Variational Inference and Generative Models

CS 285

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UC Berkeley

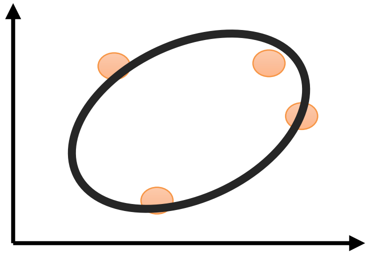
Today’s Lecture

1. Probabilistic latent variable models
2. Variational inference
3. Amortized variational inference
4. Generative models: variational autoencoders

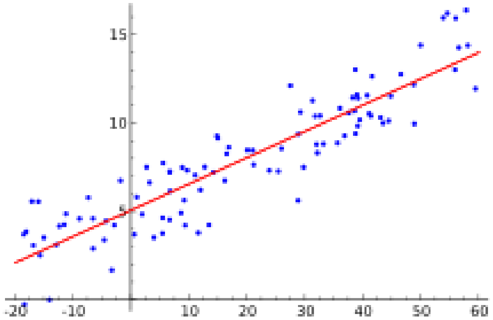
- Goals
  - Understand latent variable models in deep learning
  - Understand how to use (amortized) variational inference

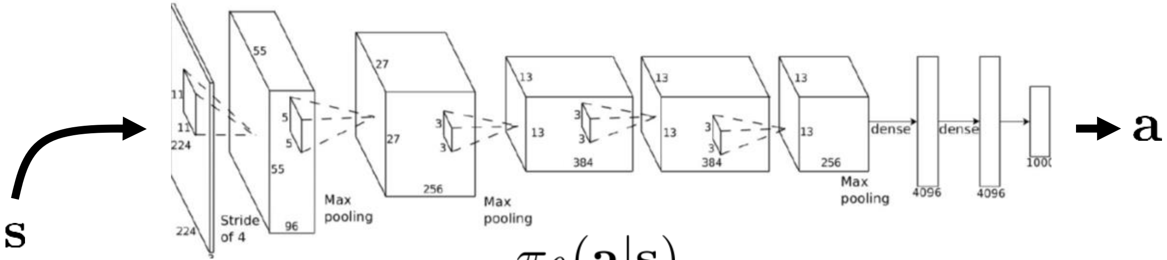
Probabilistic models

$p(x)$



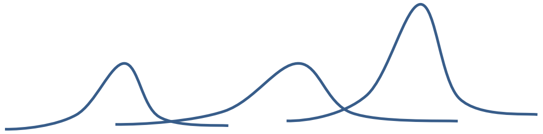
$p(y|x)$





$\pi_\theta(\mathbf{a}|\mathbf{s})$

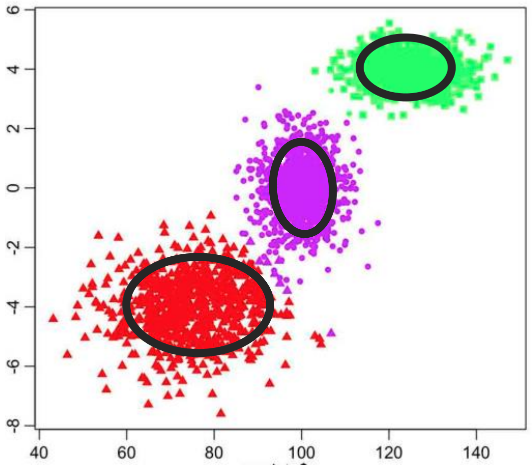
Latent variable models

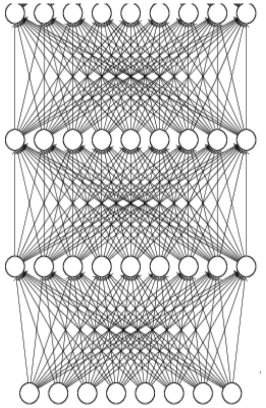


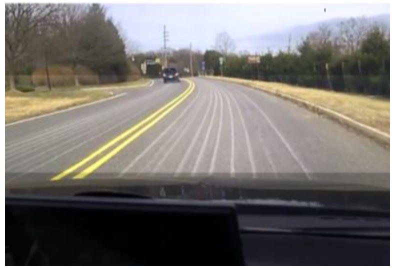
$w_1, \mu_1, \Sigma_1, \ldots, w_N, \mu_N, \sigma_N$

$$p(x) = \sum_z p(x|z)p(z)$$

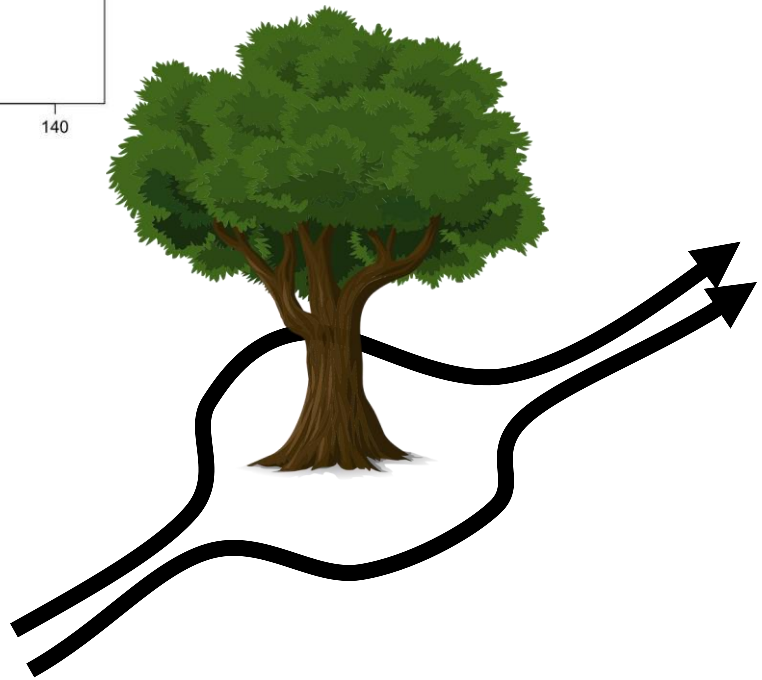
mixture element







$$p(y|x) = \sum_z p(y|x,z)p(z)$$

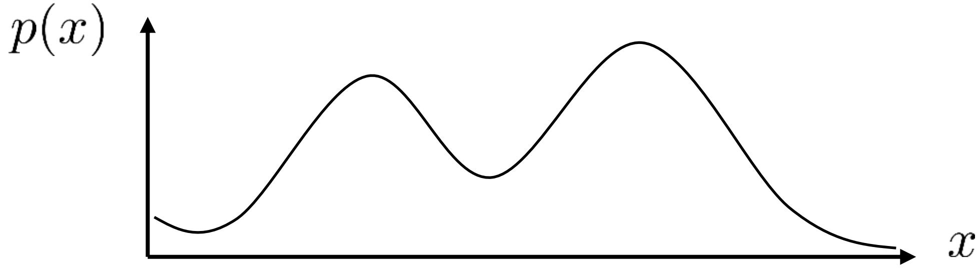


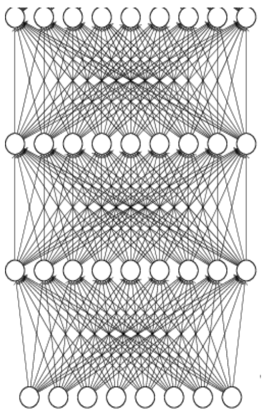
Latent variable models in general

$$p(x) = \int p(x|z)p(z)dz$$

“easy” distribution
(e.g., conditional Gaussian)

