Variational Inference and Generative Models

CS 285

Instructor: Sergey Levine

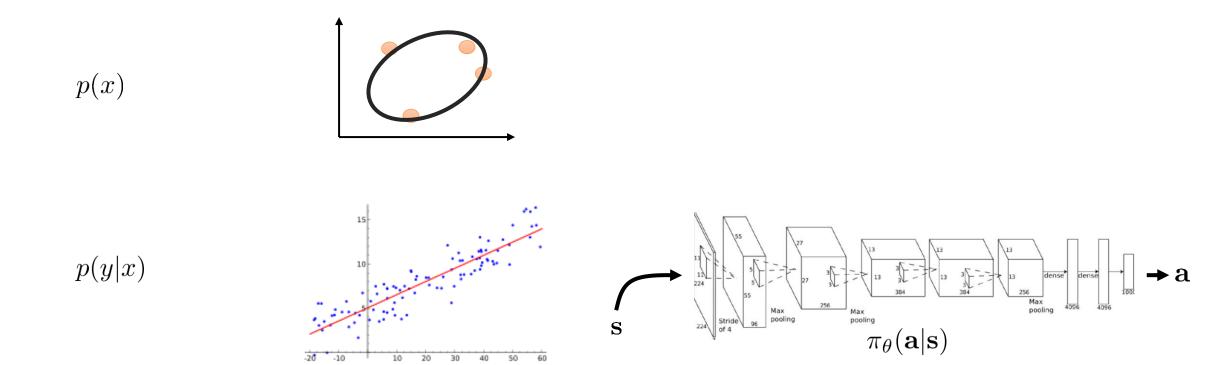
UC Berkeley



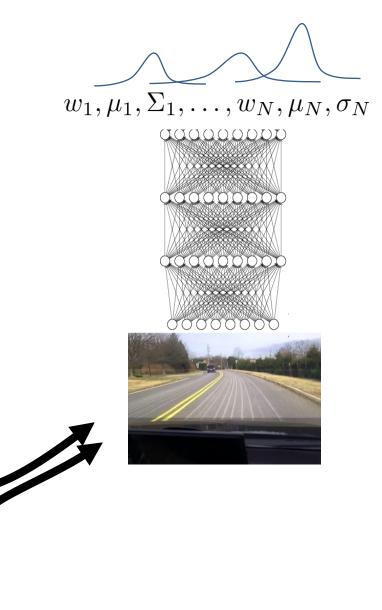
Today's Lecture

- 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



Latent variable models

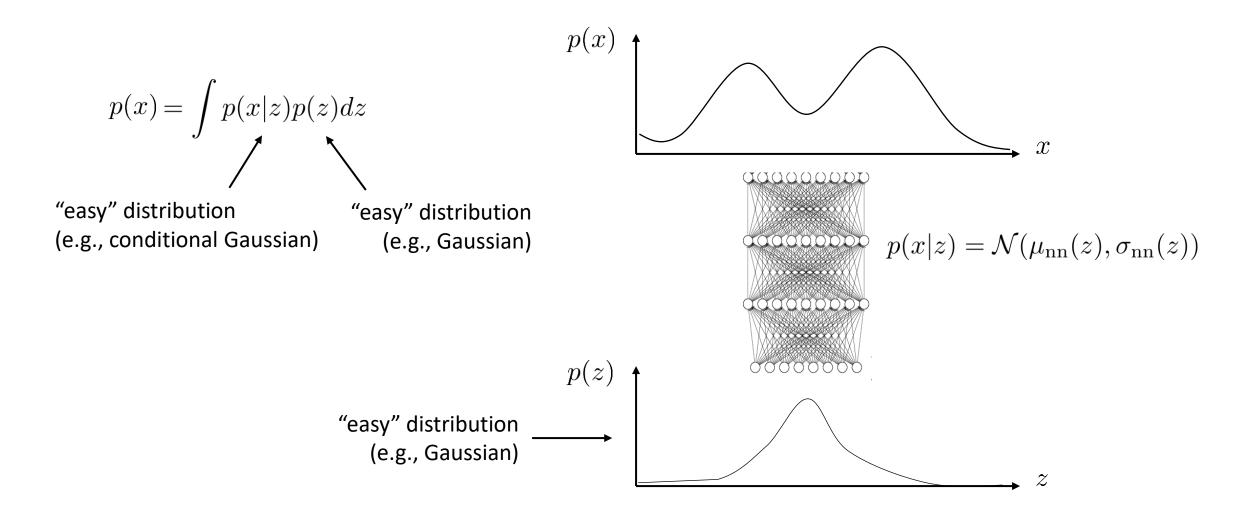


$$p(x) = \sum_{z} p(x|z)p(z)$$

$$\underset{\text{mixture element}}{\text{mixture}}$$

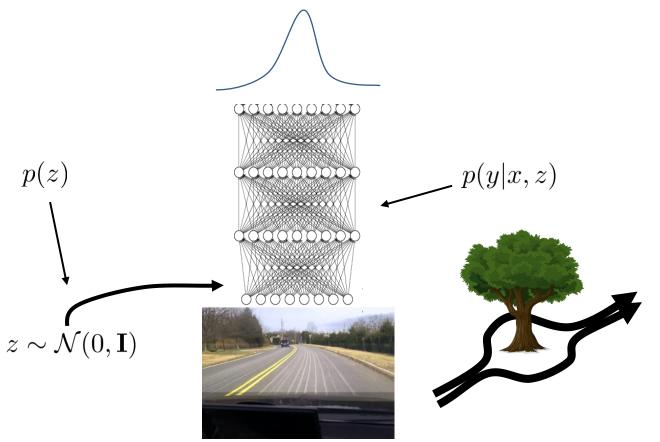
$$p(y|x) = \sum_{z} p(y|x, z)p(z)$$

Latent variable models in general

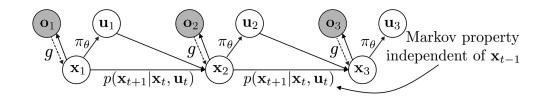


Latent variable models in RL

conditional latent variable models for multi-modal policies



latent variable models for model-based RL

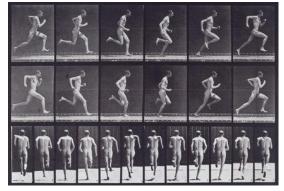


 $p(o_t|x_t)$ actually models $p(x_{t+1}|x_t)$ and $p(x_1)$

 $p(x_t)$ 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

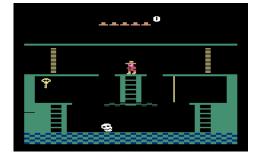


Li & Todorov '06



Ziebart '08

Using generative models and variational inference for exploration



How do we train latent variable models?

the model: $p_{\theta}(x)$

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

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

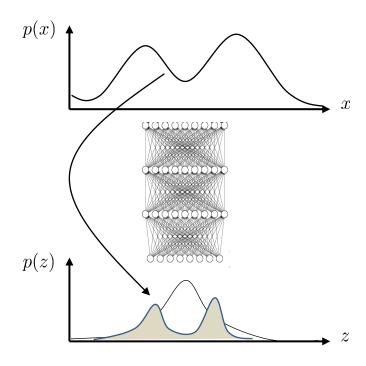
alternative: expected log-likelihood:

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

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 $p(z|x_i)$?

