}$.

$$KL(\mathbb{P}\|\mathbb{Q}) = \sum_{\boldsymbol{x}} \mathbb{P}(\boldsymbol{x}) \log \frac{\mathbb{P}(\boldsymbol{x})}{\mathbb{Q}(\boldsymbol{x})}$$

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$$\begin{aligned} KL(\mathbb{P}\|\mathbb{Q}) &= \sum_{\boldsymbol{x}} \mathbb{P}(\boldsymbol{x}) \log \frac{\mathbb{P}(\boldsymbol{x})}{\mathbb{Q}(\boldsymbol{x})} \\ &= \mathbb{E}_{\mathbb{P}(\boldsymbol{x})}\big[-\log \mathbb{Q}(\boldsymbol{x})\big] + \mathbb{E}_{\mathbb{P}(\boldsymbol{x})}\big[\log \mathbb{P}(\boldsymbol{x})\big] \end{aligned}$$

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- Old roots in calculus of variations (Euler, Lagrange, ...)

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- Which values of $\boldsymbol{h}$ is $\mathbb{Q}(\boldsymbol{h})$ encouraged to place its mass on?
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- ELBO mirrors the Bayesian trade-off between likelihood and prior.

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- Structured mean field: imposes a graphical model on $\mathbb{Q}$ capturing (some) interactions among the h_i, but still tractable. (Wainwright and Jordan, 2008).

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- Alternative: amortized variational inference!

- Key idea: instead of optimizing $\mathbb{Q}(\boldsymbol{h})$ for every example, use an encoder with shared parameters $\boldsymbol{\phi}$ and define $\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})$.

  For each example:

  - make a forward pass on the encoder to obtain $\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})$
  - backpropagate through the encoder to update $\boldsymbol{\phi}$.

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- Approximate the posterior with a variational distribution

$$\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \mathcal{N}(\boldsymbol{h}; \boldsymbol{\mu}(\boldsymbol{x}; \boldsymbol{\phi}), \boldsymbol{\sigma}^2(\boldsymbol{x}; \boldsymbol{\phi}))$$

  where $\boldsymbol{\mu}(\boldsymbol{x}; \boldsymbol{\phi})$ and $\boldsymbol{\sigma}^2(\boldsymbol{x}; \boldsymbol{\phi})$ are (learned) MLPs

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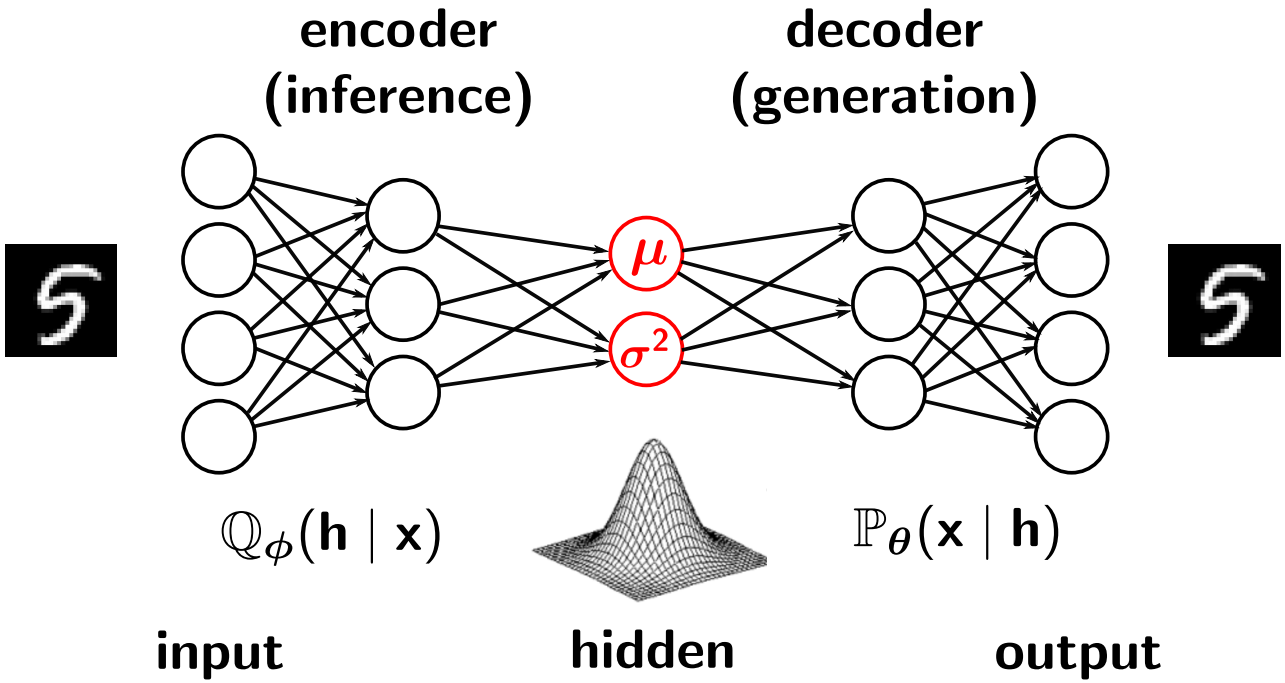
- This leads to variational auto-encoders:



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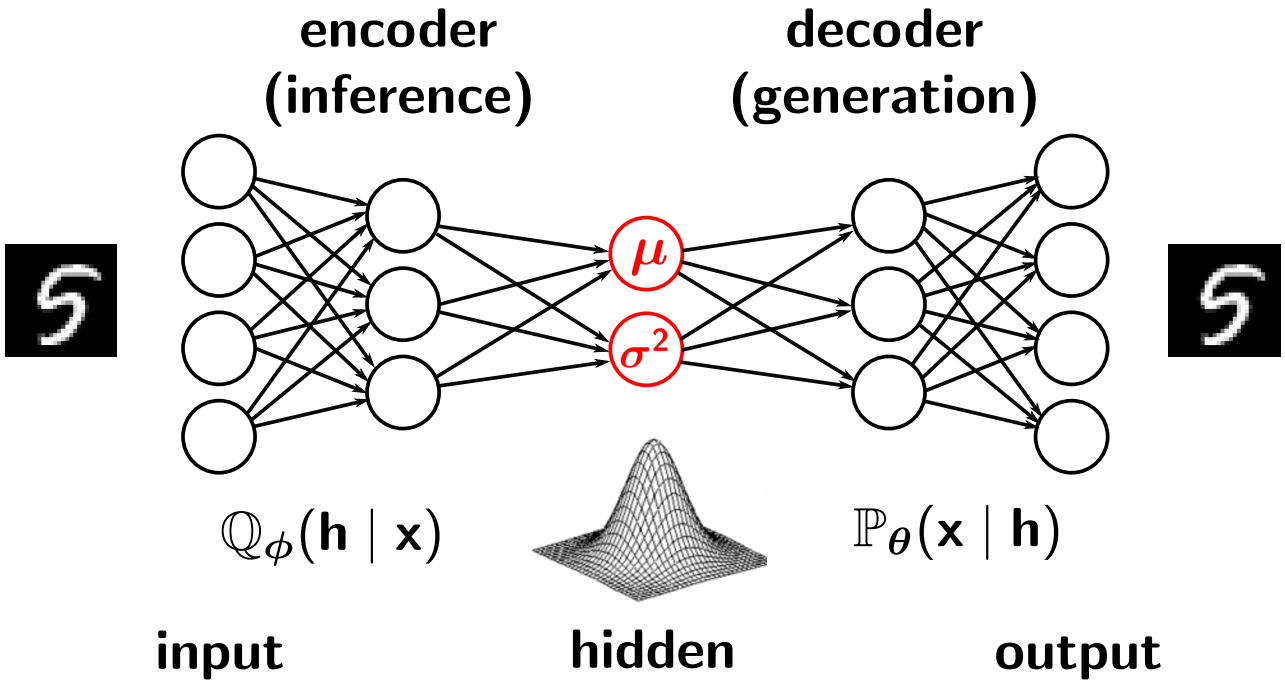

- ... we will come back to this!

Outline

Parameter Gradients

- Recall that:

$$\text{ELBO}(\boldsymbol{\phi}; \boldsymbol{\theta}) = \mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})}[\log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})].$$

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- We need to compute gradients with respect to $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$.

- Gradient w.r.t. $\boldsymbol{\theta}$, parameters of the generation (decoder) network:

$$\nabla_{\boldsymbol{\theta}} \text{ELBO}(\boldsymbol{\phi}; \boldsymbol{\theta}) = \mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})}[\nabla_{\boldsymbol{\theta}} \log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h})]$$

  - Follows from linearity of the expectation.

  - This is simple and can be well approximated with Monte Carlo samples.

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(derivation in the next slide)

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(derivation in the next slide)

  - High variance of Monte Carlo estimates due to the left part!
  - Requires variance reduction techniques.

Derivation of the Inference Network Gradient

$$
\begin{aligned}
&\nabla_{\boldsymbol{\phi}} \text{ELBO}(\boldsymbol{\phi}; \boldsymbol{\theta}) \\
&= \nabla_{\boldsymbol{\phi}} \mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})} \Big[\log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \Big] \\
&= \nabla_{\boldsymbol{\phi}} \sum_{\boldsymbol{h}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \nabla_{\boldsymbol{\phi}} \sum_{\boldsymbol{h}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \\
&= \sum_{\boldsymbol{h}} \log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) \nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) - \sum_{\boldsymbol{h}} (1 + \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})) \nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \\
&= \sum_{\boldsymbol{h}} \Big[\log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \Big] \nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \\
&= \mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})} \Big[(\log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})) \, \nabla_{\boldsymbol{\phi}} \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \Big],
\end{aligned}
$$

where we used the facts:

$$
\sum_{\boldsymbol{h}} \nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \nabla_{\boldsymbol{\phi}} \sum_{\boldsymbol{h}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \nabla_{\boldsymbol{\phi}} 1 = 0.
$$

$$
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- ... the Monte Carlo approximation has large variance.
- Is there a better strategy?
- Yes: the reparameterization trick.

