DSC190: Machine Learning with Few Labels

Unsupervised Learning
Reinforcement Learning

Zhiting Hu

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UC San Diego
HALICIOĞLU DATA SCIENCE INSTITUTE

Outline

Unsupervised learning: Variational Auto-Encoders

Reinforcement learning

Presentations

- **Jerry Xu**: Distilling the Knowledge in a Neural Network
- **Yinming Huang**: Generalizing Motion Planners with Mixture of Experts for Autonomous Driving
- **Mohit Sridhar**: Integrating Long-Range Regulatory Interactions to Predict Gene Expression Using Graph Convolutional Networks

Recap: Variational Auto-Encoders (VAEs)

- Model $p_\theta(\boldsymbol{x}, \boldsymbol{z}) = p_\theta(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})$
  - $p_\theta(\boldsymbol{x}|\boldsymbol{z})$: a.k.a., generative model, generator, (probabilistic) decoder, …
  - $p(\boldsymbol{z})$: prior, e.g., Gaussian
- Assume variational distribution $q_\phi(\boldsymbol{z}|\boldsymbol{x})$
  - E.g., a Gaussian distribution parameterized as **deep neural networks**
  - a.k.a, recognition model, inference network, (probabilistic) encoder, …
- ELBO:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}, \boldsymbol{z})] + \mathrm{H}(q_\phi(\boldsymbol{z}|\boldsymbol{x}))$$
$$= \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})] - \mathrm{KL}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}))$$

Reconstruction

Divergence from prior
(KL divergence between two Guassians has an analytic form)

Variational Auto-Encoders (VAEs)

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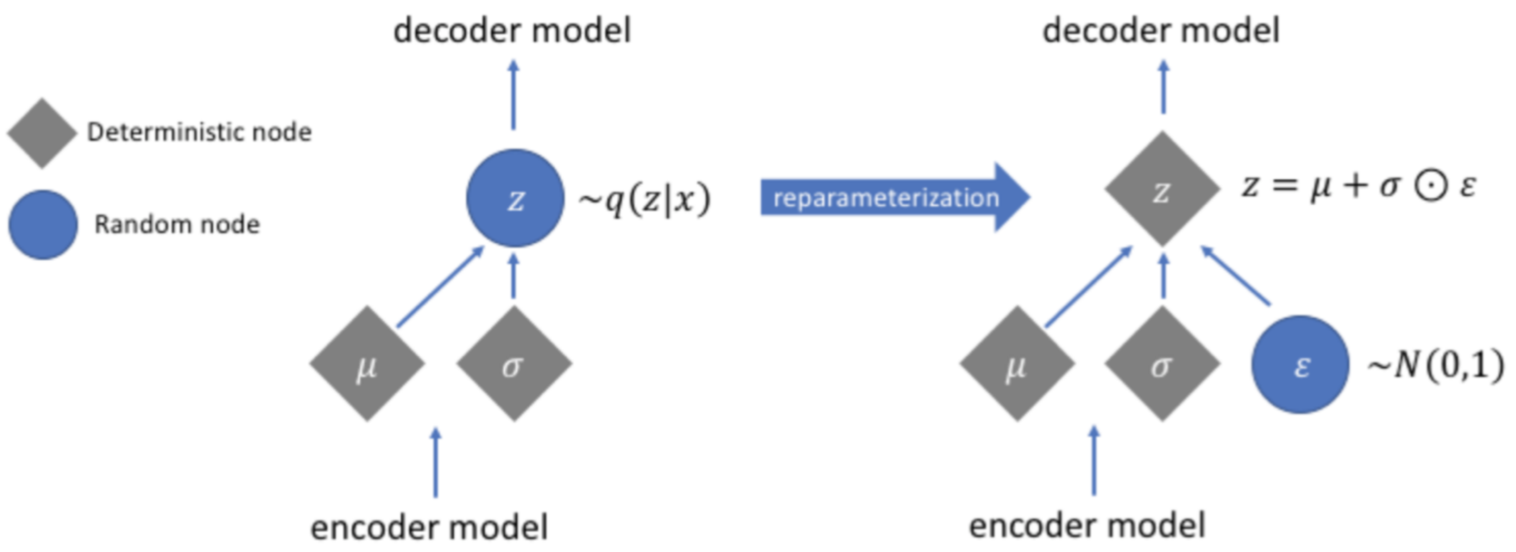
- Reparameterization:
  - $[\boldsymbol{\mu}; \boldsymbol{\sigma}] = f_\phi(\boldsymbol{x})$ (a neural network)
  - $\boldsymbol{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}, \quad \boldsymbol{\epsilon} \sim \boldsymbol{N}(\boldsymbol{0}, \boldsymbol{1})$



Variational Auto-Encoders (VAEs)

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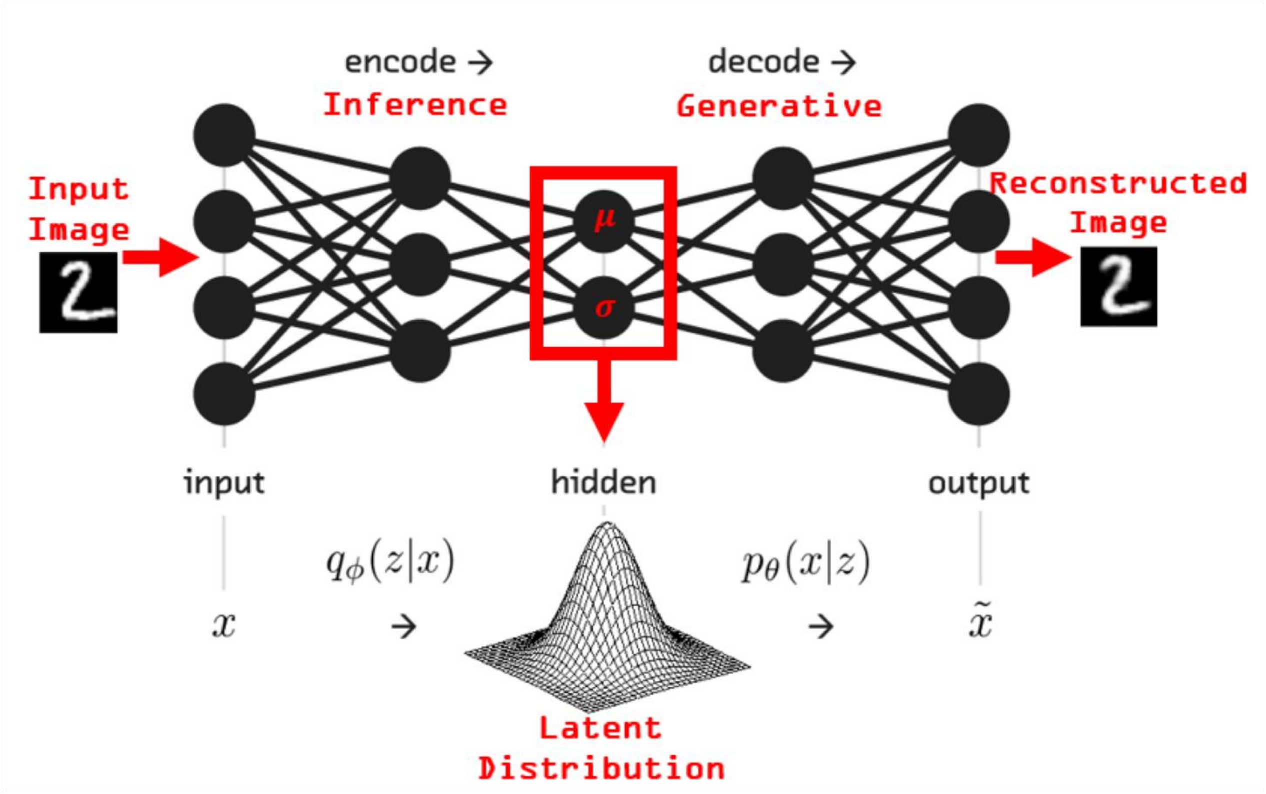
$$\nabla_{\boldsymbol{\phi}} \mathcal{L} = \mathrm{E}_{\epsilon \sim N(\boldsymbol{0},\boldsymbol{1})}[\, \nabla_{\boldsymbol{z}}\left[\log p_\theta(\boldsymbol{x}, \boldsymbol{z}) - \log q_\phi(\boldsymbol{z}|\boldsymbol{x})\right] \nabla_\phi z(\epsilon, \boldsymbol{\phi})]$$

$$\nabla_\theta \mathcal{L} = \mathrm{E}_{q_\phi(\boldsymbol{z}|\boldsymbol{x})}[\nabla_\theta \log p_\theta(\boldsymbol{x}, \boldsymbol{z})]$$

Example: VAEs for images



[https://www.kaggle.com/rvislaywade/visualizing-mnist-using-a-variational-autoencoder]