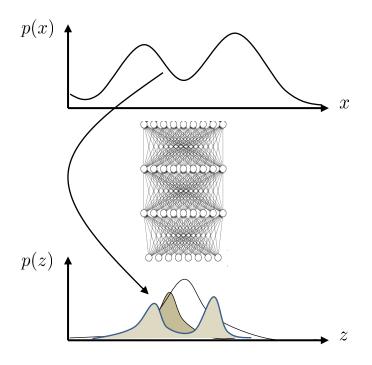
can bound $\log p(x_i)!$

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

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

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

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



The variational approximation

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

can bound $\log p(x_i)!$

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

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

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

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

Jensen's inequality

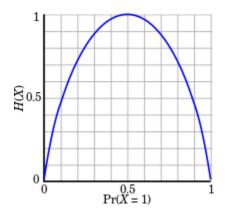
$$\log E[y] \ge E[\log y]$$

maximizing this maximizes $\log p(x_i)$



$$\geq E_{z \sim q_i(z)} \left[\log \frac{p(x_i|z)p(z)}{q_i(z)} \right] = E_{z \sim q_i(z)} [\log p(x_i|z) + \log p(z)] + \mathcal{H}_{\mathbb{A}}(q_{i_l}(z)) [\log q_i(z)]$$

A brief aside...



Entropy:

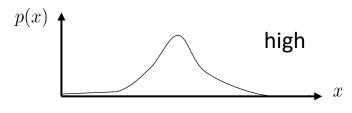
$$\mathcal{H}(p) = -E_{x \sim p(x)}[\log p(x)] = -\int_{x} p(x) \log p(x) dx$$

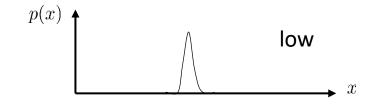
Intuition 1: how random is the random variable?

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

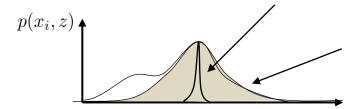
what do we expect this to do?

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





this maximizes the first part



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

A brief aside...

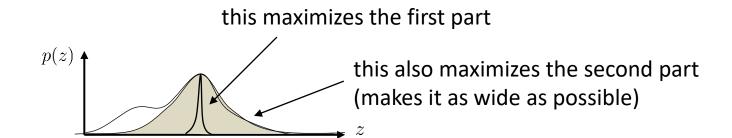
KL-Divergence:

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

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?



The variational approximation

$$\mathcal{L}_{i}(p, q_{i})$$

$$\log p(x_{i}) \geq E_{z \sim q_{i}(z)} [\log p(x_{i}|z) + \log p(z)] + \mathcal{H}(q_{i})$$

what makes a good $q_i(z)$? approximate in what sense? intuition: $q_i(z)$ should approximate $p(z|x_i)$ compare in terms of KL-divergence: $D_{KL}(q_i(z)||p(z|x))$

why?

wny?
$$D_{\text{KL}}(q_{i}(x_{i})||p(z|x_{i})) = E_{z \sim q_{i}(z)} \left[\log \frac{q_{i}(z)}{p(z|x_{i})} \right] = E_{z \sim q_{i}(z)} \left[\log \frac{q_{i}(z)p(x_{i})}{p(x_{i},z)} \right]$$

$$= -E_{z \sim q_{i}(z)} [\log p(x_{i}|z) + \log p(z)] + E_{z \sim q_{i}(z)} [\log q_{i}(z)] + E_{z \sim q_{i}(z)} [\log p(x_{i})]$$

$$= -E_{z \sim q_{i}(z)} [\log p(x_{i}|z) + \log p(z)] - \mathcal{H}(q_{i}) + \log p(x_{i})$$

$$= -\mathcal{L}_{i}(p, q_{i}) + \log p(x_{i})$$

$$\log p(x_{i}) = D_{\text{KL}}(q_{i}(z)||p(z|x_{i})) + \mathcal{L}_{i}(p, q_{i})$$

$$\log p(x_{i}) \geq \mathcal{L}_{i}(p, q_{i})$$

The variational approximation

$$\mathcal{L}_{i}(p, q_{i})$$

$$\log p(x_{i}) \geq E_{z \sim q_{i}(z)}[\log p(x_{i}|z) + \log p(z)] + \mathcal{H}(q_{i})$$

$$\log p(x_{i}) = D_{\mathrm{KL}}(q_{i}(z)||p(z|x_{i})) + \mathcal{L}_{i}(p, q_{i})$$

$$\log p(x_{i}) \geq \mathcal{L}_{i}(p, q_{i})$$

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

$$= -E_{z \sim q_{i}(z)}[\log p(x_{i}|z) + \log p(z)] - \mathcal{H}(q_{i}) + \log p(x_{i})$$

$$-\mathcal{L}_{i}(p, q_{i}) \qquad \text{independent of } q_{i}!$$

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

How do we use this?