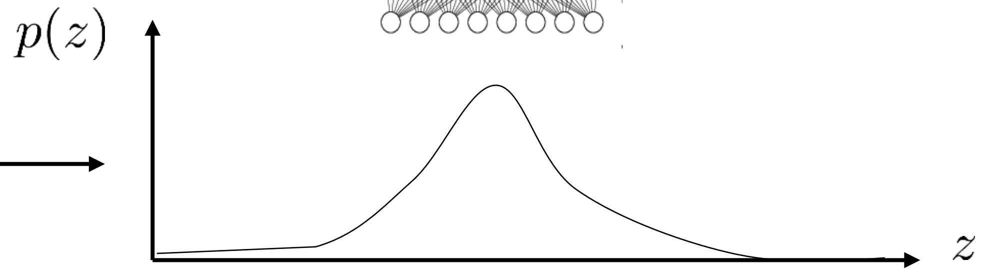
“easy” distribution
(e.g., Gaussian)





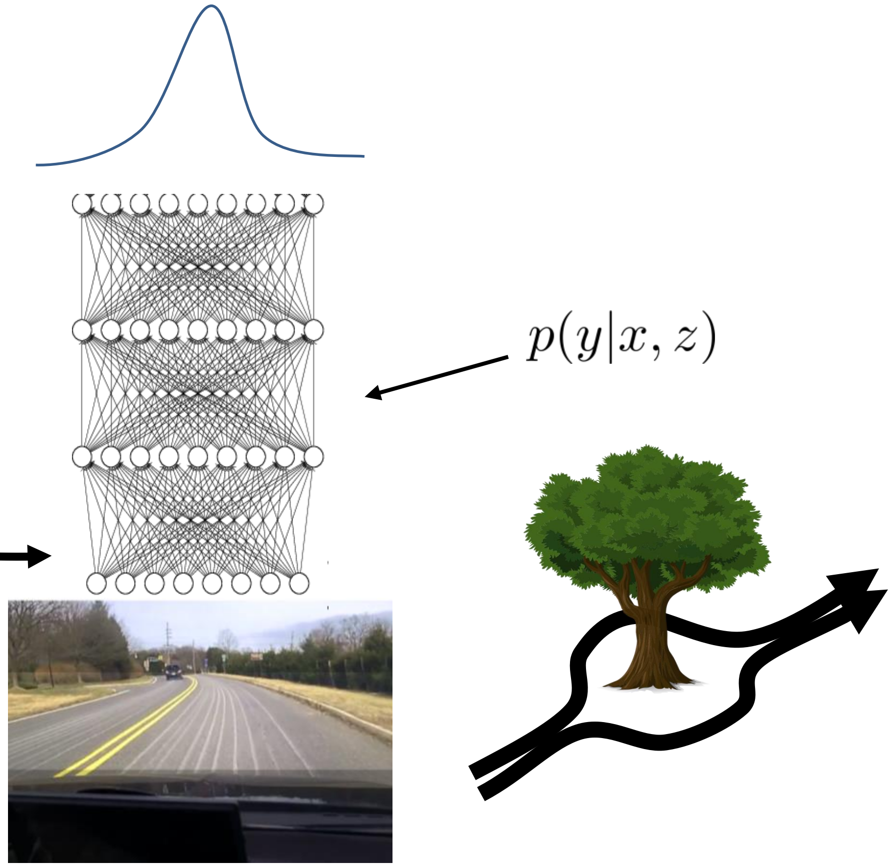
$$p(x|z) = \mathcal{N}(\mu_{\text{nn}}(z), \sigma_{\text{nn}}(z))$$

“easy” distribution
(e.g., Gaussian)



Latent variable models in RL

conditional latent variable models for multi-modal policies

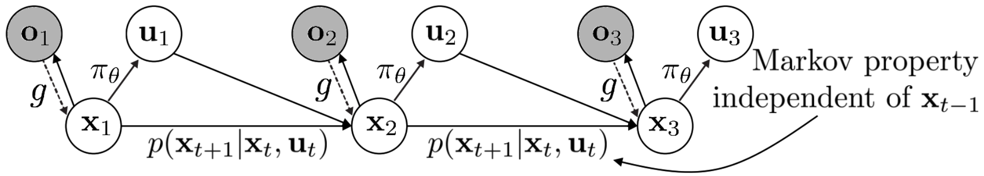


$p(z)$

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

$p(y|x, z)$

latent variable models for model-based RL

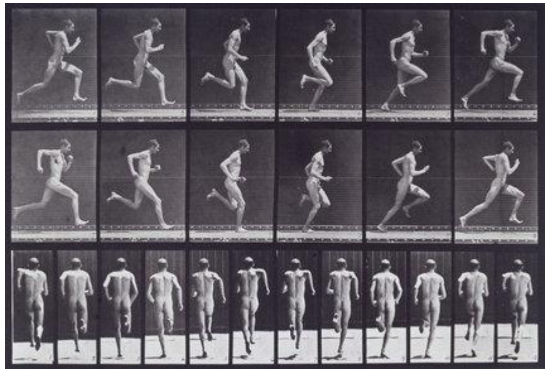


$p(o_t|x_t)$ actually models $p(x_{t+1}|x_t)$ and $p(x_1)$

$p(x_t)$ latent space has *structure*

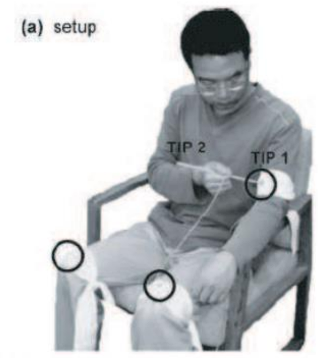
Other places we'll see latent variable models

Using RL/control + variational inference to model human behavior



Muybridge (c. 1870)