Reparameterization Trick (Kingma and Welling, 2013)

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- Consequently, for any function f,

$$\mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})}[f(\boldsymbol{h})] \approx \frac{1}{N} \sum_{i=1}^{N} f(\boldsymbol{g}_{\boldsymbol{\phi}}(\boldsymbol{x}, \boldsymbol{\epsilon}^{(i)}))$$

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- $\nabla_{\boldsymbol{\phi}}$ can be estimated with regular backpropagation over $\boldsymbol{g}_{\boldsymbol{\phi}}$.

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- This is possible in many cases for continuous latent variables:
  - exponential
  - Gaussian
  - location-scale families
  - log-normal
  - etc...

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- This is possible in many cases for continuous latent variables:
  - exponential
  - Gaussian
  - location-scale families
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  - etc...
- For discrete latent variables, it is still possible via the Gumbel-softmax trick (not covered in the course).

Example: Gaussian

1. Sample d-variate standard Gaussian $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}; 0, \boldsymbol{I})$

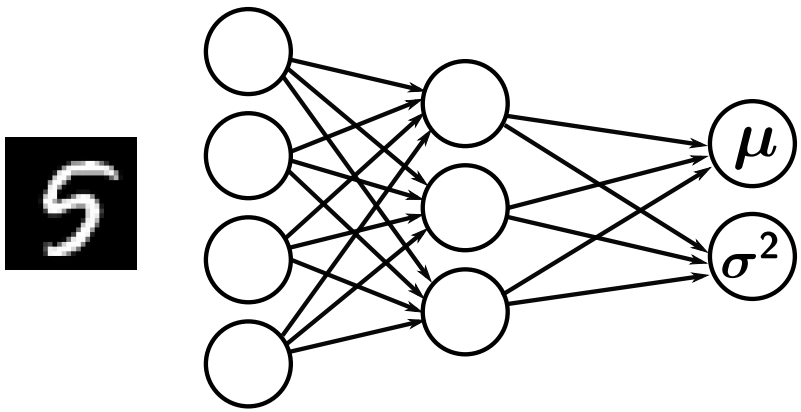
2. Use inference network $\boldsymbol{g}_\phi$ with input $\boldsymbol{x}$ to output:

   - mean $\boldsymbol{\mu}(\boldsymbol{x})$
   - component-wise variance $\boldsymbol{\sigma}^2(\boldsymbol{x}) = \text{diag}[\sigma_1^2(\boldsymbol{x}), ..., \sigma_d^2(\boldsymbol{x})]$

3. Set $\boldsymbol{h} = \boldsymbol{\mu}(\boldsymbol{x}) + \boldsymbol{\epsilon} \odot \sqrt{\sigma^2(\boldsymbol{x})}$.

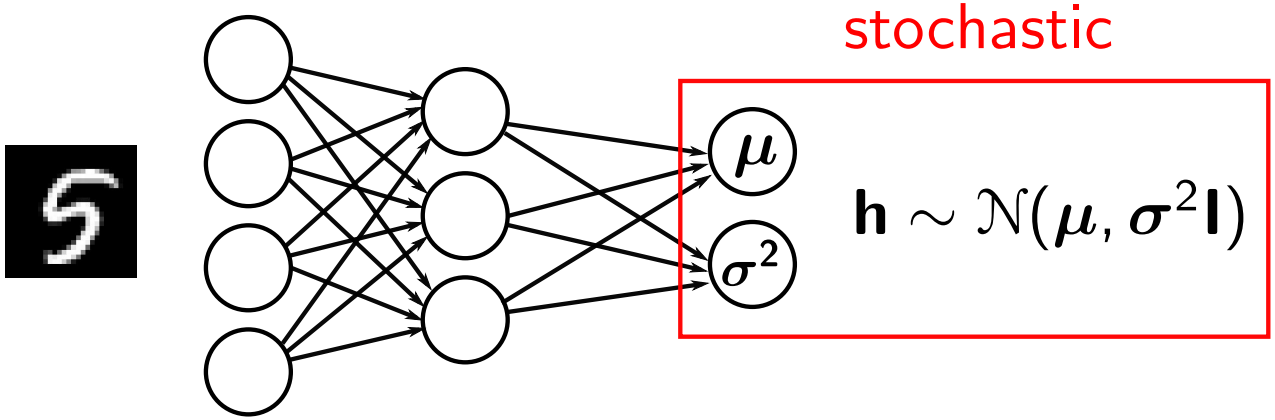
4. Thus, $\boldsymbol{h} \mid \boldsymbol{x} \sim \mathcal{N}\big(\boldsymbol{\mu}(\boldsymbol{x}), \boldsymbol{\sigma}^2(\boldsymbol{x})\big)$

Reparameterization Trick



$$\mathbf{h} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma}^2 \mathbf{I})$$

Reparameterization Trick



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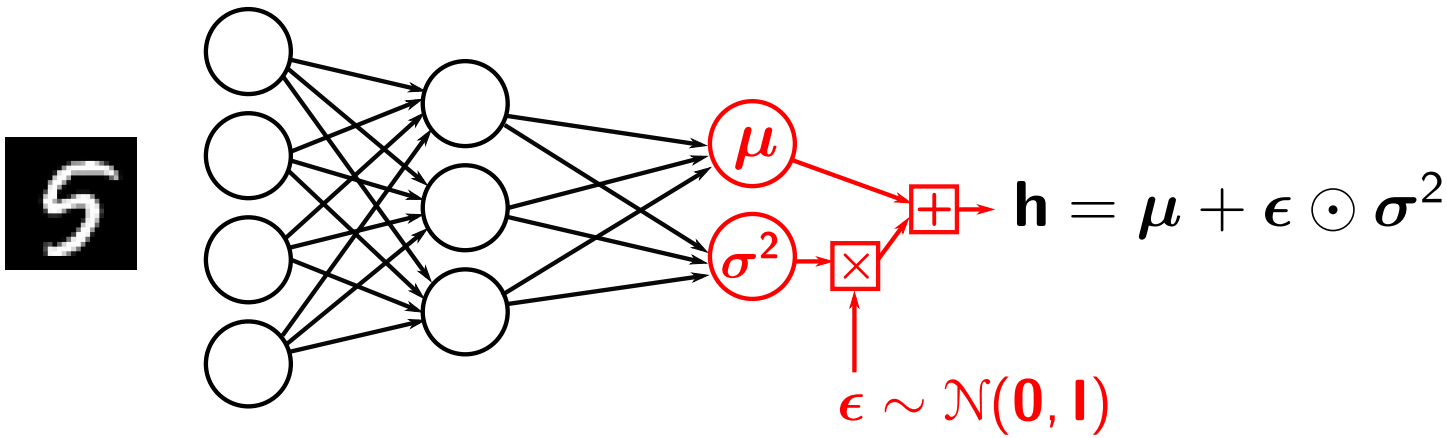

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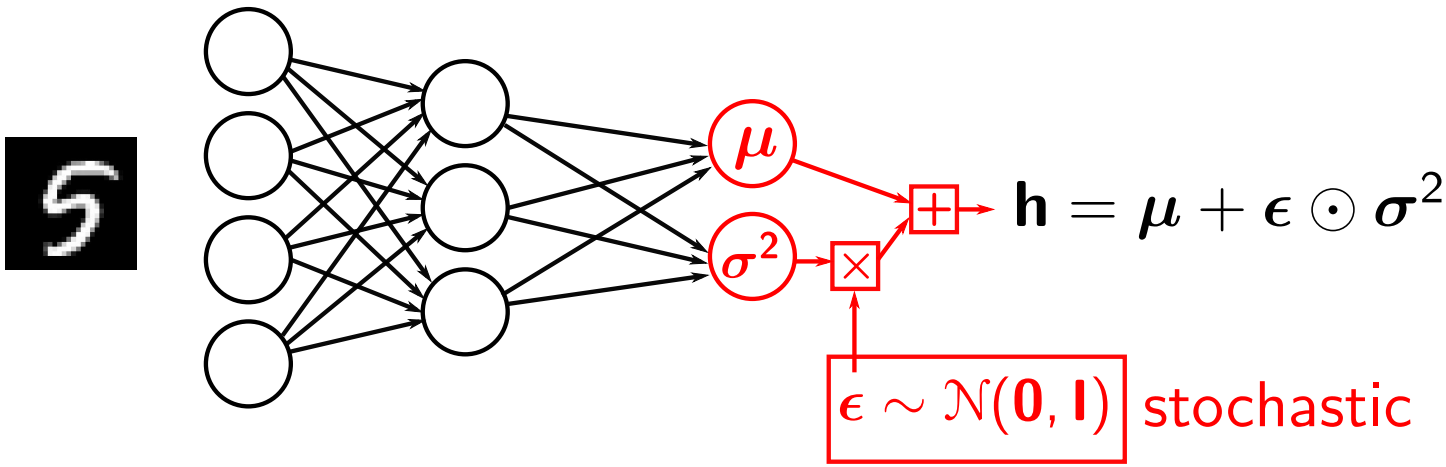