$$\mathcal{L}_{i}(p, q_{i})$$

$$\log p(x_{i}) \geq E_{z \sim q_{i}(z)} [\log p_{\theta}(x_{i}|z) + \log p(z)] + \mathcal{H}(q_{i})$$

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

$$\theta \leftarrow \arg\max_{\theta} \frac{1}{N} \sum_{i} \mathcal{L}_{i}(p, q_{i})$$

how?

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

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 $\nabla_{\sigma_i} \mathcal{L}_i(p, q_i)$

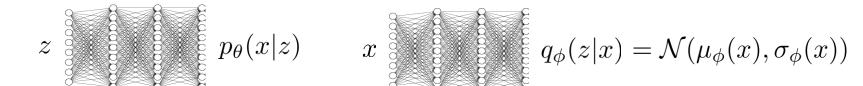
gradient ascent on μ_i , σ_i

How many parameters are there?

$$|\theta| + (|\mu_i| + |\sigma_i|) \times N$$

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

what if we learn a network $q_i(z) = q(z|x_i) \approx p(z|x_i)$?



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 $\nabla_{\sigma_i} \mathcal{L}_i(p, q_i)$

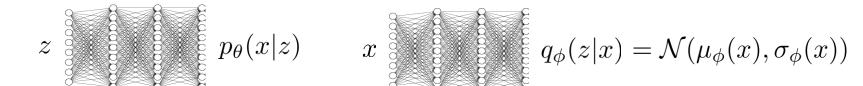
gradient ascent on μ_i , σ_i

How many parameters are there?

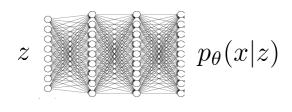
$$|\theta| + (|\mu_i| + |\sigma_i|) \times N$$

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

what if we learn a network $q_i(z) = q(z|x_i) \approx p(z|x_i)$?



Amortized variational inference



 $x = \begin{cases} 0 & \text{if } q_{\phi}(z|x) = \mathcal{N}(\mu_{\phi}(x), \sigma_{\phi}(x)) \end{cases}$

for each
$$x_i$$
 (or mini-batch):
calculate $\nabla_{\theta} \mathcal{L}(p_{\theta}(x_i|z), q_{\phi}(z|x_i))$:
sample $z \sim q_{\phi}(z|x_i)$
 $\nabla_{\theta} \mathcal{L} \approx \nabla_{\theta} \log p_{\theta}(x_i|z)$

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

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

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

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

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 $z \sim q_{\phi}(z|x_i)$

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

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

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

$$\mathcal{L}(\phi) = E_{z \sim q_{\phi}(z|x_i)}[r(x_i, z)]$$

can just use policy gradient!

What's wrong with this gradient?

$$\nabla J(\phi) \approx \frac{1}{M} \sum_{i} \nabla_{\phi} \log q_{\phi}(z_{j}|x_{i}) r(x_{i}, z_{j})$$

The reparameterization trick

Is there a better way?