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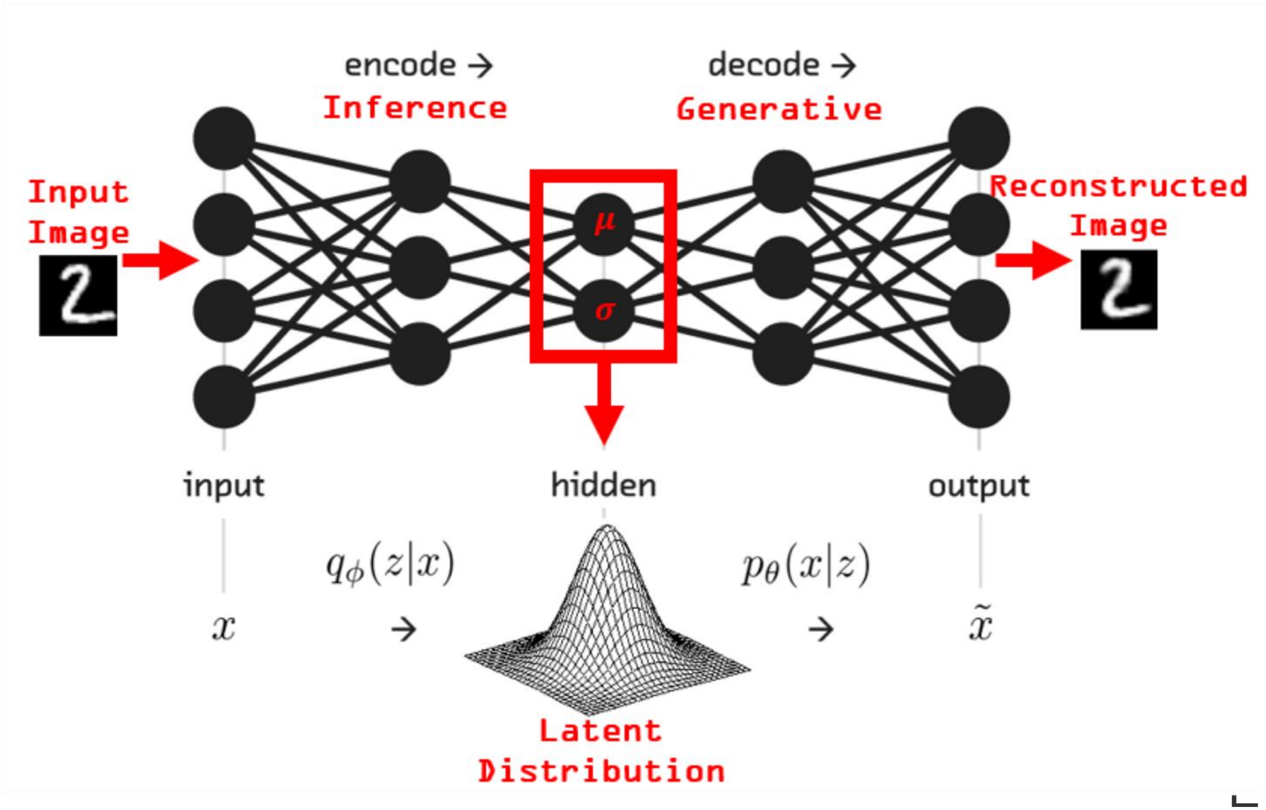

[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

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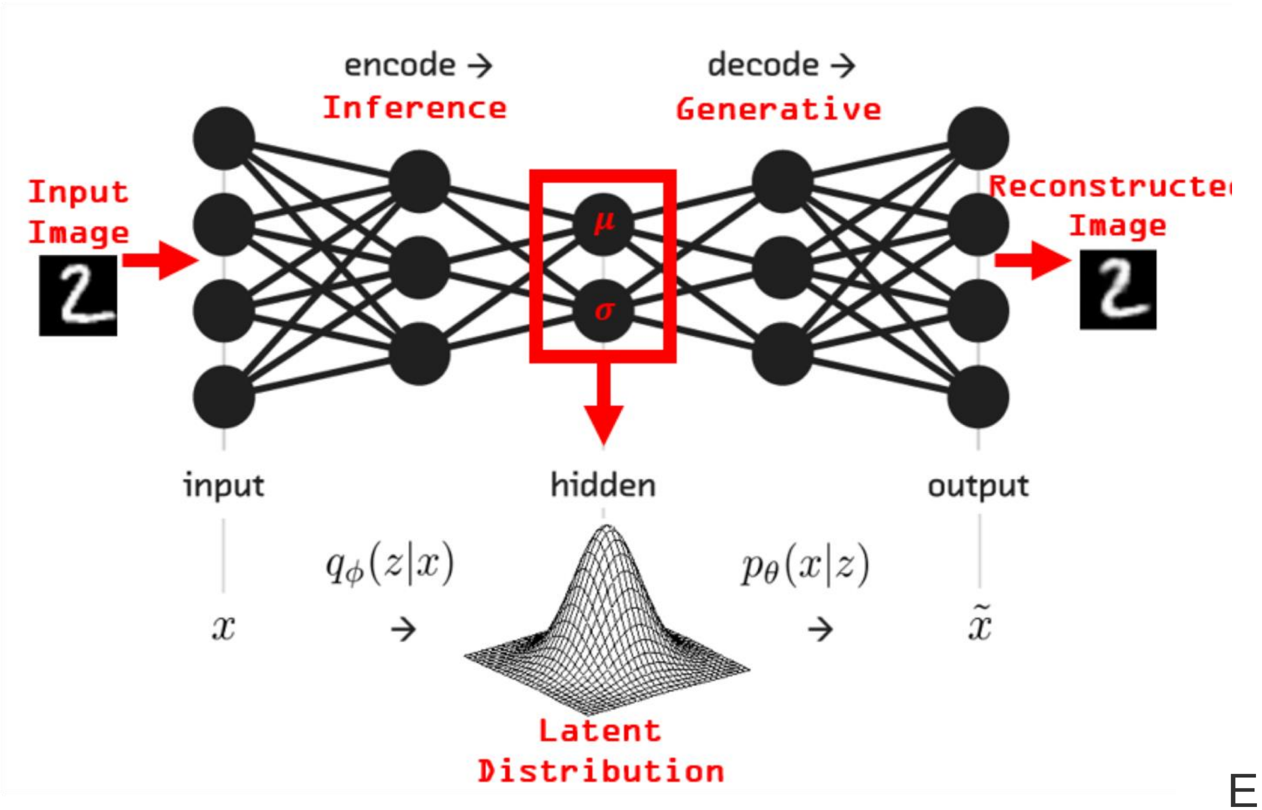

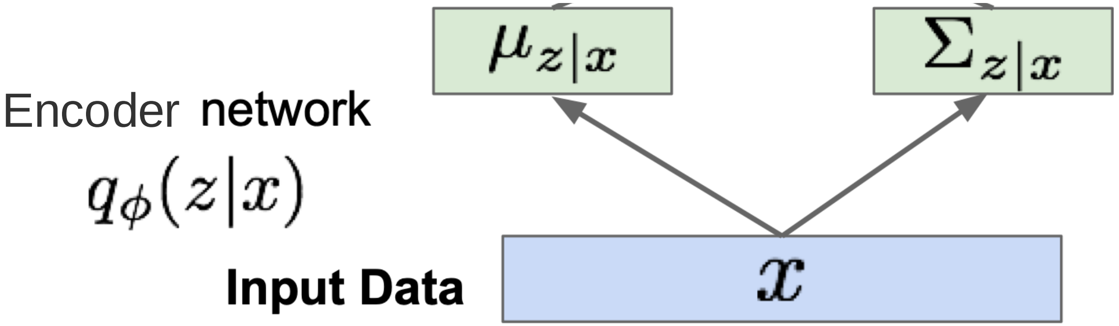

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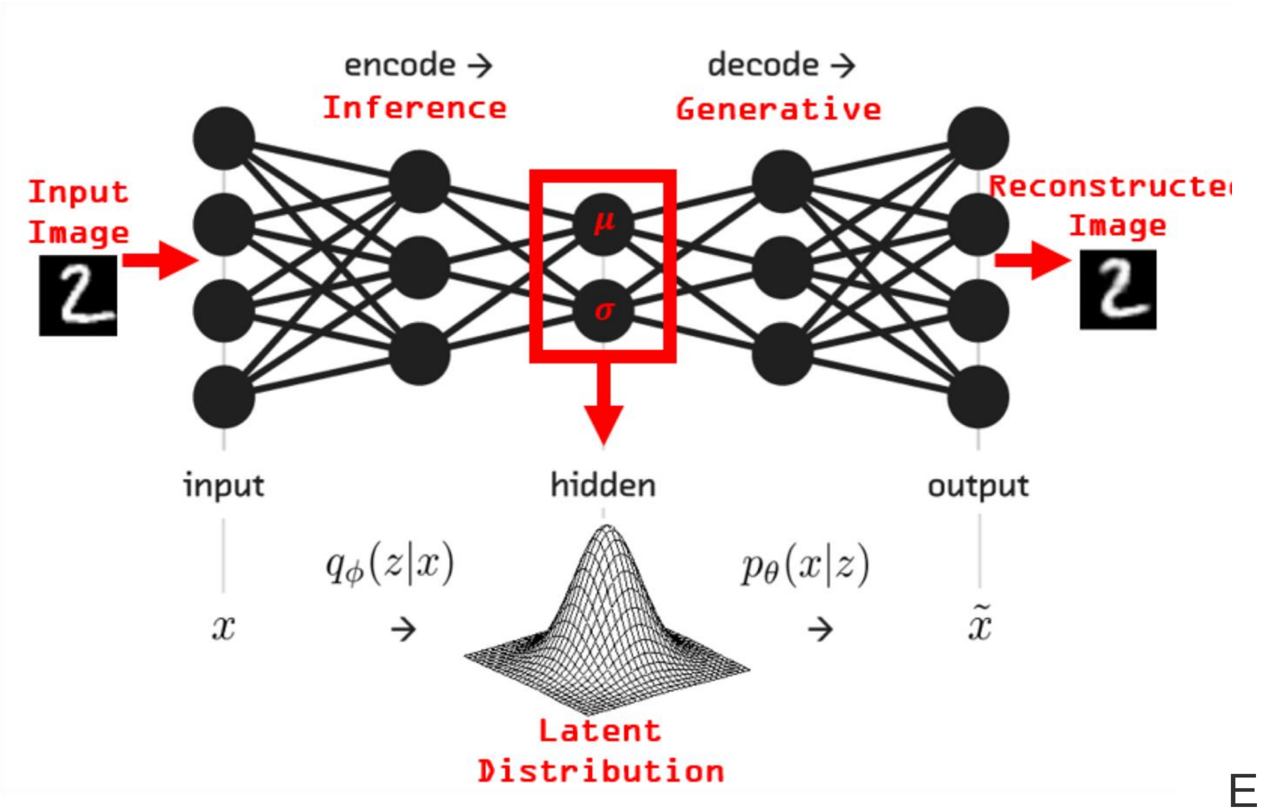