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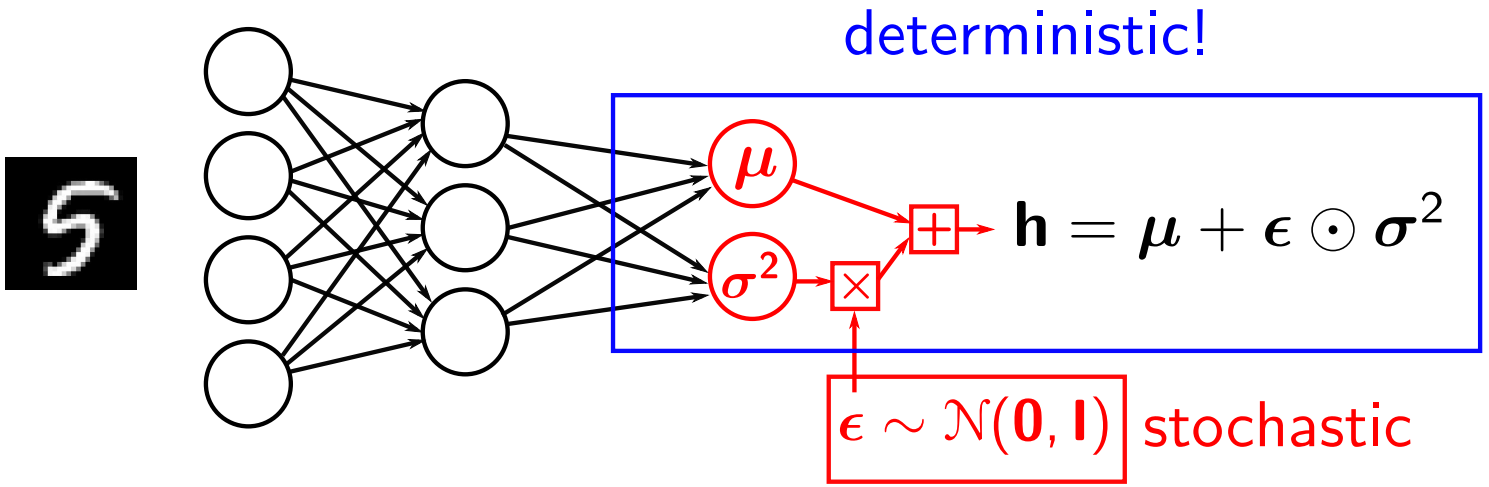
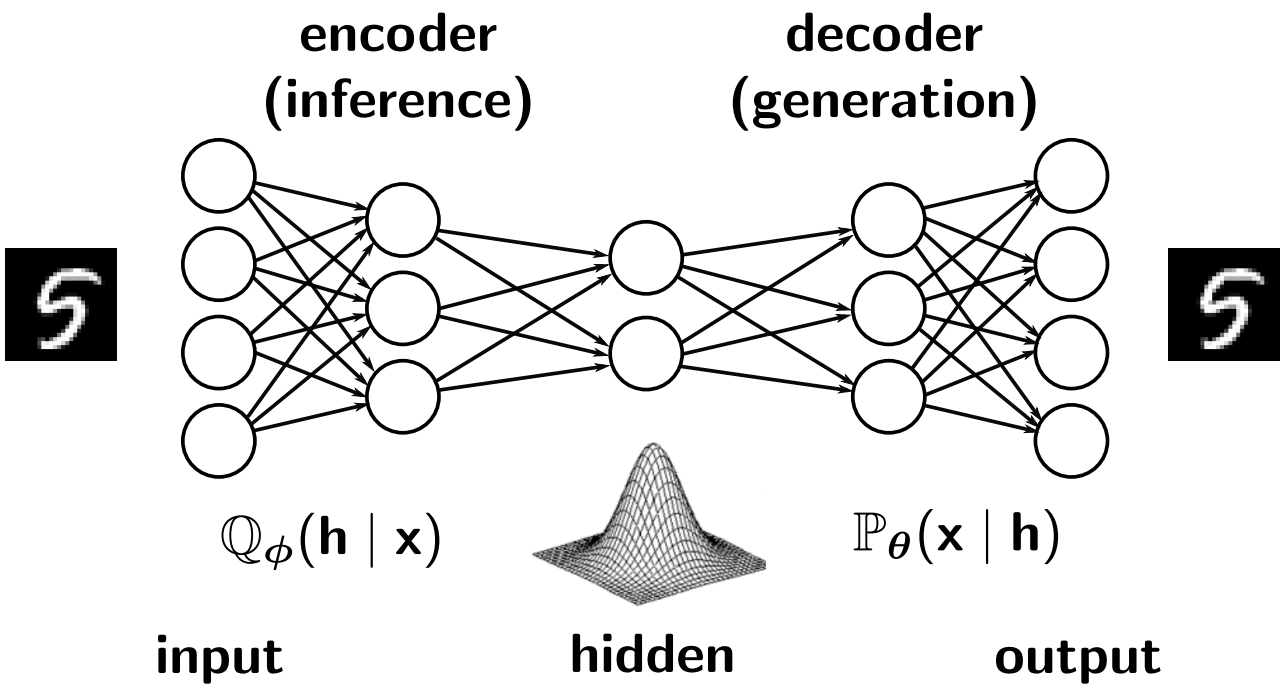


Variational Auto-Encoders (Kingma and Welling, 2013)



- Decoder computes $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h})$ and $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{h})$
- Encoder computes $\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \mathcal{N}(\boldsymbol{h}; \boldsymbol{\mu}_{\boldsymbol{\phi}}(\boldsymbol{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\phi}}(\boldsymbol{x}))$
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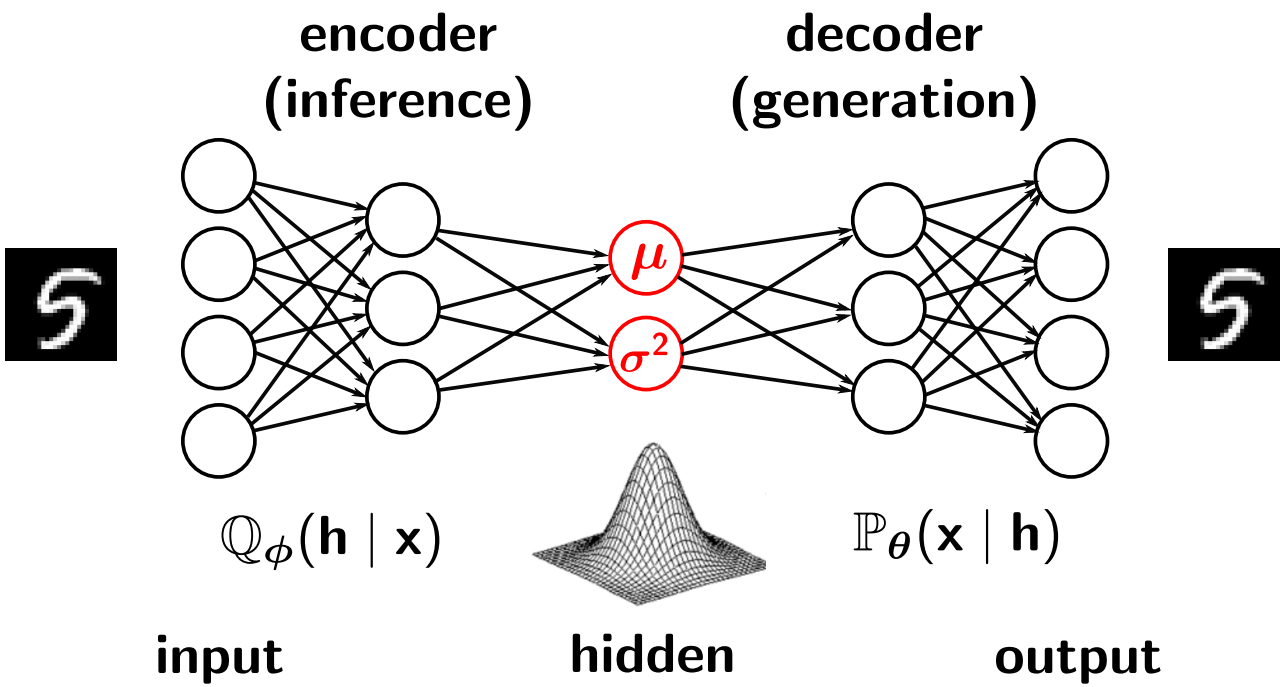