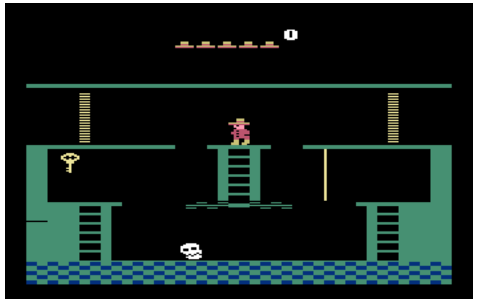
Mombaur et al. '09



Li & Todorov '06

Ziebart '08

Using generative models and variational inference for exploration



How do we train latent variable models?

the model: $p_\theta(x)$

the data: $\mathcal{D} = \{x_1, x_2, x_3, \ldots, x_N\}$

maximum likelihood fit:

$$\theta \leftarrow \arg\max_\theta \frac{1}{N} \sum_i \log p_\theta(x_i)$$

$$p(x) = \int p(x|z)p(z)dz$$

$$\theta \leftarrow \arg\max_\theta \frac{1}{N} \sum_i \log \left(\int p_\theta(x_i|z)p(z)dz \right)$$

completely intractable

Estimating the log-likelihood

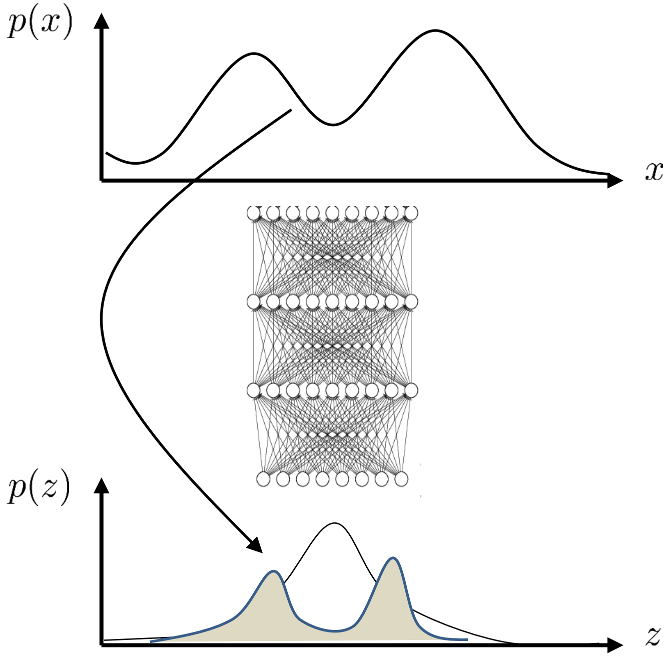
alternative: *expected* log-likelihood:

$$\theta \leftarrow \arg\max_\theta \frac{1}{N} \sum_i E_{z \sim p(z|x_i)}[\log p_\theta(x_i, z)]$$

but... how do we calculate $p(z|x_i)$?

intuition: "guess" most likely z given x_i, and pretend it's the right one

...but there are many possible values of z so use the distribution $p(z|x_i)$



Variational Inference

The variational approximation

but... how do we calculate $p(z|x_i)$?

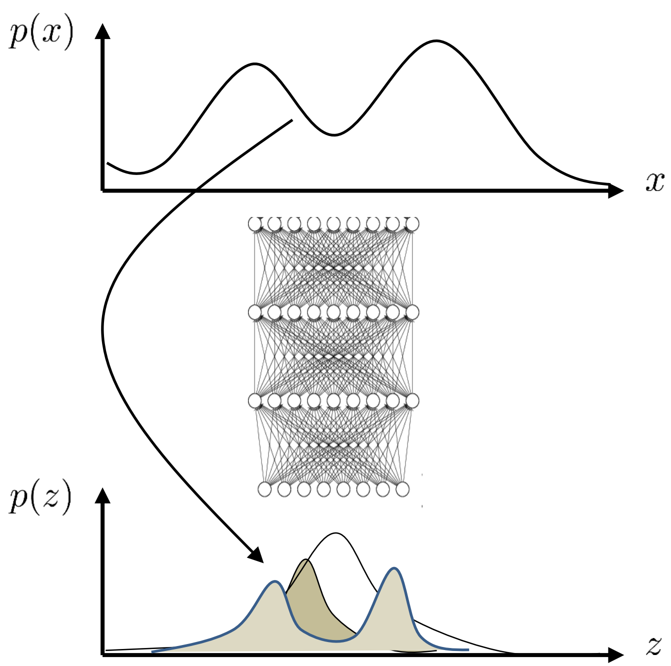
what if we approximate with $q_i(z) = \mathcal{N}(\mu_i, \sigma_i)$

can bound $\log p(x_i)$!

$$\log p(x_i) = \log \int_z p(x_i|z)p(z)$$

$$= \log \int_z p(x_i|z)p(z)\frac{q_i(z)}{q_i(z)}$$

$$= \log E_{z\sim q_i(z)}\left[\frac{p(x_i|z)p(z)}{q_i(z)}\right]$$



The variational approximation

Jensen's inequality

$$\log E[y] \geq E[\log y]$$

but... how do we calculate $p(z|x_i)$?

can bound $\log p(x_i)$!

$$\log p(x_i) = \log \int_z p(x_i|z)p(z)$$

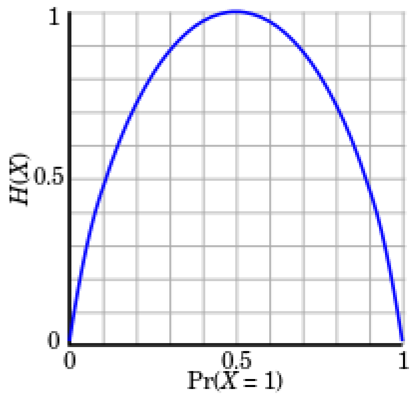
$$= \log \int_z p(x_i|z)p(z)\frac{q_i(z)}{q_i(z)}$$

$$= \log E_{z\sim q_i(z)}\left[\frac{p(x_i|z)p(z)}{q_i(z)}\right]$$

maximizing this maximizes $\log p(x_i)$

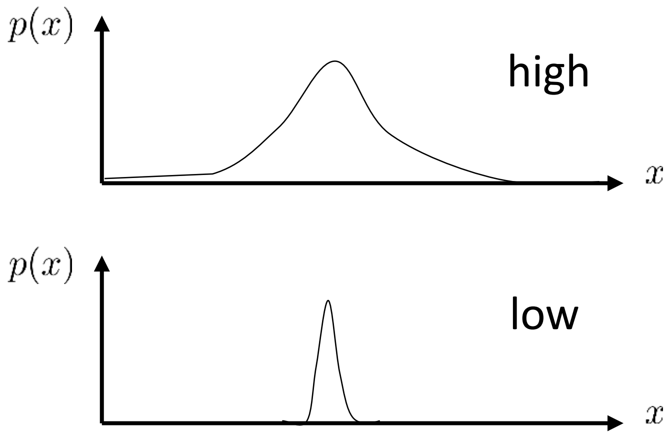
$$\geq E_{z\sim q_i(z)}\left[\log \frac{p(x_i|z)p(z)}{q_i(z)}\right] = E_{z\sim q_i(z)}[\log p(x_i|z) + \log p(z)] + H(q_i) E_{z\sim q_i(z)}[\log q_i(z)]$$