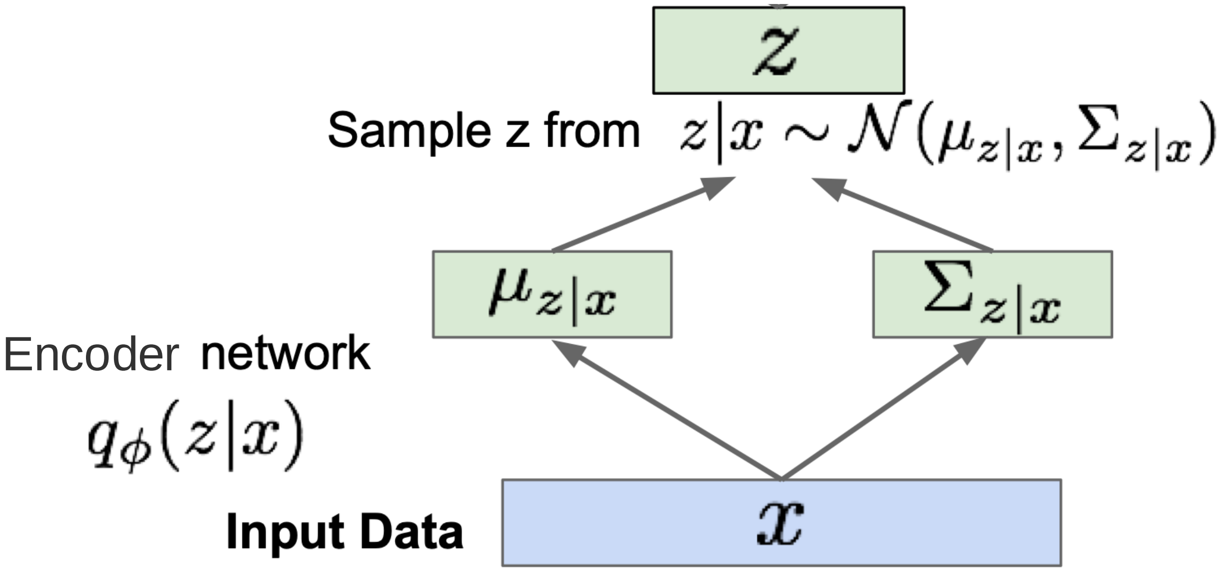

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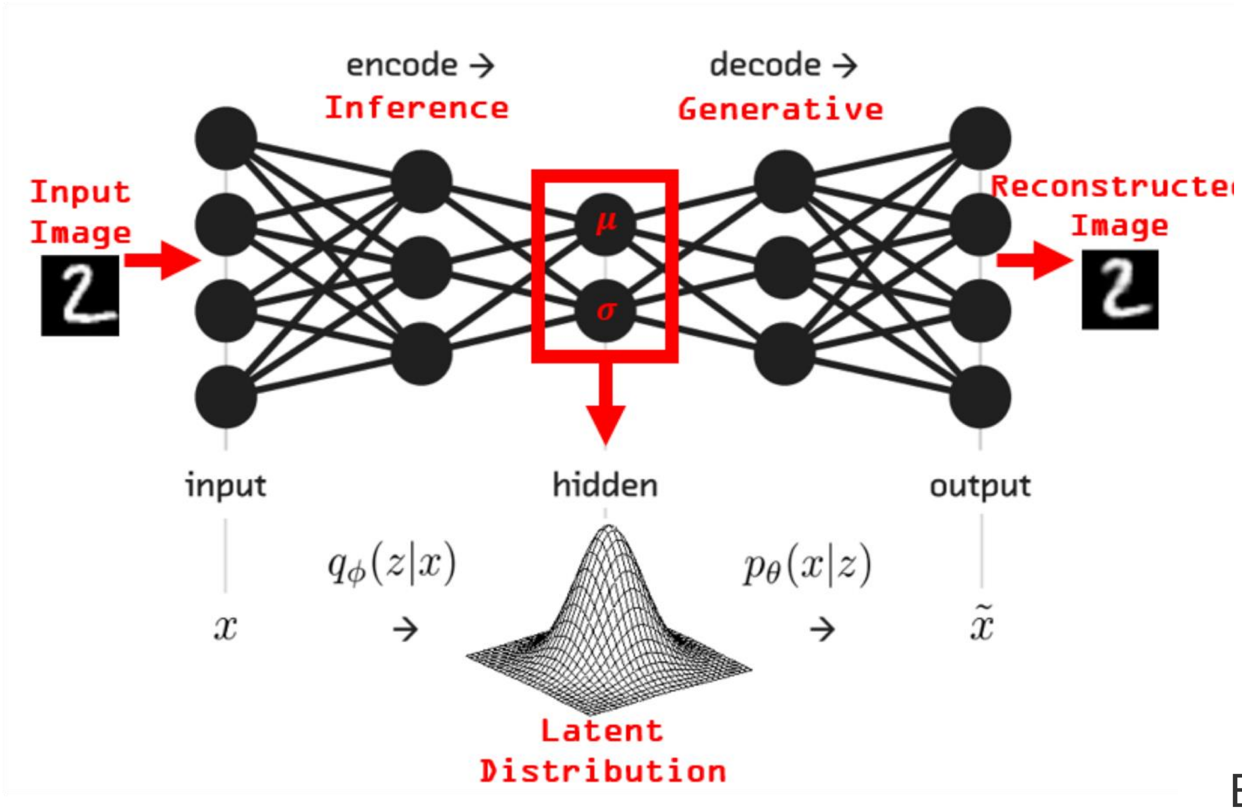