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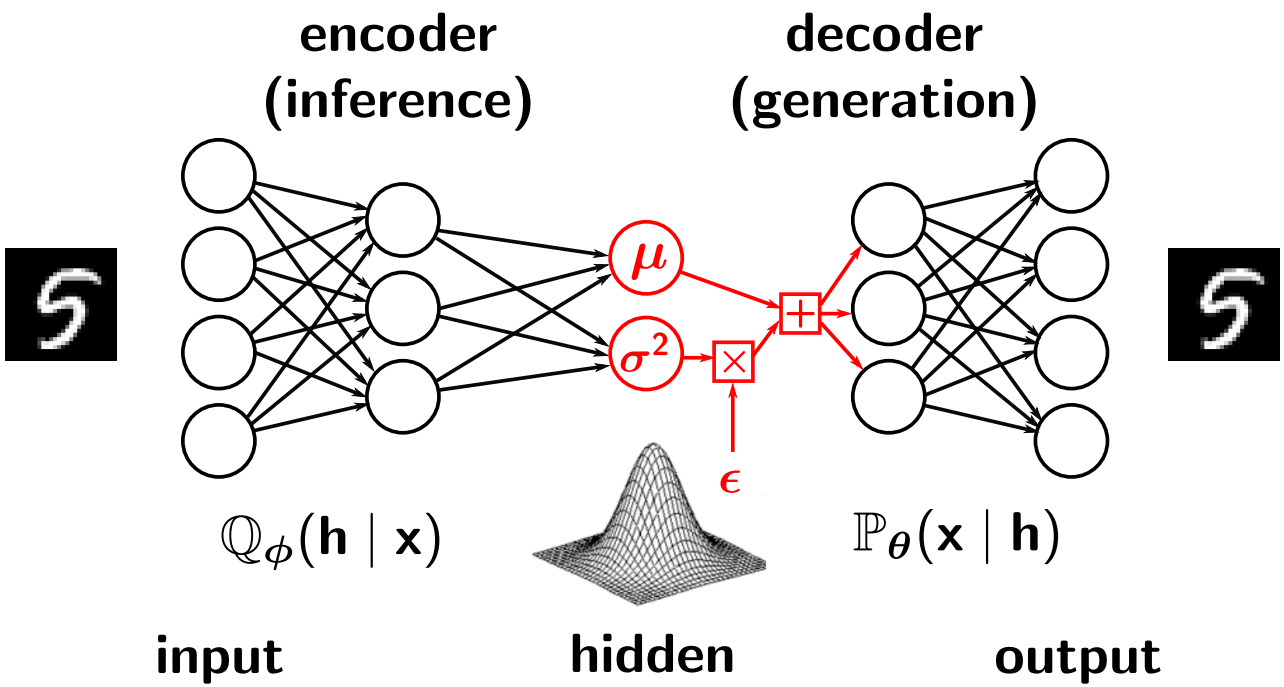

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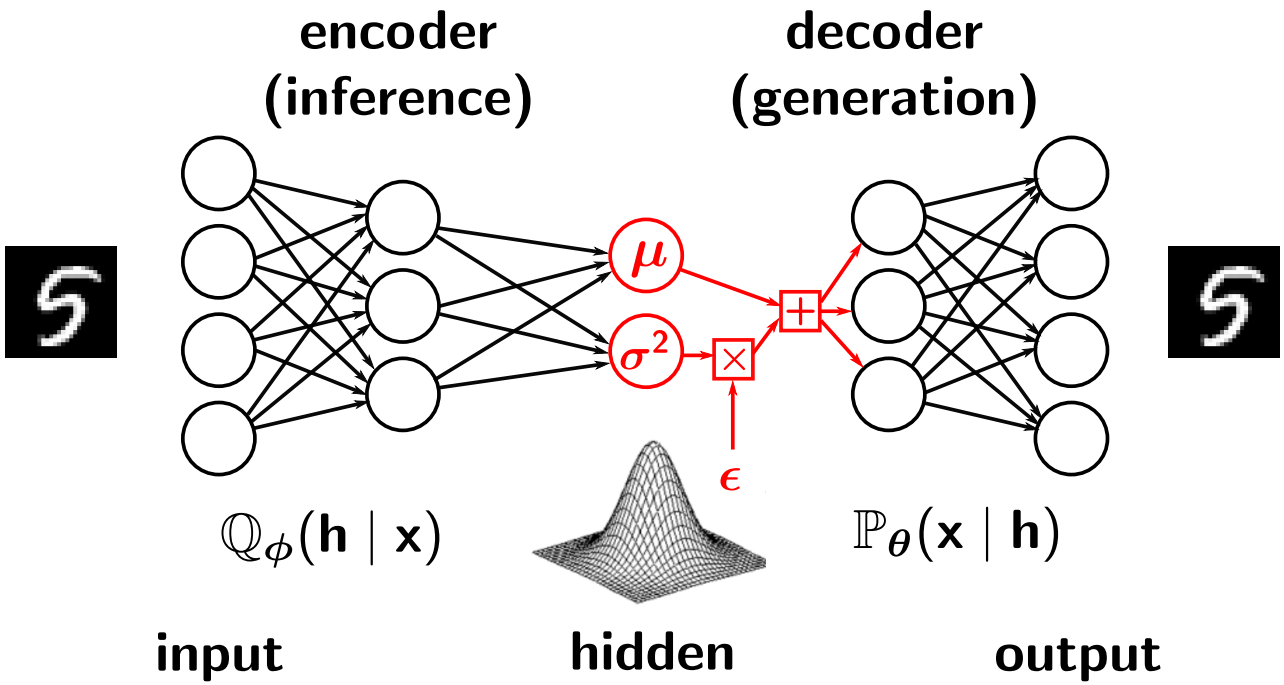
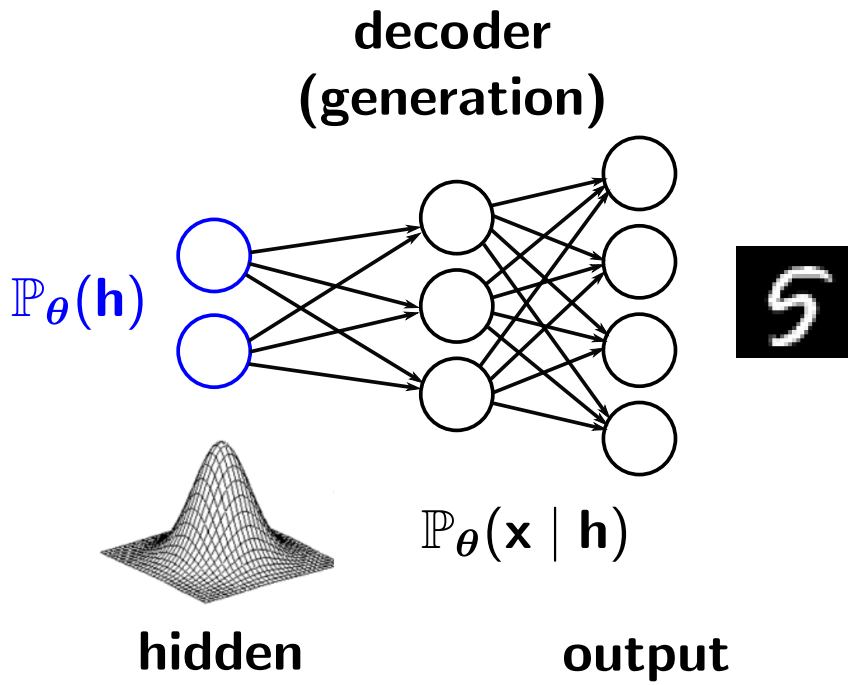
Summing Up: VAEs at Training Time



Summing Up: VAEs at Test Time



What is the Latent Variable Representing?

- Nice property of VAE: simultaneously training a parametric encoder in combination with a generator network forces the model to learn a predictable coordinate system that the encoder can capture.
- This makes it an excellent manifold learning algorithm.
- Example: the algorithm discovered two independent factors of variation present in images of faces: angle of rotation and emotional expression.

What is the Latent Variable Representing?

From Kingma and Welling (2013).

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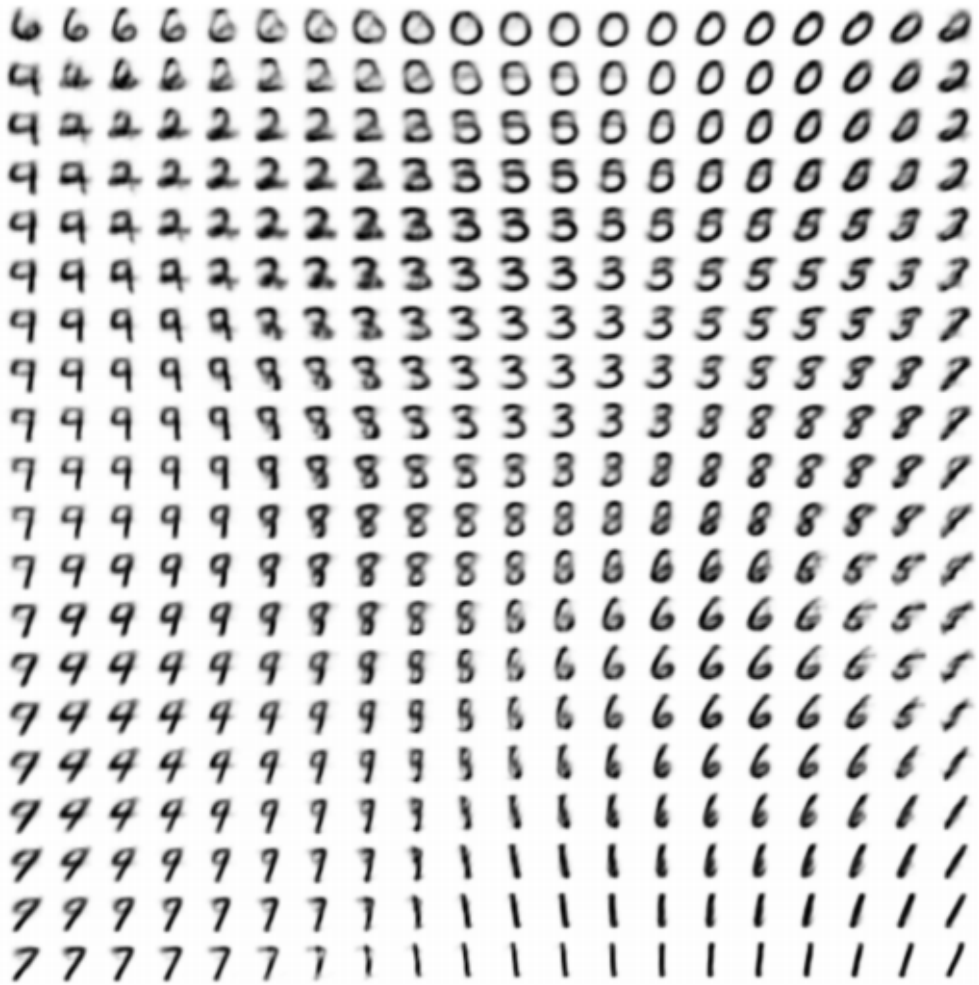

(b) Learned MNIST manifold

From Kingma and Welling (2013).