A brief aside…



Entropy:

$$\mathcal{H}(p) = -E_{x \sim p(x)}[\log p(x)] = -\int_x p(x) \log p(x) dx$$

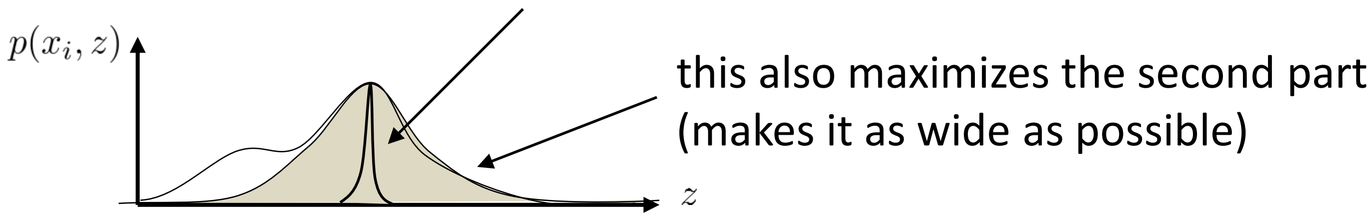


Intuition 1: how *random* is the random variable?

Intuition 2: how large is the log probability in expectation *under itself*

what do we expect this to do?

$$E_{z \sim q_i(z)}[\log p(x_i|z) + \log p(z)] + \mathcal{H}(q_i)$$



A brief aside…

KL-Divergence:

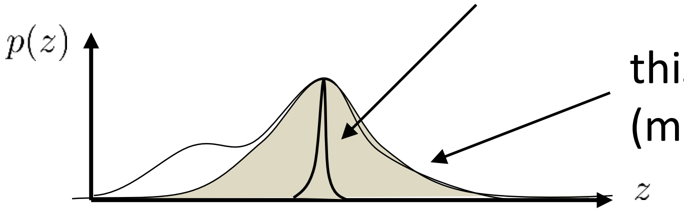
$$D_{\mathrm{KL}}(q\|p) = E_{x\sim q(x)}\left[\log \frac{q(x)}{p(x)}\right] = E_{x\sim q(x)}[\log q(x)] - E_{x\sim q(x)}[\log p(x)] = -E_{x\sim q(x)}[\log p(x)] - \mathcal{H}(q)$$

Intuition 1: how *different* are two distributions?

Intuition 2: how small is the expected log probability of one distribution under another, minus entropy?

why entropy?

this maximizes the first part



this also maximizes the second part
(makes it as wide as possible)

The variational approximation

$$\log p(x_i) \geq \overbrace{E_{z\sim q_i(z)}[\log p(x_i|z) + \log p(z)] + \mathcal{H}(q_i)}^{\mathcal{L}_i(p, q_i)}$$

what makes a good $q_i(z)$?

approximate in what sense?

why?

intuition: $q_i(z)$ should approximate $p(z|x_i)$

compare in terms of KL-divergence: $D_{\mathrm{KL}}(q_i(z)\|p(z|x))$

$$D_{\mathrm{KL}}(q_i(x_i)\|p(z|x_i)) = E_{z\sim q_i(z)}\left[\log \frac{q_i(z)}{p(z|x_i)}\right] = E_{z\sim q_i(z)}\left[\log \frac{q_i(z)p(x_i)}{p(x_i, z)}\right]$$

$$= -E_{z\sim q_i(z)}[\log p(x_i|z) + \log p(z)] + E_{z\sim q_i(z)}[\log q_i(z)] + E_{z\sim q_i(z)}[\log p(x_i)]$$

$$= -E_{z\sim q_i(z)}[\log p(x_i|z) + \log p(z)] - \mathcal{H}(q_i) + \log p(x_i)$$

$$= -\mathcal{L}_i(p, q_i) + \log p(x_i)$$

$$\log p(x_i) = D_{\mathrm{KL}}(q_i(z)\|p(z|x_i)) + \mathcal{L}_i(p, q_i)$$

$$\log p(x_i) \geq \mathcal{L}_i(p, q_i)$$

The variational approximation

$$\log p(x_i) \geq \overbrace{E_{z\sim q_i(z)}[\log p(x_i|z) + \log p(z)] + \mathcal{H}(q_i)}^{\mathcal{L}_i(p, q_i)}$$

$$\log p(x_i) = D_{\mathrm{KL}}(q_i(z)\|p(z|x_i)) + \mathcal{L}_i(p, q_i)$$

$$\log p(x_i) \geq \mathcal{L}_i(p, q_i)$$

$$D_{\mathrm{KL}}(q_i(z)\|p(z|x_i)) = E_{z\sim q_i(z)}\left[\log \frac{q_i(z)}{p(z|x_i)}\right] = E_{z\sim q_i(z)}\left[\log \frac{q_i(z)p(x_i)}{p(x_i, z)}\right]$$

$$= \underbrace{-E_{z\sim q_i(z)}[\log p(x_i|z) + \log p(z)] - \mathcal{H}(q_i)}_{-\mathcal{L}_i(p, q_i)} + \log p(x_i)$$

independent of q_i!

$\Rightarrow$ maximizing $\mathcal{L}_i(p, q_i)$ w.r.t. q_i minimizes KL-divergence!

How do we use this?

$$\log p(x_i) \geq \underbrace{E_{z \sim q_i(z)}[\log p_\theta(x_i|z) + \log p(z)] + \mathcal{H}(q_i)}_{\mathcal{L}_i(p, q_i)}$$

$$\theta \leftarrow \arg\max_\theta \frac{1}{N} \sum_i \log p_\theta(x_i)$$

$$\theta \leftarrow \arg\max_\theta \frac{1}{N} \sum_i \mathcal{L}_i(p, q_i)$$

for each x_i (or mini-batch):

calculate $\nabla_\theta \mathcal{L}_i(p, q_i)$:

sample $z \sim q_i(z)$

$\nabla_\theta \mathcal{L}_i(p, q_i) \approx \nabla_\theta \log p_\theta(x_i|z)$

$\theta \leftarrow \theta + \alpha \nabla_\theta \mathcal{L}_i(p, q_i)$

update q_i to maximize $\mathcal{L}_i(p, q_i)$

how?