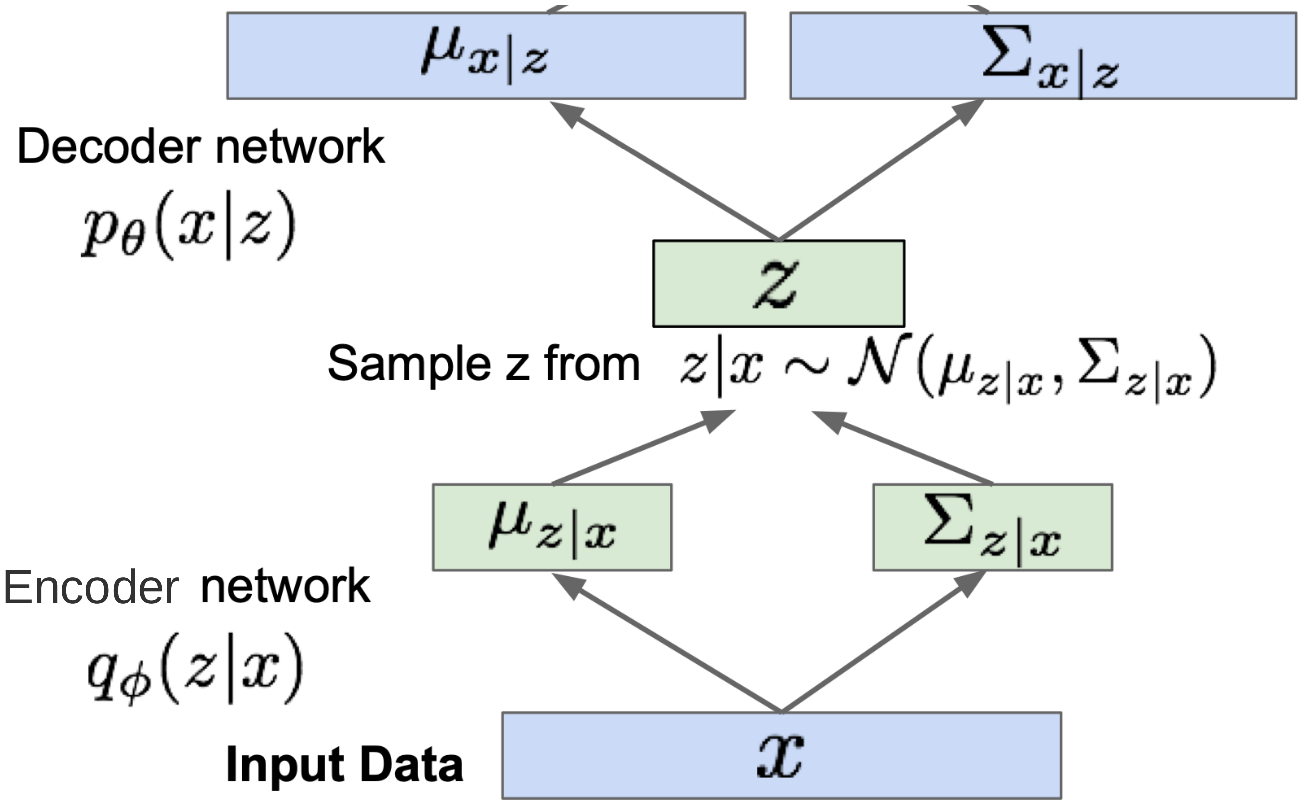

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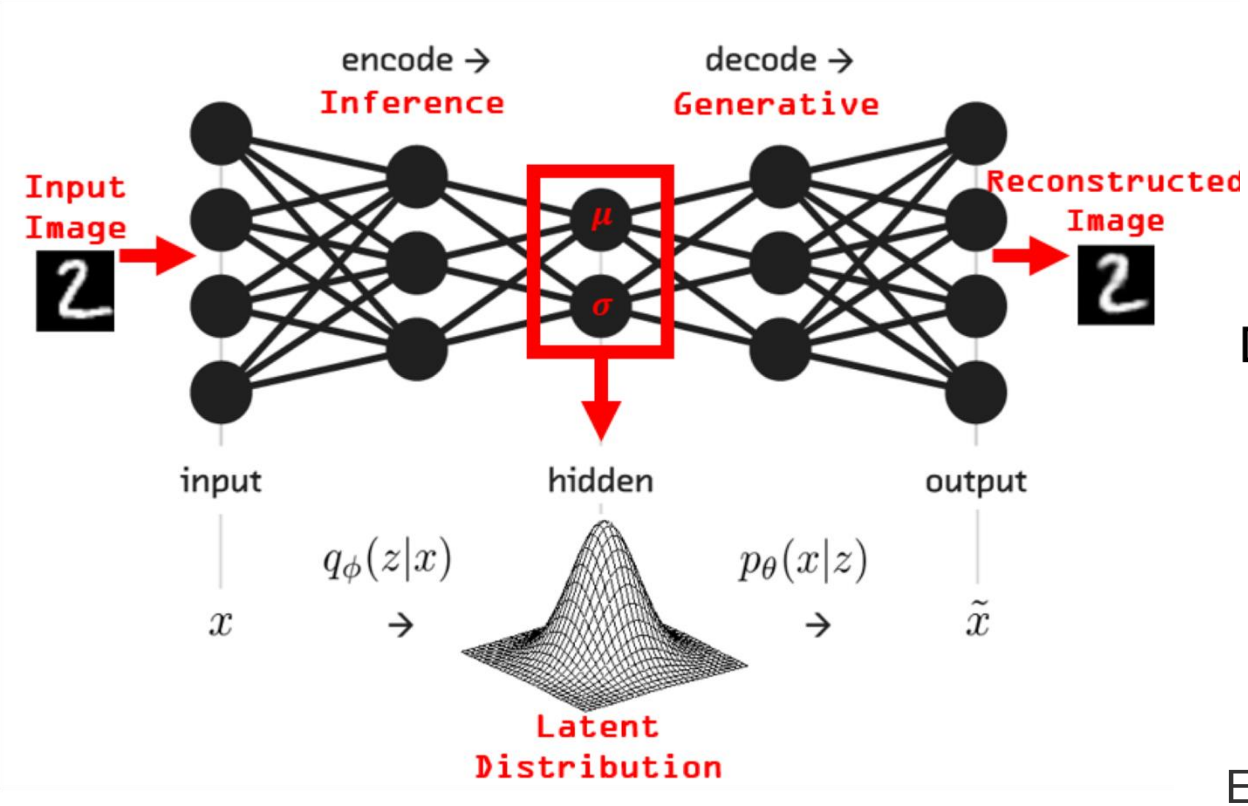
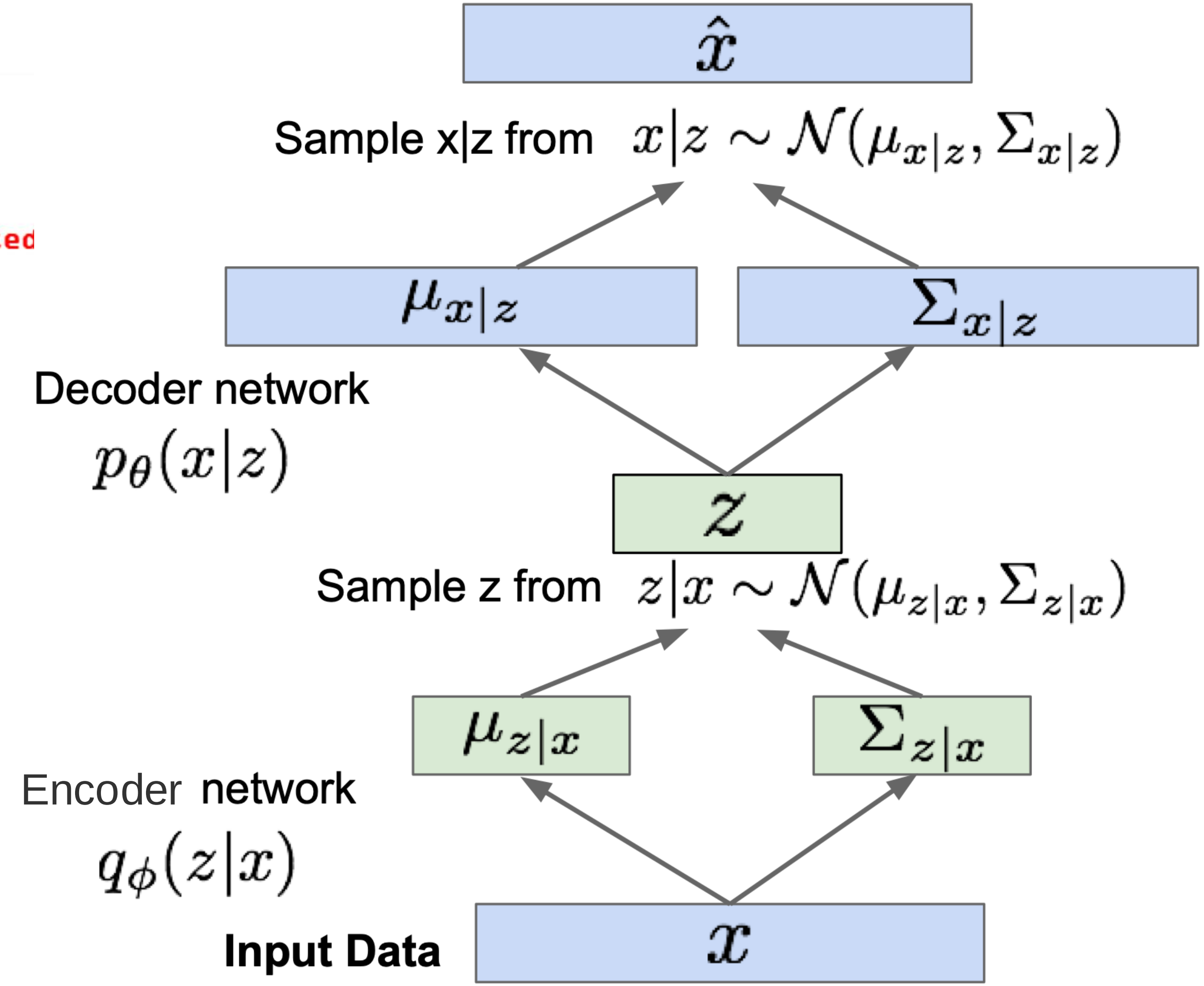