Issues with VAEs

- Posterior collapse: if the generative part is strong, the model may learn to ignore the latent variables:

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- Can be mitigated with a few tricks:
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  - Combine stochastic and amortized inference.

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  - Use auxiliary losses
  - Combine stochastic and amortized inference.
- In general, reporting both reconstruction loss and the KL term is needed to assess if the model makes use of the latent variables.

Examples of Deep Generative Models

- Auto-Regressive Networks ✓
- Restricted Boltzmann Machines ✓
- Deep Belief Networks
- Deep Boltzmann Machines
- Gaussian-Bernoulli RBMs
- Convolutional Boltzmann Machines
- Sigmoid Belief Nets
- Variational Auto-Encoders ✓
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Outline

Why Maximum Likelihood?

- All models discussed aim to maximize the likelihood (evidence) $\mathbb{P}(\boldsymbol{x})$
- In fact, since this is intractable, they maximize a lower bound (ELBO)
- But if we want to build a generator, is this really the best criterion?
- Maximum likelihood tends to produce blurry images

Generative Adversarial Networks (GANs) (Goodfellow et al., 2014)

- **Key idea:**
  - keep the generation network $G = \{\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h}), \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{h})\}$
  - drop the inference network: use a discriminator network $D : \mathcal{X} \to \{0, 1\}$

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- Sort of like a Turing test: distinguish artificial from real.

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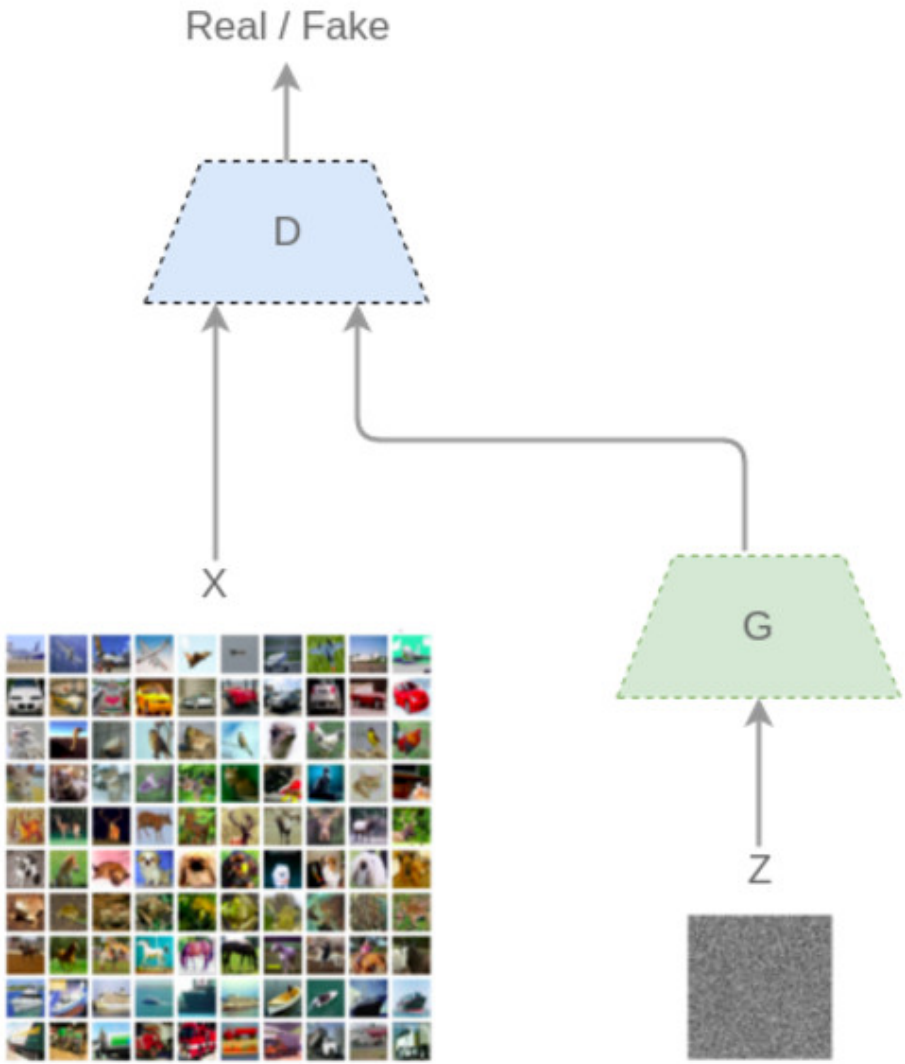

Minimax Game

- Saddle point problem:

$$\min_G \max_D V(D, G) = \mathbb{E}_{\mathbb{P}_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h})}[\log(1 - D(G(\boldsymbol{h})))].$$

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- The optimal generator $G^\star$ minimizes the Jensen-Shannon divergence between $\mathbb{P}_{\text{data}}(\boldsymbol{x})$ and $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})$:

$$JS(\mathbb{P}_{\text{data}}(\boldsymbol{x}), \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})) = \frac{1}{2} KL\left(\mathbb{P}_{\text{data}}(\boldsymbol{x}) \| \bar{\mathbb{P}}(\boldsymbol{x})\right) + \frac{1}{2} KL\left(\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}) \| \bar{\mathbb{P}}(\boldsymbol{x})\right),$$

where $\bar{\mathbb{P}}(\boldsymbol{x}) = \frac{\mathbb{P}_{\text{data}}(\boldsymbol{x}) + \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})}{2}$.

Wasserstein GANs (WGANs)

- Find the saddle point ($\min_G \max_D$) of

$$V(D, G) \quad = \quad \mathbb{E}_{\boldsymbol{x} \sim \mathbb{P}_{\text{data}}(\boldsymbol{x})}[D(\boldsymbol{x})] - \mathbb{E}_{\boldsymbol{h} \sim \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h})}[D(G(\boldsymbol{h}))].$$

- This is related to the Wasserstein distance (also called Earth mover's distance).

- A technical condition is that ∇D is bounded; in practice this is ensured with gradient clipping.

- This improves stability and mitigates the mode collapse problem.

Training GANs

- Use stochastic gradient descent! Alternate between:
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- Several variants and schedules have been proposed.
- Caveats:
  - no convergence guarantees
  - optimization in GANs is often difficult

Images Generated by GANs

(https://tryolabs.com/blog/2016/12/06/major-advancements-deep-learning-2016/)

Remarkable Improvement from 2014 to 2017

Ian Goodfellow
@goodfellow_ian

Follow

4 years of GAN progress (source: eff.org/files/2018/02/ …)