let's say $q_i(z) = \mathcal{N}(\mu_i, \sigma_i)$

use gradient $\nabla_{\mu_i} \mathcal{L}_i(p, q_i)$ and $\nabla_{\sigma_i} \mathcal{L}_i(p, q_i)$

gradient ascent on μ_i, σ_i

What’s the problem?

for each x_i (or mini-batch):

calculate $\nabla_\theta \mathcal{L}_i(p, q_i)$:

sample $z \sim q_i(z)$

$\nabla_\theta \mathcal{L}_i(p, q_i) \approx \nabla_\theta \log p_\theta(x_i|z)$

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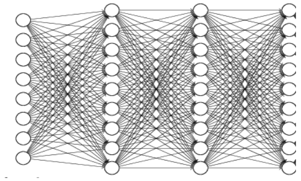
use gradient $\nabla_{\mu_i} \mathcal{L}_i(p, q_i)$ and $\nabla_{\sigma_i} \mathcal{L}_i(p, q_i)$

gradient ascent on μ_i, σ_i

How many parameters are there? $|\theta| + (|\mu_i| + |\sigma_i|) \times N$

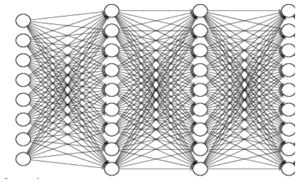
intuition: $q_i(z)$ should approximate $p(z|x_i)$ what if we learn a *network* $q_i(z) = q(z|x_i) \approx p(z|x_i)$?

z



$p_\theta(x|z)$

x



$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$

Amortized Variational Inference

What’s the problem?

for each x_i (or mini-batch):

calculate $\nabla_\theta \mathcal{L}_i(p, q_i)$:

sample $z \sim q_i(z)$

$\nabla_\theta \mathcal{L}_i(p, q_i) \approx \nabla_\theta \log p_\theta(x_i|z)$

$\theta \leftarrow \theta + \alpha \nabla_\theta \mathcal{L}_i(p, q_i)$

update q_i to maximize $\mathcal{L}_i(p, q_i)$

let’s say $q_i(z) = \mathcal{N}(\mu_i, \sigma_i)$

use gradient $\nabla_{\mu_i} \mathcal{L}_i(p, q_i)$ and $\nabla_{\sigma_i} \mathcal{L}_i(p, q_i)$

gradient ascent on μ_i, σ_i

How many parameters are there? $|\theta| + (|\mu_i| + |\sigma_i|) \times N$

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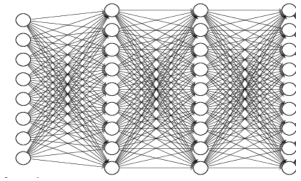
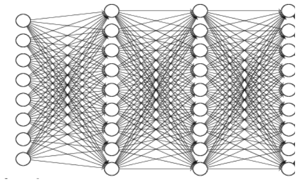
z



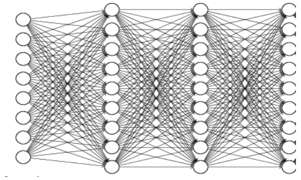
$p_\theta(x|z)$

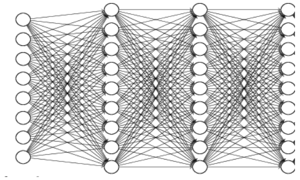
x



$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$

Amortized variational inference

z  $p_\theta(x|z)$

x  $q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$

$$\log p(x_i) \geq \underbrace{E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z) + \log p(z)] + \mathcal{H}(q_\phi(z|x_i))}_{\mathcal{L}(p_\theta(x_i|z), q_\phi(z|x_i))}$$

for each x_i (or mini-batch):

calculate $\nabla_\theta \mathcal{L}(p_\theta(x_i|z), q_\phi(z|x_i))$:

sample $z \sim q_\phi(z|x_i)$

$\nabla_\theta \mathcal{L} \approx \nabla_\theta \log p_\theta(x_i|z)$

$\theta \leftarrow \theta + \alpha \nabla_\theta \mathcal{L}$

$\phi \leftarrow \phi + \alpha \nabla_\phi \mathcal{L}$ ← how do we calculate this?

Amortized variational inference

for each x_i (or mini-batch):

calculate $\nabla_\theta \mathcal{L}(p_\theta(x_i|z), q_\phi(z|x_i))$:

sample $z \sim q_\phi(z|x_i)$

$\nabla_\theta \mathcal{L} \approx \nabla_\theta \log p_\theta(x_i|z)$

$\theta \leftarrow \theta + \alpha \nabla_\theta \mathcal{L}$

$\phi \leftarrow \phi + \alpha \nabla_\phi \mathcal{L}$

$$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$$

look up formula for entropy of a Gaussian

$$\mathcal{L}_i = \underbrace{E_{z\sim q_\phi(z|x_i)}[\log p_\theta(x_i|z) + \log p(z)]}_{J(\phi) = E_{z\sim q_\phi(z|x_i)}[r(x_i, z)]} + \mathcal{H}(q_\phi(z|x_i))$$

can just use policy gradient!

What's wrong with this gradient?

$$\nabla J(\phi) \approx \frac{1}{M} \sum_j \nabla_\phi \log q_\phi(z_j|x_i) r(x_i, z_j)$$

The reparameterization trick

Is there a better way?

$$J(\phi) = E_{z \sim q_\phi(z|x_i)}[r(x_i, z)]$$
$$= E_{\epsilon \sim \mathcal{N}(0,1)}[r(x_i, \mu_\phi(x_i) + \epsilon\sigma_\phi(x_i))]$$

$$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$$

$$z = \mu_\phi(x) + \epsilon\sigma_\phi(x)$$

$\epsilon \sim \mathcal{N}(0,1)$

independent of ϕ!

estimating $\nabla_\phi J(\phi)$:

sample $\epsilon_1, \ldots, \epsilon_M$ from $\mathcal{N}(0,1)$ (a single sample works well!)

$$\nabla_\phi J(\phi) \approx \frac{1}{M} \sum_j \nabla_\phi r(x_i, \mu_\phi(x_i) + \epsilon_j \sigma_\phi(x_i))$$

most autodiff software (e.g., TensorFlow) will compute this for you!