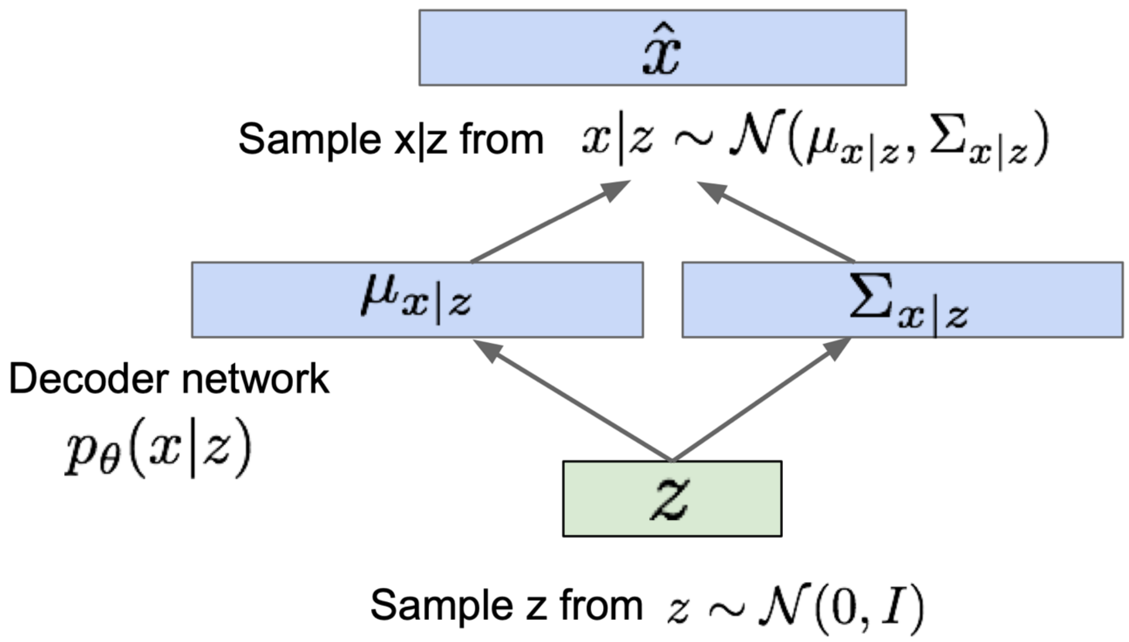


[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

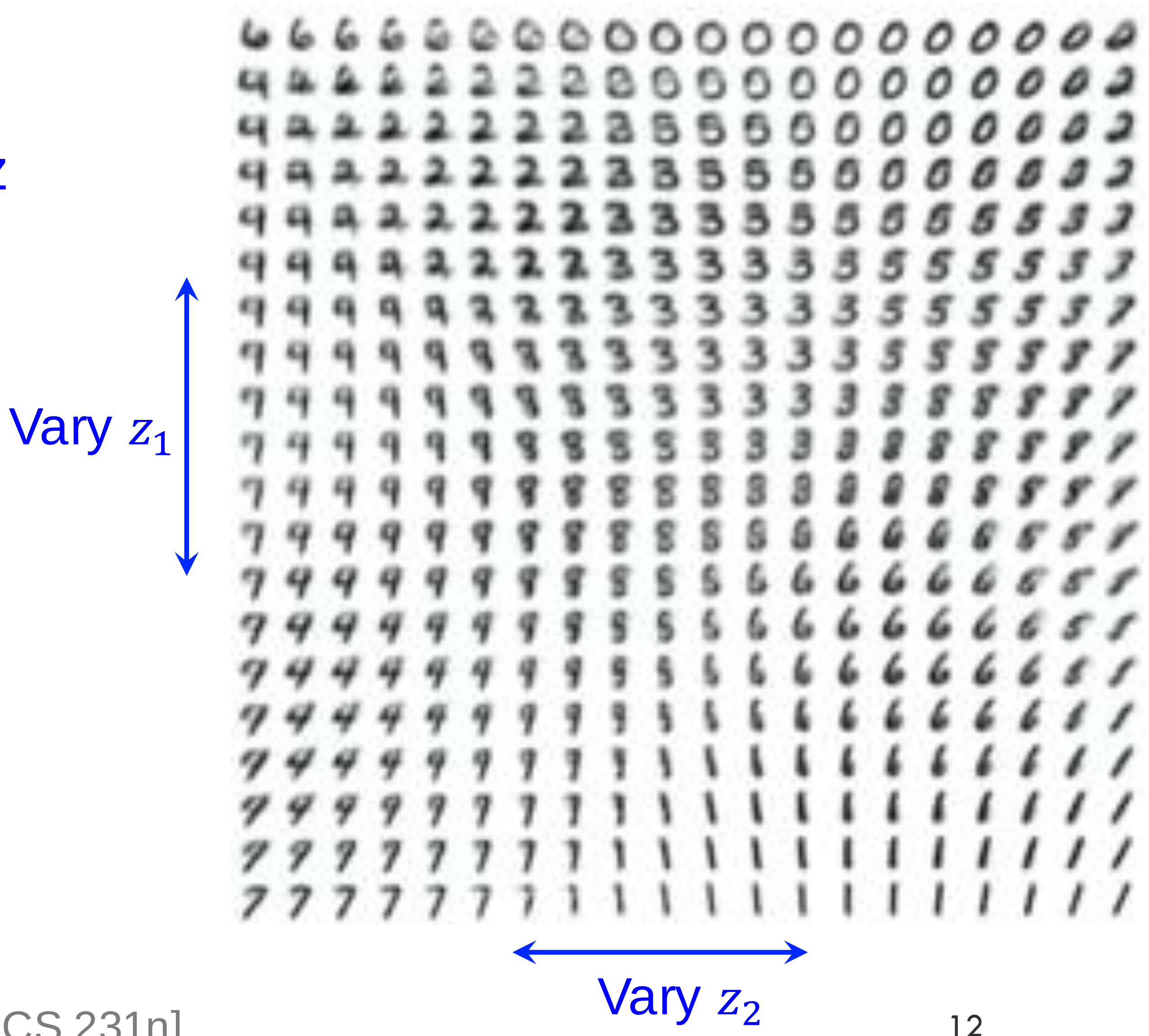
Example: VAEs for images

Generating samples:

- Use decoder network. Now sample z from prior!



Data manifold for 2-d **z**



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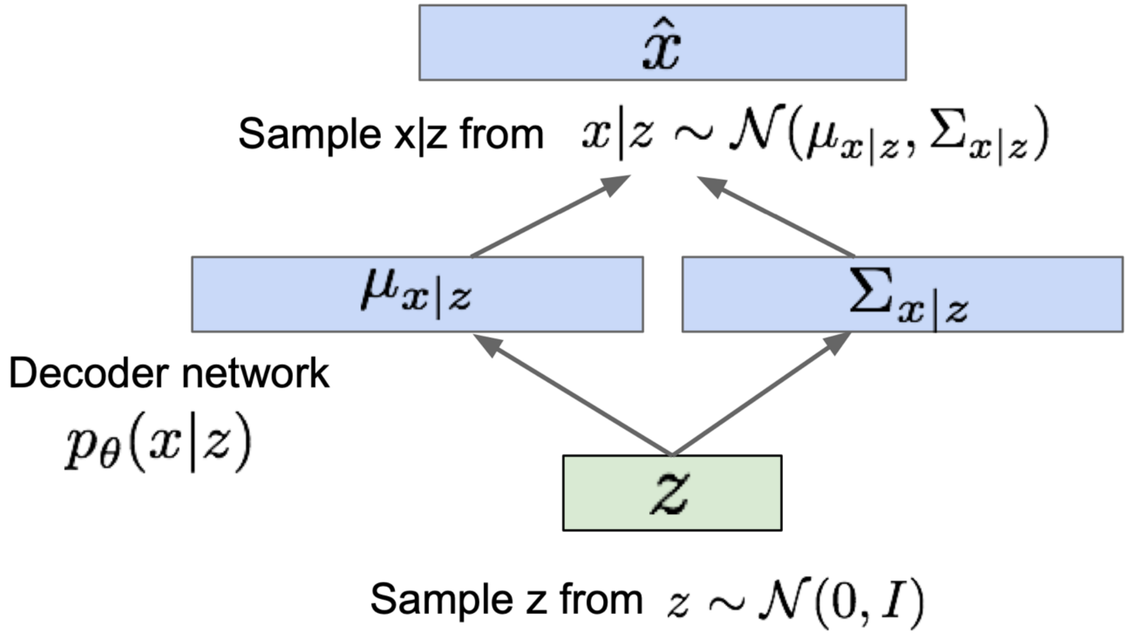


Data manifold for 2-d **z**

Vary z_1
(Degree of smile)

Vary z_2 (head pose)

[Courtesy: Fei-Fei Li, Justin Johnson, Serena Yeung, CS 231n]

Example: VAEs for text

- Latent code interpolation and sentences generation from VAEs [Bowman et al., 2015].

“ i want to talk to you . ”
“i want to be with you . ”
“i do n’t want to be with you . ”
i do n’t want to be with you .
she did n’t want to be with him .

Note: Amortized Variational Inference

- Variational distribution as an inference model $q_{\phi}(\boldsymbol{z}|\boldsymbol{x})$ with parameters $\boldsymbol{\phi}$ (which was traditionally factored over samples)
- Amortize the cost of inference by learning a **single** data-dependent inference model
- The trained inference model can be used for quick inference on new data

Variational Auto-encoders: Summary

- A combination of the following ideas:
  - Variational Inference: ELBO
  - Variational distribution parametrized as neural networks
  - Reparameterization trick

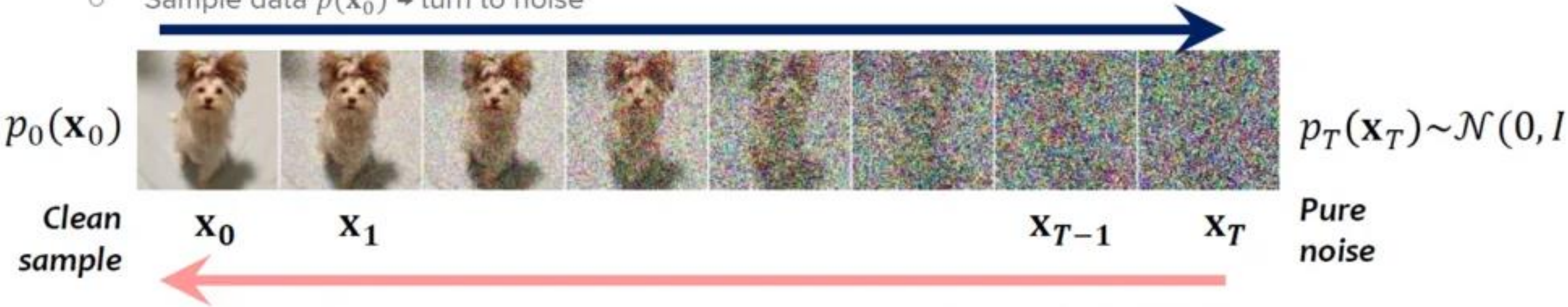
$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = \underbrace{[\log p_\theta(\boldsymbol{x}|\boldsymbol{z})]}_{\text{Reconstruction}} - \underbrace{\mathrm{KL}(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,||\, p(\boldsymbol{z}))}_{\text{Divergence from prior}}$$

(Razavi et al., 2019)

- Pros:
  - Principled approach to generative models
  - Allows inference of $q(z|x)$, can be useful feature representation for other tasks
- Cons:
  - Samples blurrier and lower quality compared to GANs
  - Tend to collapse on text data

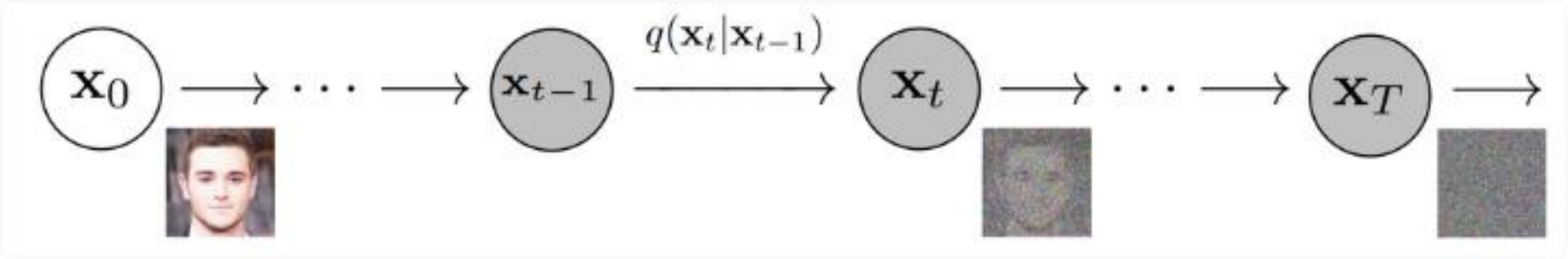
Diffusion model

- **Forward / noising process**
  - Sample data $p(\mathbf{x}_0)$ → turn to noise



- **Reverse / denoising process**
  - Sample noise $p_T(\mathbf{x}_T)$ → turn into data