2014

2015

2016

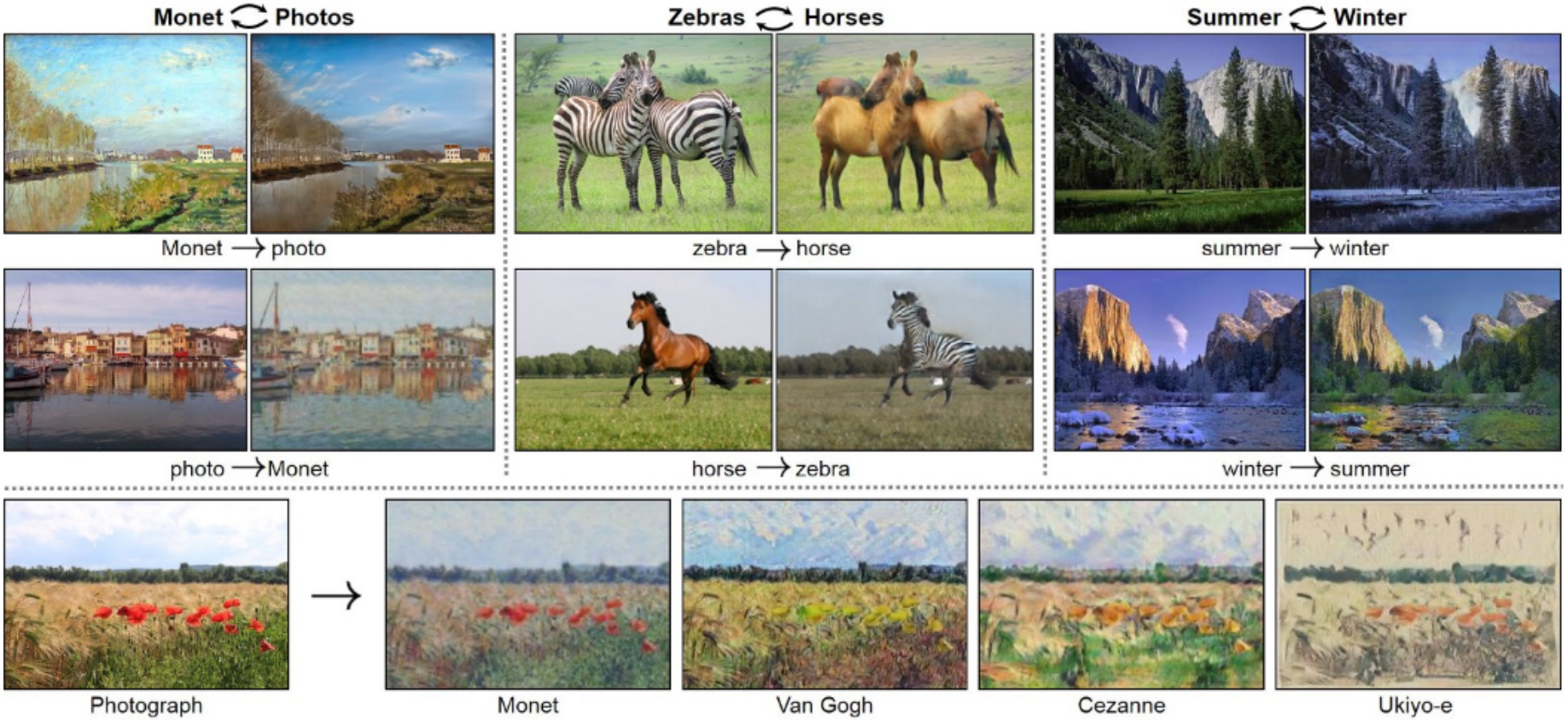
2017

7:26 PM - 2 Mar 2018

Some Extensions of GANs

- Augmenting GANs with an inference network (Dumoulin et al., 2016; Donahue et al., 2016)
- Domain adversarial training for domain adaptation (Ganin et al., 2016)
- Conditional GANs and semi-supervised GANs (Salimans et al., 2016)
- CycleGAN (Zhu et al., 2017): "translate" images from a source domain $\mathcal{X}$ to a target domain $\mathcal{Y}$ without paired examples. Use two generators $G : \mathcal{Y} \rightarrow \mathcal{X}$ and $F : \mathcal{X} \rightarrow \mathcal{Y}$ and introduce a **cycle consistency loss** to push $F(G(\boldsymbol{y})) \approx \boldsymbol{y}$ and $G(F(\boldsymbol{x})) \approx \boldsymbol{x}$.

Image-to-Image Translation with CycleGAN (Zhu et al., 2017)



(https://junyanz.github.io/CycleGAN)

Failure Cases

(https://junyanz.github.io/CycleGAN)

Examples of Deep Generative Models

- Auto-Regressive Networks ✓
- Restricted Boltzmann Machines ✓
- Deep Belief Networks
- Deep Boltzmann Machines
- Gaussian-Bernoulli RBMs
- Convolutional Boltzmann Machines
- Sigmoid Belief Nets
- Variational Auto-Encoders ✓
- Generative Adversarial Networks ✓
- Denoising diffusion models

Examples of Deep Generative Models

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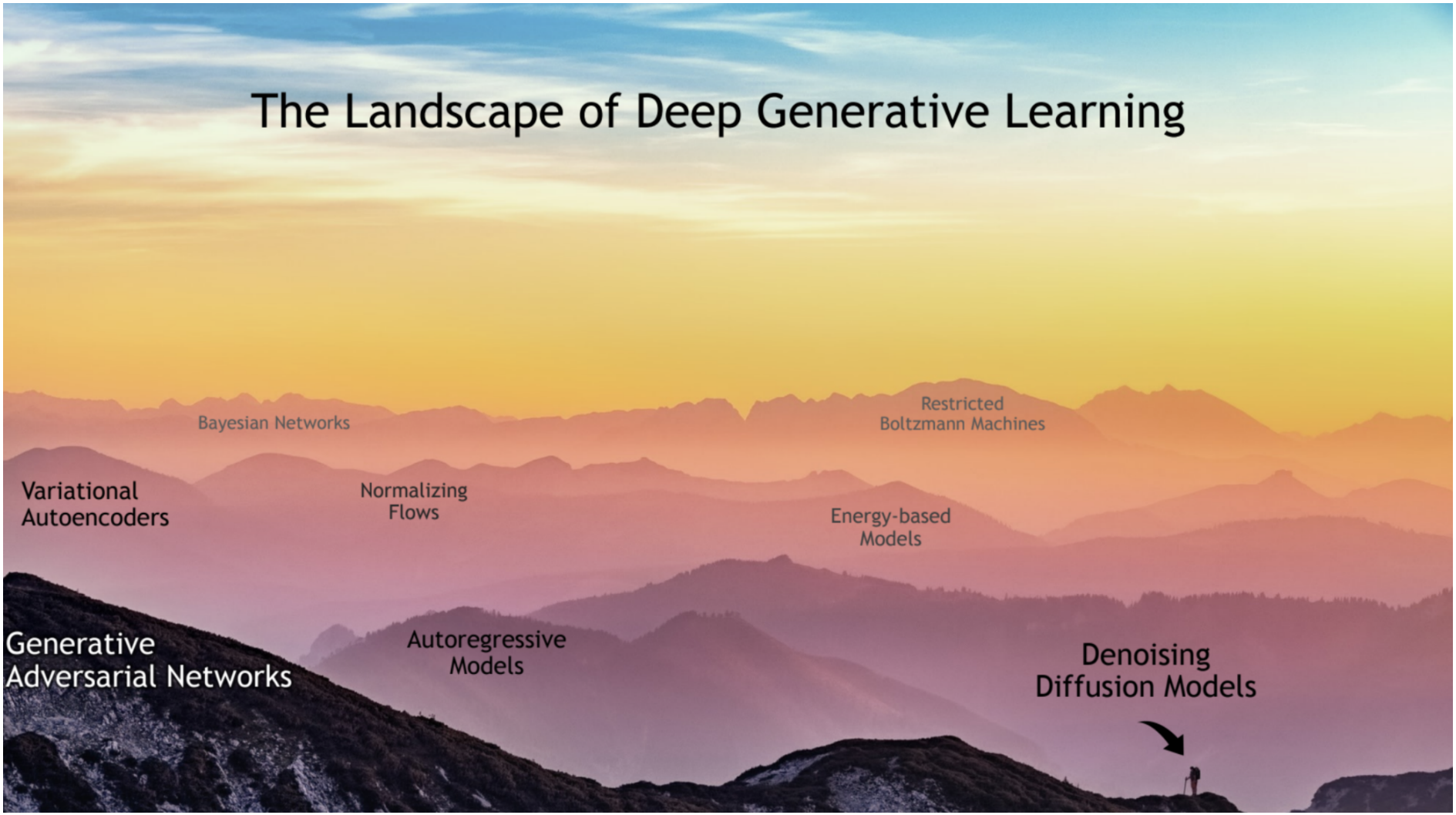
Outline

Denoising Diffusion Models

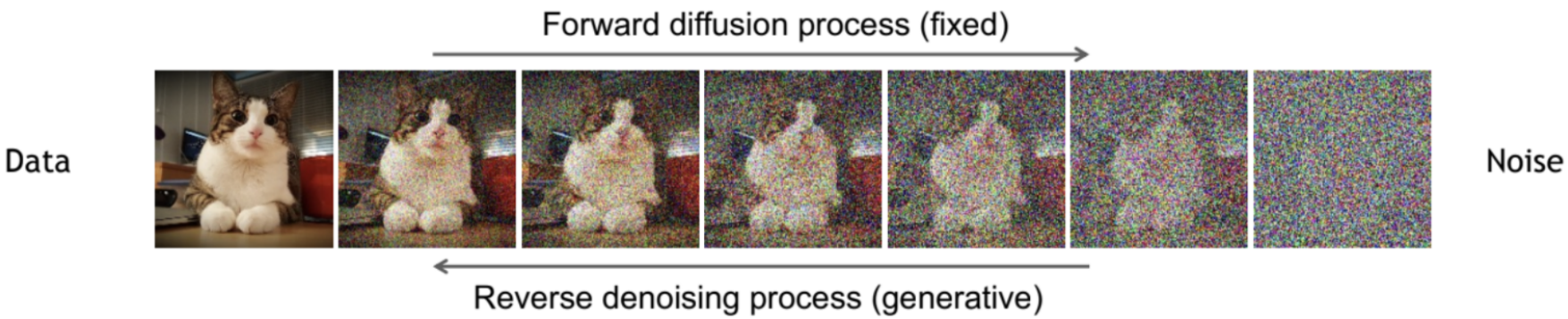


This and the next 10 slides: Diffusion Models Tutorial, CVPR2023, J. Song, C. Meng, A. Vahdat. `https://cvpr2023-tutorial-diffusion-models.github.io/`

Denoising Diffusion Models: Basic Idea

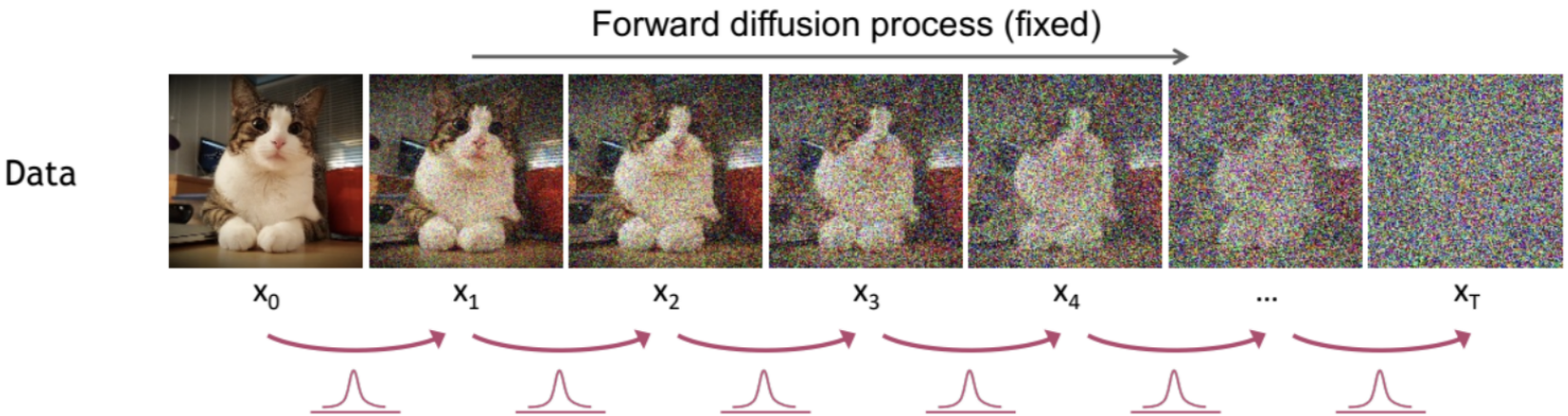
Denoising diffusion models consist of two processes:

- Forward diffusion process that gradually adds noise to input
- Reverse denoising process that learns to generate data by denoising



Forward Diffusion

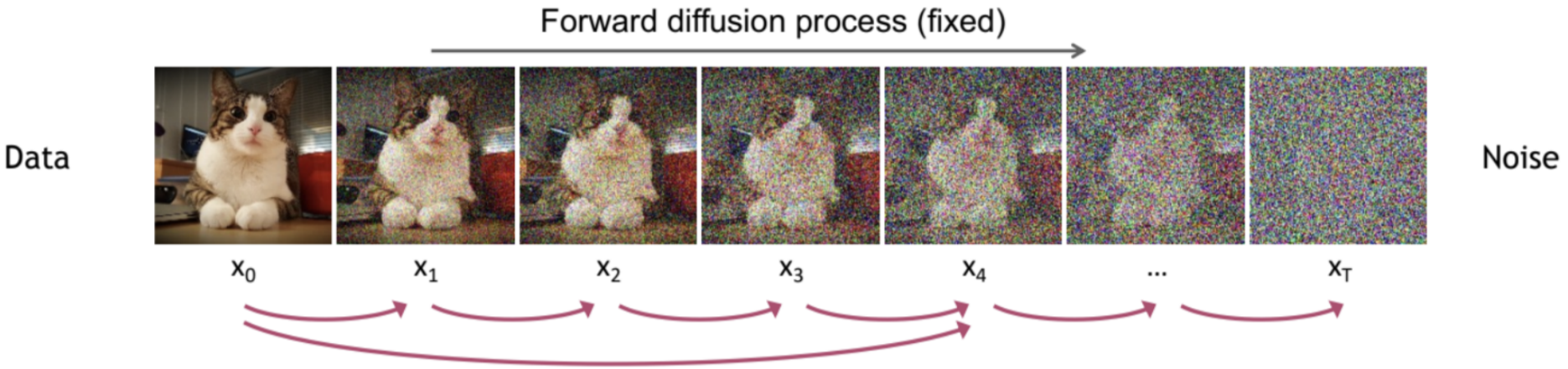
The formal definition of the forward process in T steps:



$$q(\mathbf{x}_t|\mathbf{x}_{t-1}) = \mathcal{N}(\mathbf{x_t}; \sqrt{1-\beta_t}\mathbf{x_{t-1}}, \beta_t\mathbf{I}) \quad \Rightarrow \quad q(\mathbf{x}_{1:T}|\mathbf{x}_0) = \prod_{t=1}^{T} q(\mathbf{x}_t|\mathbf{x}_{t-1}) \qquad \text{(joint)}$$

14

Diffusion Kernel



Define $\bar{\alpha}_t = \prod_{s=1}^{t}(1-\beta_s)$ ➡ $q(\mathbf{x}_t|\mathbf{x}_0) = \mathcal{N}(\mathbf{x}_t; \sqrt{\bar{\alpha}_t}\mathbf{x}_0, (1-\bar{\alpha}_t)\mathbf{I}))$ (Diffusion Kernel)

For sampling: $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\,\epsilon$ where $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

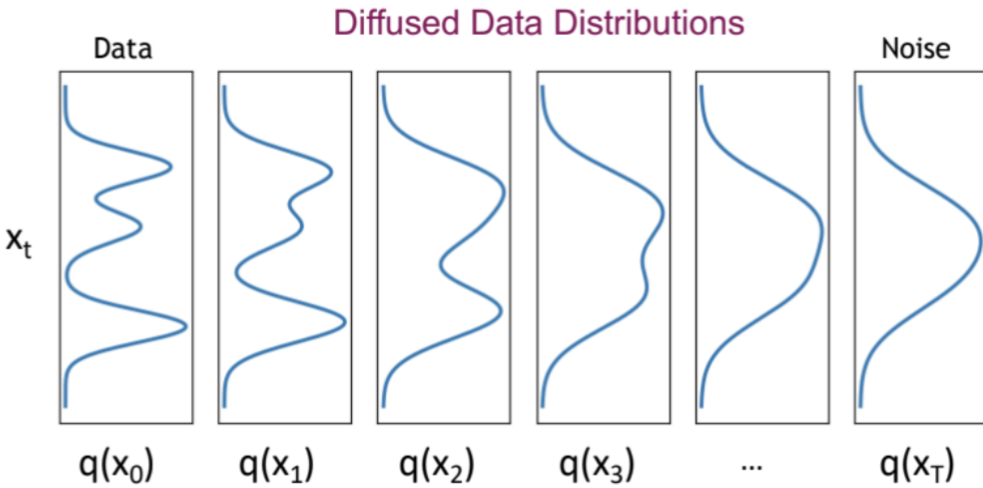
β_t values schedule (i.e., the noise schedule) is designed such that $\bar{\alpha}_T \to 0$ and $q(\mathbf{x}_T|\mathbf{x}_0) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

Diffusions are Convolutions

So far, we discussed the diffusion kernel $q(\mathbf{x}_t|\mathbf{x}_0)$ but what about $q(\mathbf{x}_t)$?

$$\underbrace{q(\mathbf{x}_t)}_{\text{Diffused data dist.}} = \int \underbrace{q(\mathbf{x}_0, \mathbf{x}_t)}_{\text{Joint dist.}} d\mathbf{x}_0 = \int \underbrace{q(\mathbf{x}_0)}_{\text{Input data dist.}} \underbrace{q(\mathbf{x}_t|\mathbf{x}_0)}_{\text{Diffusion kernel}} d\mathbf{x}_0$$

The diffusion kernel is Gaussian convolution.



We can sample $\mathbf{x}_t \sim q(\mathbf{x}_t)$ by first sampling $\mathbf{x}_0 \sim q(\mathbf{x}_0)$ and then sampling $\mathbf{x}_t \sim q(\mathbf{x}_t|\mathbf{x}_0)$ (i.e., ancestral sampling).

16

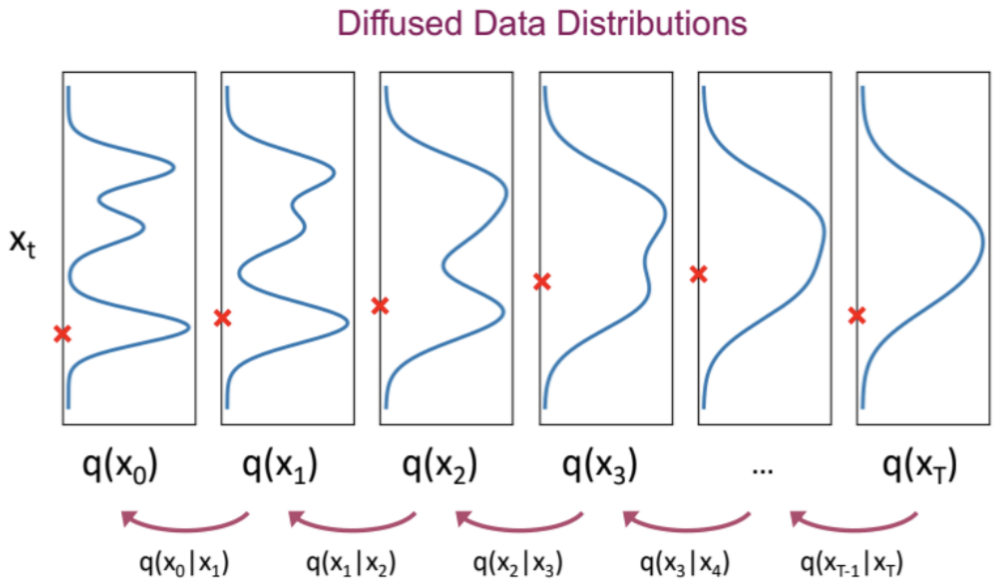
Generative Learning by Learning to Denoise

Recall, that the diffusion parameters are designed such that $q(\mathbf{x}_T) \approx \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I}))$

Generation:

Sample $\mathbf{x}_T \sim \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$

Iteratively sample $\mathbf{x}_{t-1} \sim \underbrace{q(\mathbf{x}_{t-1}|\mathbf{x}_t)}_{\text{True Denoising Dist.}}$