Another way to look at it...

$$\mathcal{L}_i = E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z) + \log p(z)] + \mathcal{H}(q_\phi(z|x_i))$$

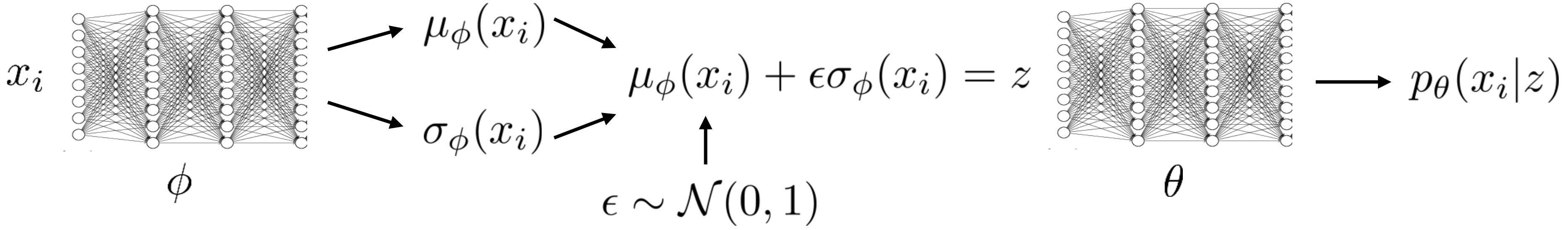
$$= E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z)] + \underbrace{E_{z \sim q_\phi(z|x_i)}[\log p(z)] + \mathcal{H}(q_\phi(z|x_i))}_{-D_{\mathrm{KL}}(q_\phi(z|x_i)\|p(z))}$$

$-D_{\mathrm{KL}}(q_\phi(z|x_i)\|p(z))$ ← this often has a convenient analytical form (e.g., KL-divergence for Gaussians)

$$= E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z)] - D_{\mathrm{KL}}(q_\phi(z|x_i)\|p(z))$$

$$= E_{\epsilon \sim \mathcal{N}(0,1)}[\log p_\theta(x_i|\mu_\phi(x_i) + \epsilon\sigma_\phi(x_i))] - D_{\mathrm{KL}}(q_\phi(z|x_i)\|p(z))$$

$$\approx \log p_\theta(x_i|\mu_\phi(x_i) + \epsilon\sigma_\phi(x_i)) - D_{\mathrm{KL}}(q_\phi(z|x_i)\|p(z))$$



Reparameterization trick vs. policy gradient

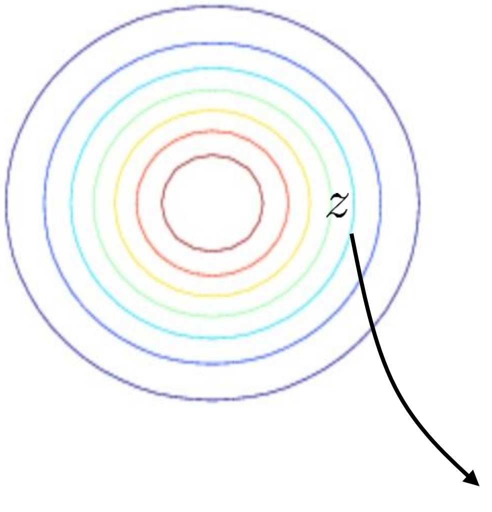
- Policy gradient
  - Can handle both discrete and continuous latent variables
  - High variance, requires multiple samples & small learning rates
- Reparameterization trick
  - Only continuous latent variables
  - Very simple to implement
  - Low variance

$$J(\phi) \approx \frac{1}{M} \sum_j \nabla_\phi \log q_\phi(z_j|x_i) r(x_i, z_j)$$

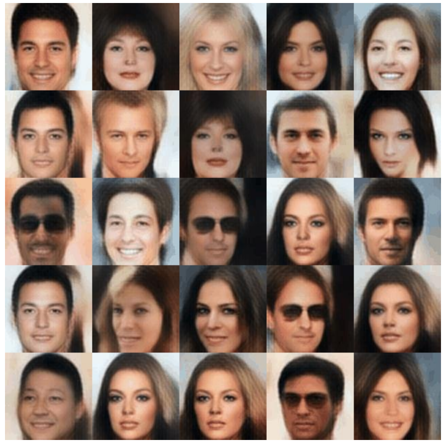
$$\nabla_\phi J(\phi) \approx \frac{1}{M} \sum_j \nabla_\phi r(x_i, \mu_\phi(x_i) + \epsilon_j \sigma_\phi(x_i))$$

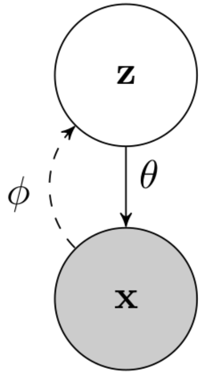
Example Models

The *variational* autoencoder

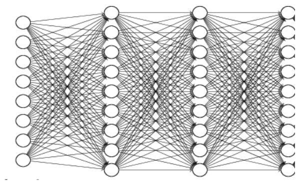


$p_\theta(x|z)$



$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$ 

$p_\theta(x|z) = \mathcal{N}(\mu_\theta(z), \sigma_\theta(z))$

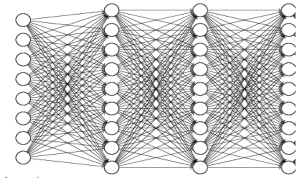
x_i  ϕ

$\mu_\phi(x_i)$

$\sigma_\phi(x_i)$

$\mu_\phi(x_i) + \epsilon\sigma_\phi(x_i) = z$

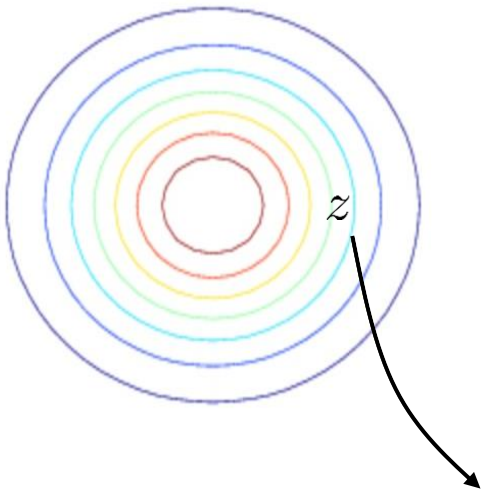
$\epsilon \sim \mathcal{N}(0, 1)$

 θ

$\longrightarrow p_\theta(x|z)$

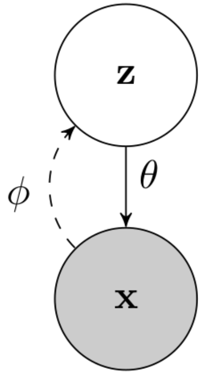
$$\max_{\theta,\phi} \frac{1}{N} \sum_i \log p_\theta(x_i|\mu_\phi(x_i) + \epsilon\sigma_\phi(x_i)) - D_{\mathrm{KL}}(q_\phi(z|x_i) \| p(z))$$