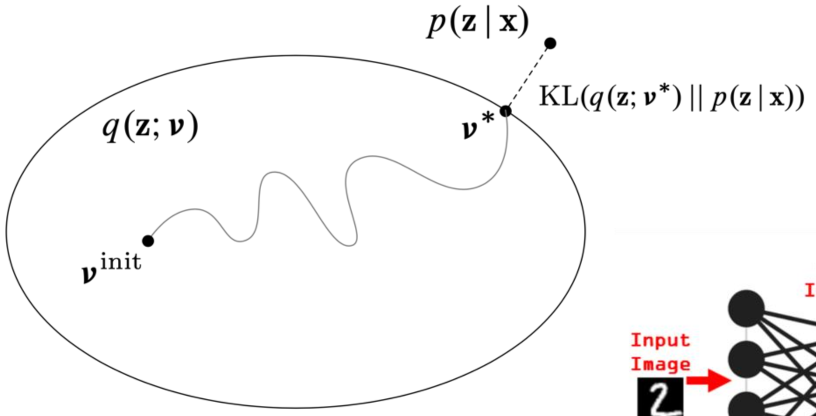
Diffusion model

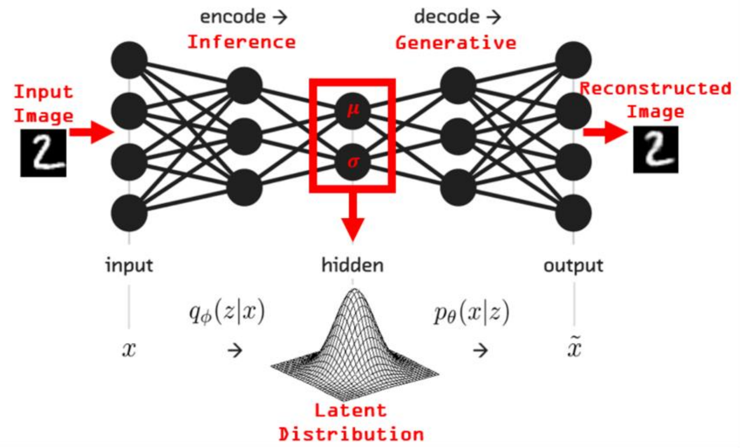


Summary: Supervised / Unsupervised Learning

- Supervised Learning
  - Maximum likelihood estimation (MLE)

- Unsupervised learning
  - Maximum likelihood estimation (MLE) with latent variables
    - Marginal log-likelihood
  - EM algorithm for MLE
    - ELBO / Variational free energy
  - Variational Inference
    - ELBO / Variational free energy
    - Variational distributions
      - Factorized (mean-field VI)
      - Mixture of Gaussians (Black-box VI)
      - Neural-based (VAEs)

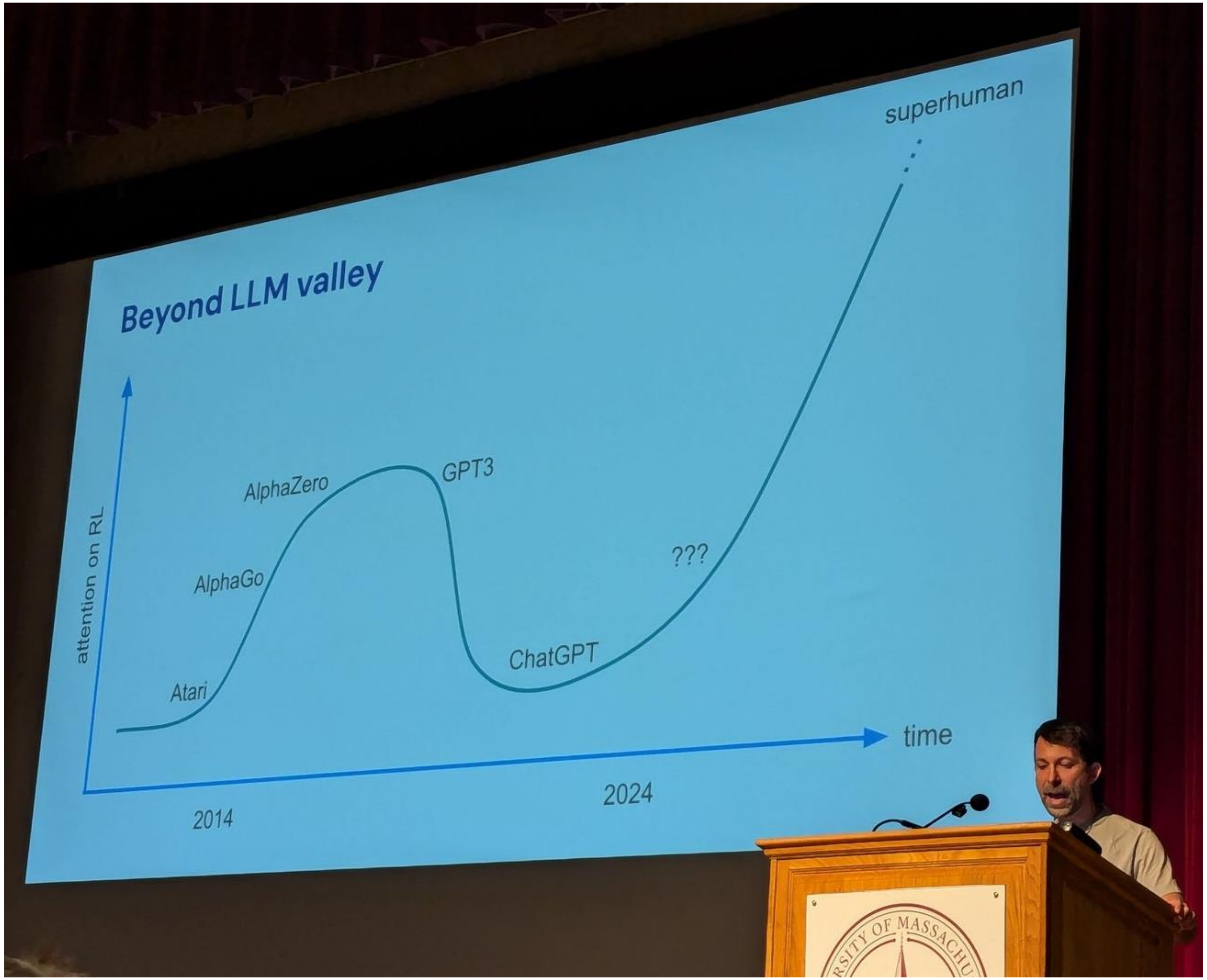




Reinforcement Learning

RL Conference 2024

RL Conference 2024



So far… Supervised Learning

Data: (x, y)
x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.

Cat

Classification

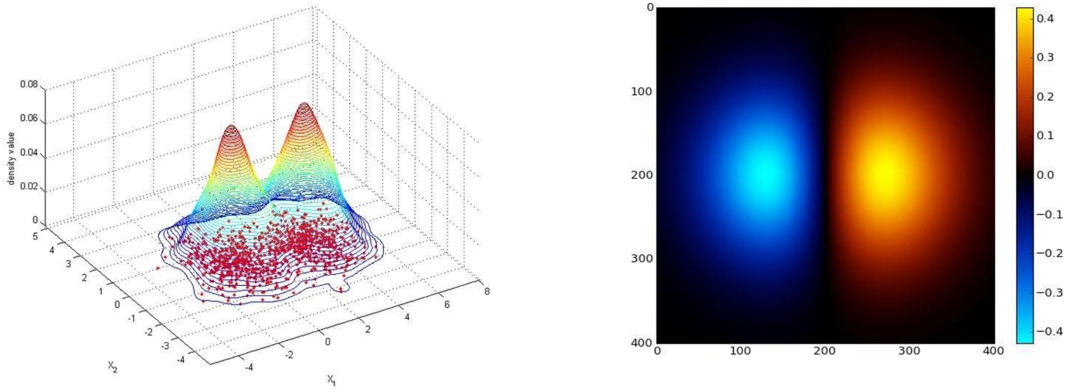
So far… Unsupervised Learning

Data: x
no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.

1-d density estimation

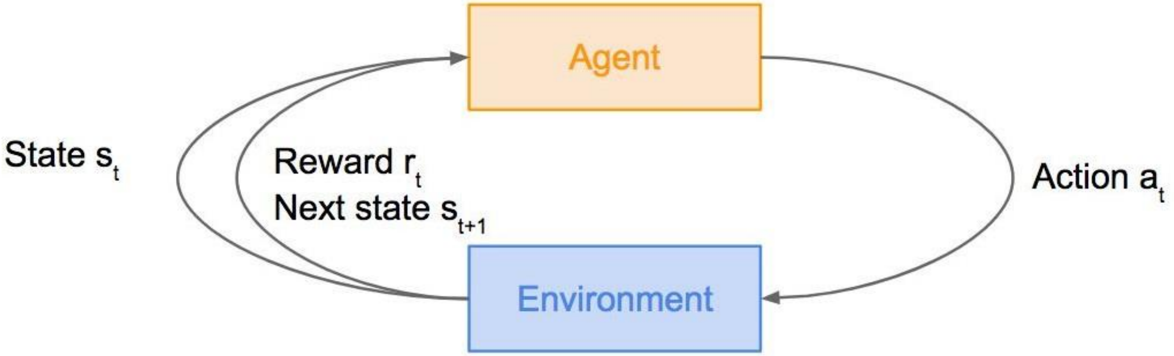


2-d density estimation

Today: Reinforcement Learning

Problems involving an **agent** interacting with an **environment**, which provides numeric **reward** signals

Goal: Learn how to take actions in order to maximize reward



Atari games figure copyright Volodymyr Mnih et al., 2013. Reproduced with permission.