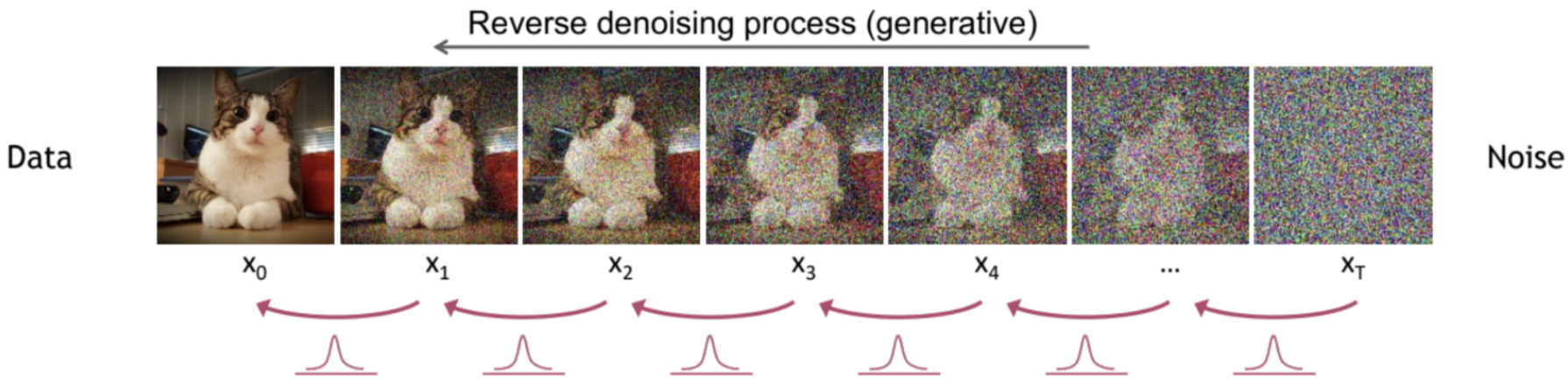


Can we approximate $q(\mathbf{x}_{t-1}|\mathbf{x}_t)$? Yes, we can use a Normal distribution if β_t is small in each forward diffusion step.

18

Reverse Denoising Process

Formal definition of forward and reverse processes in T steps:



$$p(\mathbf{x}_T) = \mathcal{N}(\mathbf{x}_T; \mathbf{0}, \mathbf{I})$$

$$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t) = \mathcal{N}(\mathbf{x}_{t-1}; \underbrace{\mu_\theta(\mathbf{x}_t, t)}_{\text{Trainable network}}, \sigma_t^2\mathbf{I})$$

$$\Rightarrow \quad p_\theta(\mathbf{x}_{0:T}) = p(\mathbf{x}_T) \prod_{t=1}^{T} p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$$

Generative Learning by Learning to Denoise

For training, we can form variational upper bound that is commonly used for training variational autoencoders:

$$\mathbb{E}_{q(\mathbf{x}_0)}\left[-\log p_\theta(\mathbf{x}_0)\right] \leq \mathbb{E}_{q(\mathbf{x}_0)q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\left[-\log \frac{p_\theta(\mathbf{x}_{0:T})}{q(\mathbf{x}_{1:T}|\mathbf{x}_0)}\right] =: L$$

Recall that $\mathbf{x}_t = \sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{(1-\bar{\alpha}_t)}\,\epsilon$. Ho et al. NeurIPS 2020 parameterized the mean of denoising model via:

$$\mu_\theta(\mathbf{x}_t, t) = \frac{1}{\sqrt{1-\beta_t}}\left(\mathbf{x}_t - \frac{\beta_t}{\sqrt{1-\bar{\alpha}_t}}\,\epsilon_\theta(\mathbf{x}_t, t)\right)$$

Using a few simple arithmetic operations, we can write down the variational objective as:

$$L = \mathbb{E}_{\mathbf{x}_0\sim q(\mathbf{x}_0), t\sim\mathcal{U}\{1,T\}, \epsilon\sim\mathcal{N}(\mathbf{0},\mathbf{I})}\left[\lambda_t||\epsilon - \epsilon_\theta(\sqrt{\bar{\alpha}_t}\,\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\,\epsilon, t)||^2\right]$$

Ho et al. NeurIPS 2020 observe that simply setting λ_t to 1 for all t works best in practice.

Algorithm 1 Training

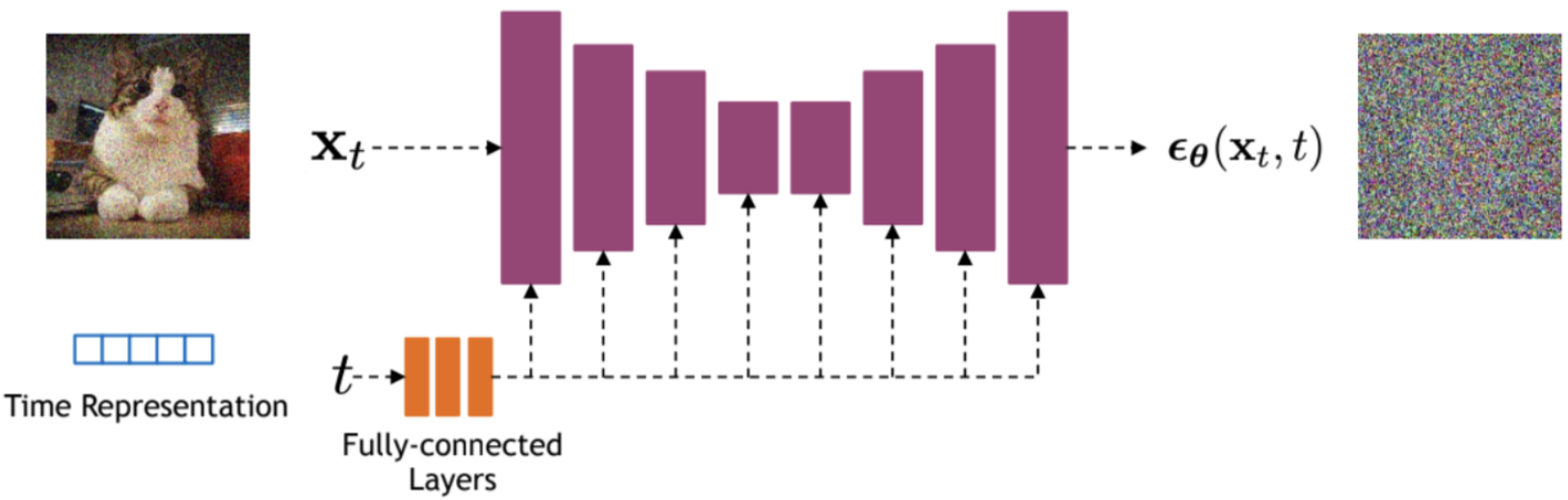
1: **repeat**
2: $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
3: $t \sim \text{Uniform}(\{1, \dots, T\})$
4: $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
5: Take gradient descent step on
$$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
6: **until** converged

Algorithm 2 Sampling

1: $\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
2: **for** $t = T, \dots, 1$ **do**
3: $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
4: $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}} \left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}} \boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t) \right) + \sigma_t \mathbf{z}$
5: **end for**
6: **return** $\mathbf{x}_0$

Implementation of the Denoisers

Diffusion models often use U-Net architectures with ResNet blocks and self-attention layers to represent $\epsilon_\theta(\mathbf{x}_t, t)$



Time representation: sinusoidal positional embeddings or random Fourier features.

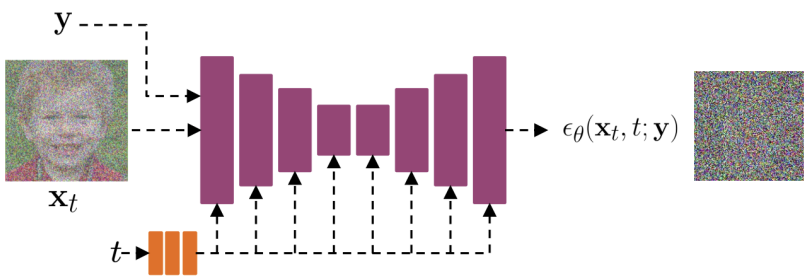
Conditional Training and Generation

Conditional sampling can be considered as training $p(\mathbf{x}|\mathbf{y})$ where $\mathbf{y}$ is the input conditioning (e.g., text) and $\mathbf{x}$ is generated output (e.g., image)

Train the score model for $\mathbf{x}$ conditioned on $\mathbf{y}$ using:

$$\mathbb{E}_{(\mathbf{x},\mathbf{y})\sim p_{\text{data}}(\mathbf{x},\mathbf{y})}\mathbb{E}_{\epsilon\sim\mathcal{N}(\mathbf{0},\mathbf{I})}\mathbb{E}_{t\sim\mathcal{U}[0,T]}\ ||\epsilon_\theta(\mathbf{x}_t, t; \mathbf{y}) - \epsilon||_2^2$$

The conditional score is simply a U-Net with $\mathbf{x_t}$ and $\mathbf{y}$ together in the input.



Text-to-Image Generation Examples

DALL·E 2

"a propaganda poster depicting a cat dressed as french emperor napoleon holding a piece of cheese"

IMAGEN

"A photo of a raccoon wearing an astronaut helmet, looking out of the window at night."

TIME

← THE BEST INVENTIONS OF 2022

Artificial Imagination

OpenAI DALL-E 2

DALL·E

Outline

Conclusions

- Generative models are useful to model high-dimensional data.
- Latent-variable generative models are appealing since they are more compact.
- Often, computing evidence and posterior distributions is intractable.
- A common surrogate for maximum likelihood is the evidence lower bound (ELBO).
- Variational auto-encoders optimize the ELBO with amortized VI.
- Generative adversarial networks (GANs) are formulated as a game between a generator and a discriminator.
- Denoising diffusion models have impressive results and can be conditioned by text.
- Open problem (for VAE, GAN, and diffusion models): discrete data.

Thank you!

Questions?

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