Using the variational autoencoder

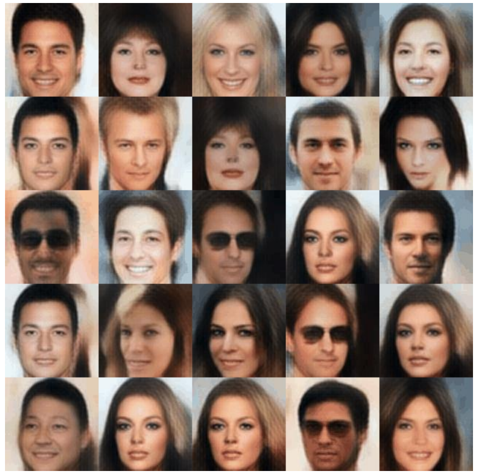


$p_\theta(x|z)$

$q_\phi(z|x) = \mathcal{N}(\mu_\phi(x), \sigma_\phi(x))$



$p_\theta(x|z) = \mathcal{N}(\mu_\theta(z), \sigma_\theta(z))$



$$p(x) = \int p(x|z)p(z)dz$$

why does this work?

sampling:

$z \sim p(z)$

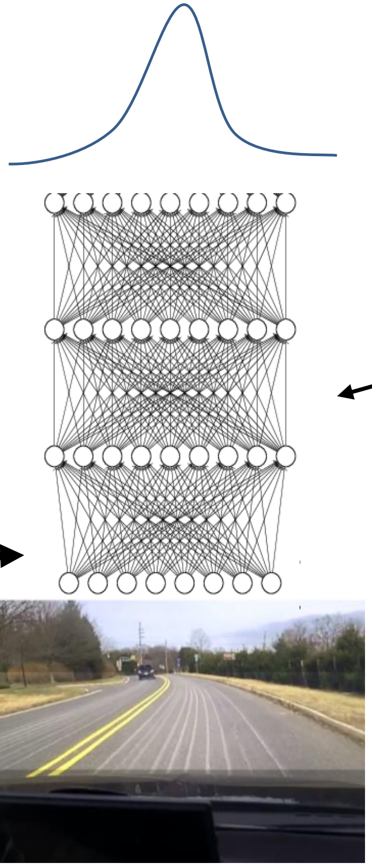
$x \sim p(x|z)$

$$\mathcal{L}_i = E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z)] - D_{\mathrm{KL}}(q_\phi(z|x_i) \| p(z))$$

Conditional models

$$\mathcal{L}_i = E_{z \sim q_\phi(z|x_i,y_i)}[\log p_\theta(y_i|x_i,z) + \log p(z|x_i)] + \mathcal{H}(q_\phi(z|x_i,y_i))$$

just like before, only now generating y_i
and *everything* is conditioned on x_i



$p(y|x,z)$

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

$p(z)$

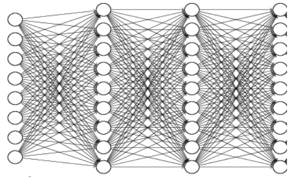
can *optionally* depend on x

at test time:

$z \sim p(z|x_i)$

$y \sim p(y|x_i, z)$

x_i
y_i



ϕ

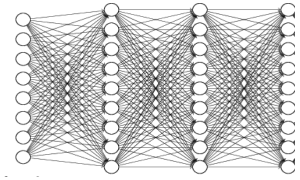
$\mu_\phi(x_i, y_i)$

$\sigma_\phi(x_i, y_i)$

$\mu_\phi + \epsilon\sigma_\phi = z$

$\epsilon \sim \mathcal{N}(0, 1)$

x_i



θ

$p_\theta(y_i|x_i, z)$

Examples

Embed to Control: A Locally Linear Latent Dynamics Model for Control from Raw Images

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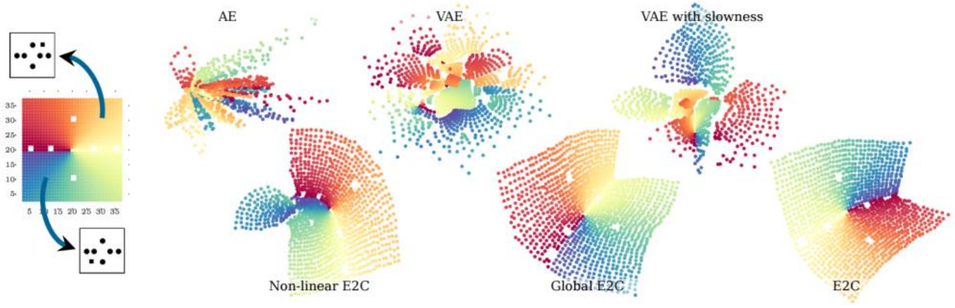
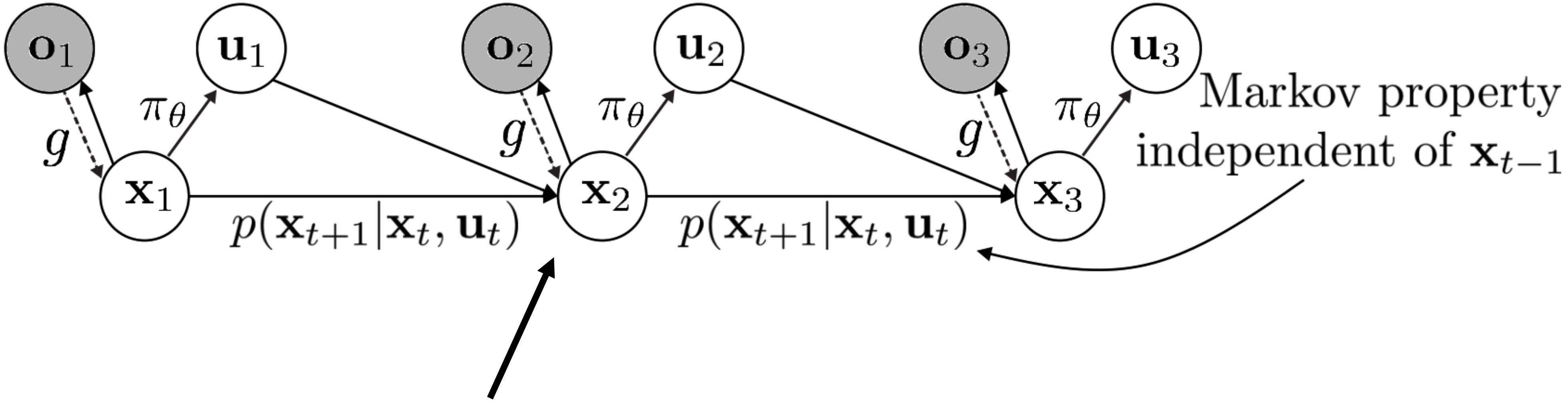