Overview

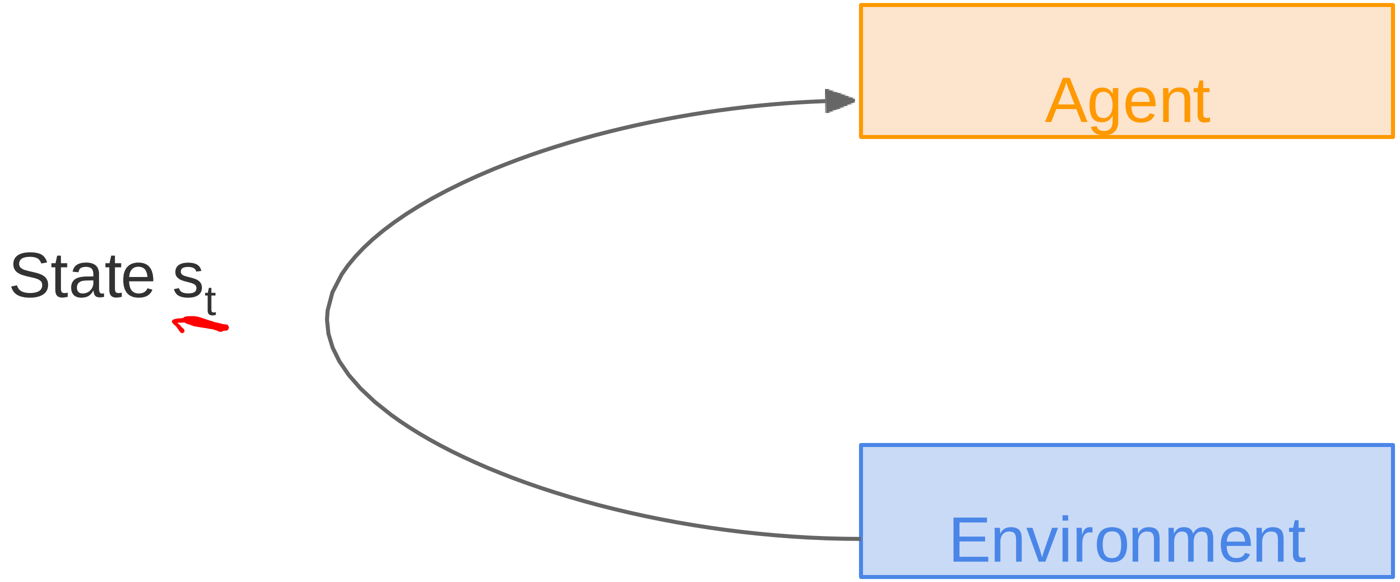
- What is Reinforcement Learning?
- Markov Decision Processes
- Q-Learning
- Policy Gradients