Swing-up with the E2C algorithm

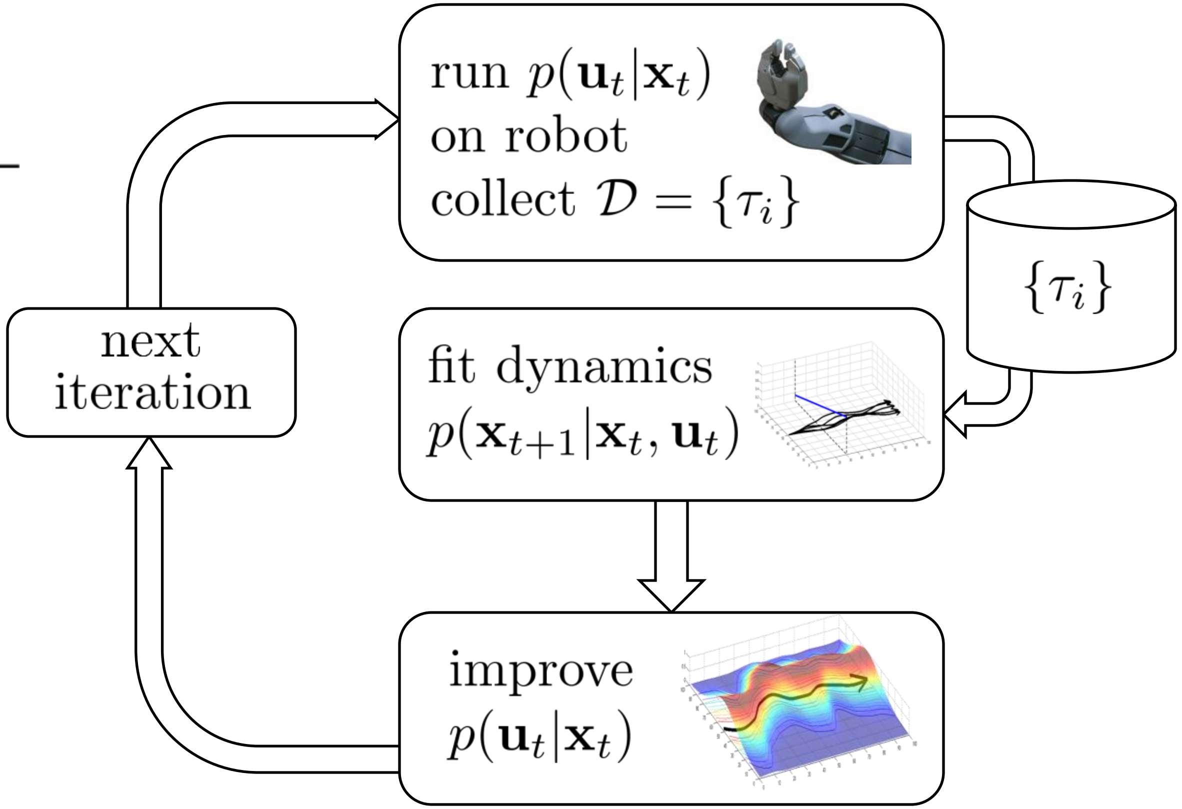
1. collect data
2. learn embedding of image & dynamics model (**jointly**)
3. run iLQG to learn to reach image of goal



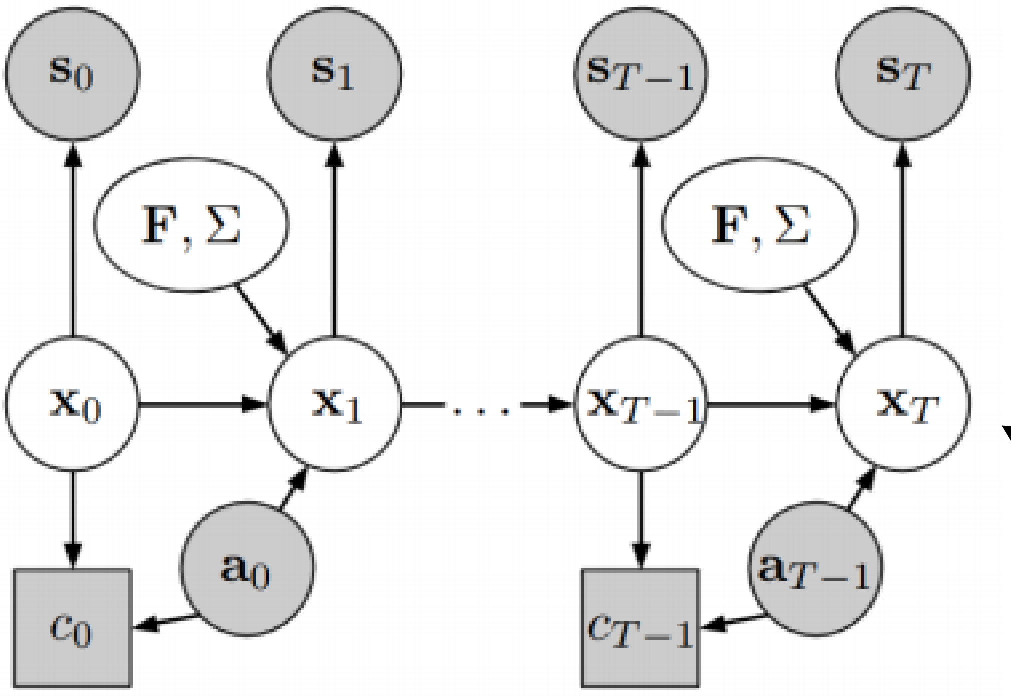
a type of variational autoencoder with temporally decomposed latent state!

Local models with images

SOLAR: Deep Structured Latent Representations for Model-Based Reinforcement Learning



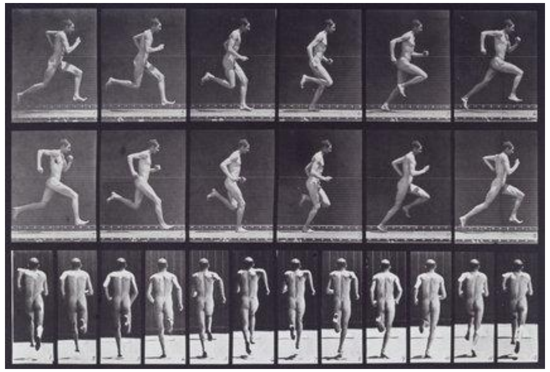
Local models with images



variational autoencoder with stochastic dynamics

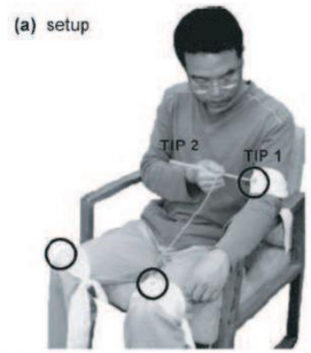
We’ll see more of this for…

Using RL/control + variational inference to model human behavior



Muybridge (c. 1870)

Mombaur et al. ‘09



Li & Todorov ‘06

Ziebart ‘08

Using generative models and variational inference for exploration