Reinforcement Learning

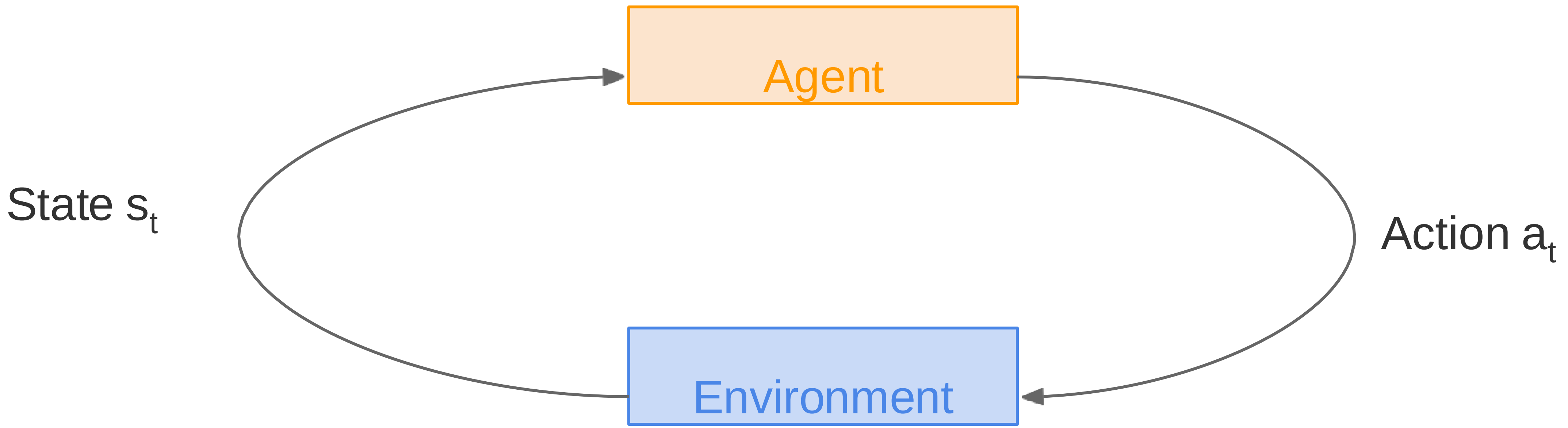
Agent

Environment

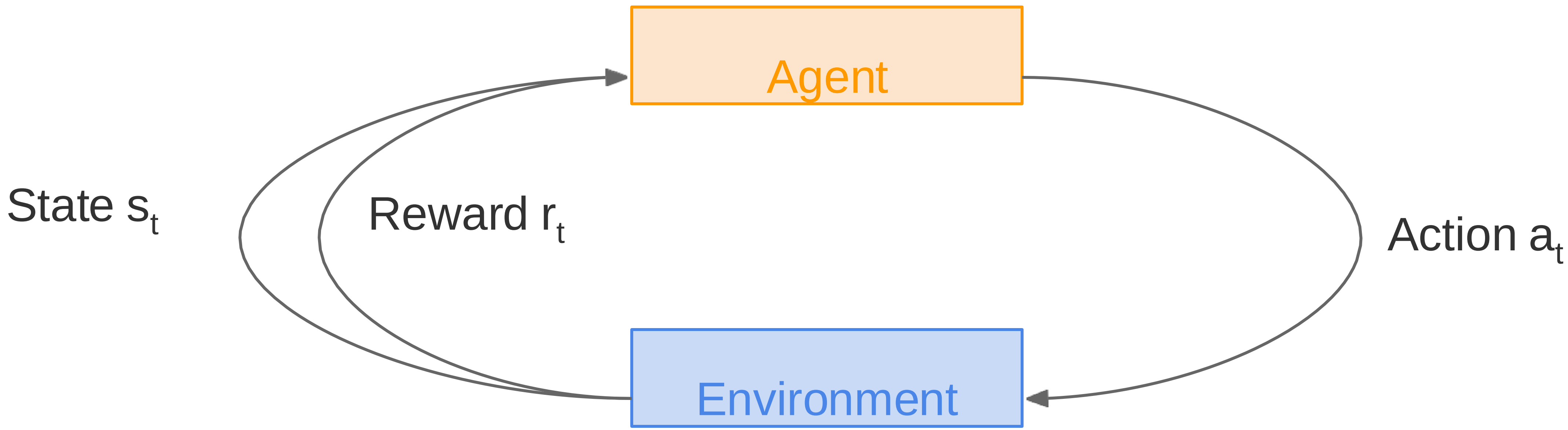
Reinforcement Learning



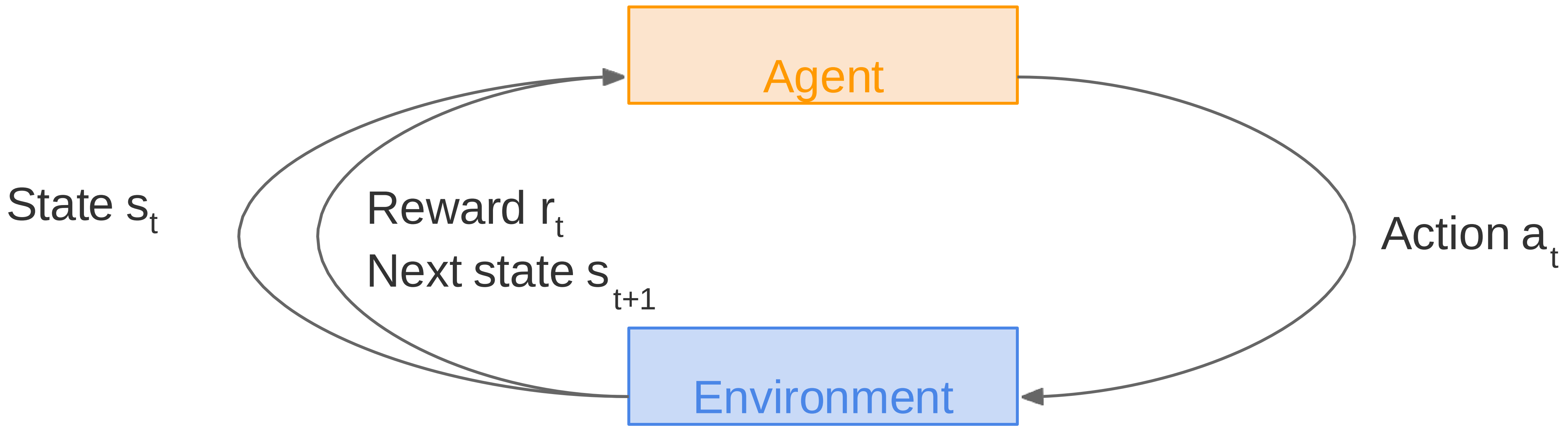
Reinforcement Learning



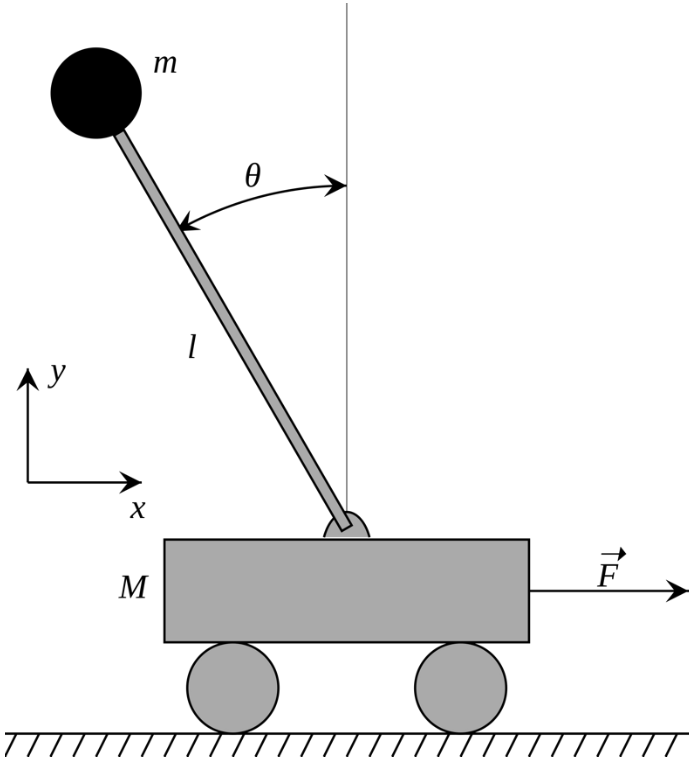
Reinforcement Learning



Reinforcement Learning



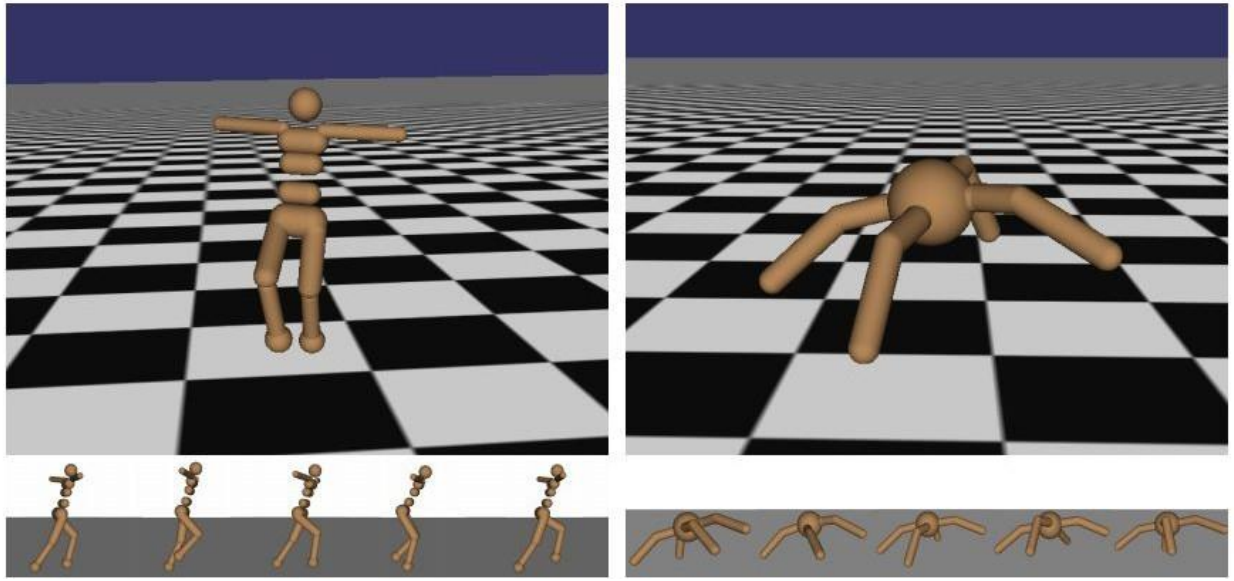
Cart-Pole Problem



Objective: Balance a pole on top of a movable cart

State: angle, angular speed, position, horizontal velocity
Action: horizontal force applied on the cart
Reward: 1 at each time step if the pole is upright

Robot Locomotion



Objective: Make the robot move forward

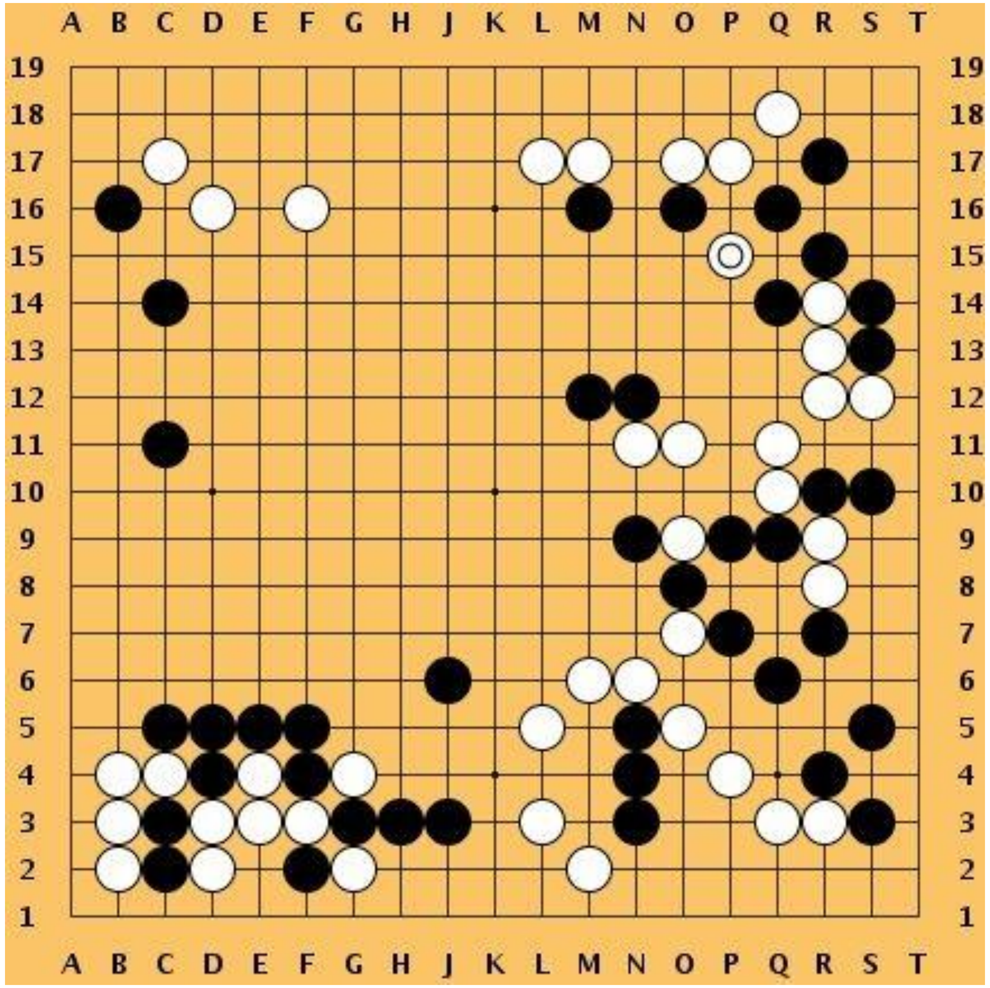
State: Angle and position of the joints
Action: Torques applied on joints
Reward: 1 at each time step upright + forward movement

Atari Games

Objective: Complete the game with the highest score

State: Raw pixel inputs of the game state
Action: Game controls e.g. Left, Right, Up, Down
Reward: Score increase/decrease at each time step

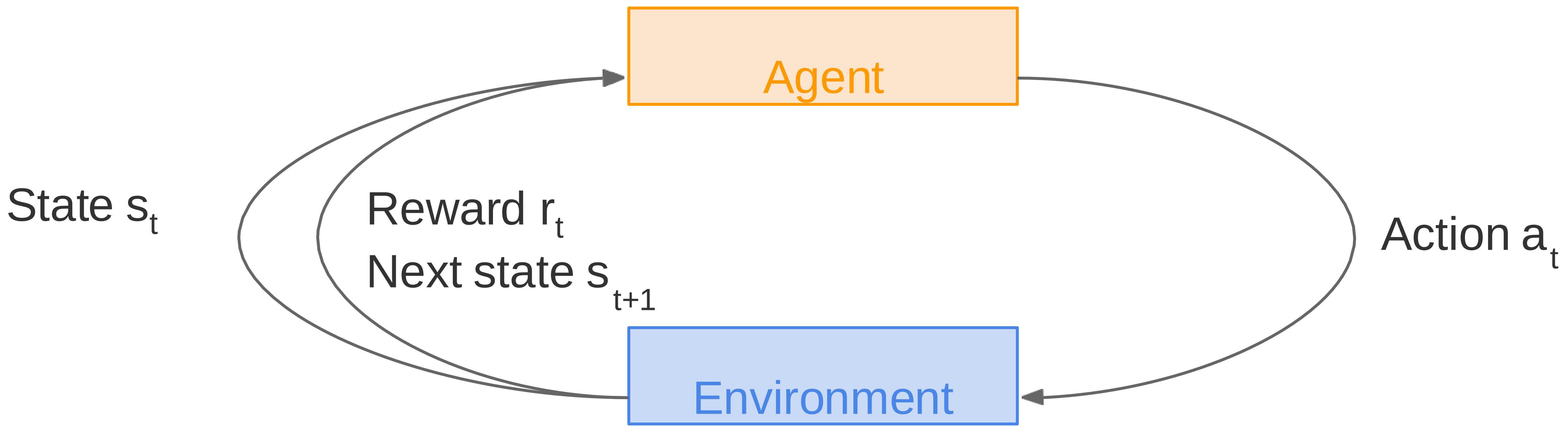
Go



Objective: Win the game!

State: Position of all pieces
Action: Where to put the next piece down
Reward: 1 if win at the end of the game, 0 otherwise

How can we mathematically formalize the RL problem?



Presentations

Questions?