$$J(\phi) = E_{z \sim q_{\phi}(z|x_{i})}[r(x_{i}, z)] \qquad q_{\phi}(z|x) = \mathcal{N}(\mu_{\phi}(x), \sigma_{\phi}(x))$$

$$= E_{\epsilon \sim \mathcal{N}(0,1)}[r(x_{i}, \mu_{\phi}(x_{i}) + \epsilon \sigma_{\phi}(x_{i}))] \qquad z = \mu_{\phi}(x) + \epsilon \sigma_{\phi}(x)$$
estimating $\nabla_{\phi}J(\phi)$:
$$\text{sample } \epsilon_{1}, \dots, \epsilon_{M} \text{ from } \mathcal{N}(0, 1) \quad \text{(a single sample works well!)} \qquad \epsilon \sim \mathcal{N}(0, 1)$$

$$\nabla_{\phi}J(\phi) \approx \frac{1}{M} \sum_{i} \nabla_{\phi}r(x_{i}, \mu_{\phi}(x_{i}) + \epsilon_{j}\sigma_{\phi}(x_{i})) \qquad \text{independent of } \phi!$$

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

Another way to look at it...

$$\begin{split} \mathcal{L}_i &= E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z) + \log p(z)] + \mathcal{H}(q_\phi(z|x_i)) \\ &= E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z)] + E_{z \sim q_\phi(z|x_i)}[\log p(z)] + \mathcal{H}(q_\phi(z|x_i)) \\ &\qquad \qquad - D_{\mathrm{KL}}(q_\phi(z|x_i) \| p(z)) &\longleftarrow \text{ this often has a convenient analytical form (e.g., KL-divergence for Gaussians)} \\ &= E_{z \sim q_\phi(z|x_i)}[\log p_\theta(x_i|z)] - D_{\mathrm{KL}}(q_\phi(z|x_i) \| p(z)) \\ &= E_{\epsilon \sim \mathcal{N}(0,1)}[\log p_\theta(x_i|\mu_\phi(x_i) + \epsilon \sigma_\phi(x_i))] - D_{\mathrm{KL}}(q_\phi(z|x_i) \| p(z)) \\ &\approx \log p_\theta(x_i|\mu_\phi(x_i) + \epsilon \sigma_\phi(x_i)) - D_{\mathrm{KL}}(q_\phi(z|x_i) \| p(z)) \end{split}$$

$$x_{i} = \begin{array}{c} \mu_{\phi}(x_{i}) \\ \downarrow \\ \phi \end{array} \qquad \begin{array}{c} \mu_{\phi}(x_{i}) \\ \uparrow \\ \epsilon \sim \mathcal{N}(0, 1) \end{array} \qquad \begin{array}{c} \mu_{\phi}(x_{i}) \\ \downarrow \\ \theta \end{array} \qquad \begin{array}{c} \mu_{\phi}(x_{i}) \\ \downarrow \\ \theta \end{array} \qquad \begin{array}{c} \mu_{\theta}(x_{i}|z) \\ \downarrow \\ \theta \end{array}$$

Reparameterization trick vs. policy gradient

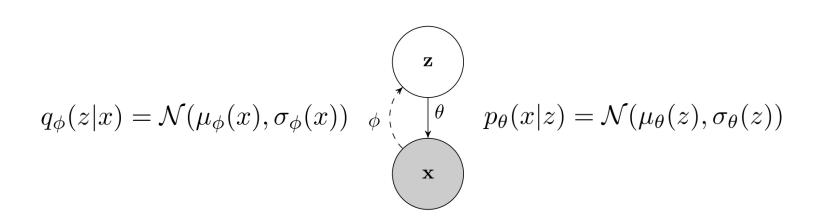
- Policy gradient
 - Can handle both discrete and continuous latent variables
 - High variance, requires multiple samples & small learning rates
- Reparameterization trick
 - Only continuous latent variables
 - Very simple to implement
 - Low variance

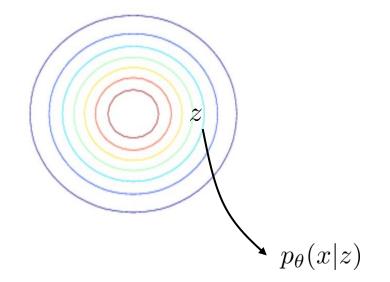
$$J(\phi) \approx \frac{1}{M} \sum_{j} \nabla_{\phi} \log q_{\phi}(z_{j}|x_{i}) r(x_{i}, z_{j})$$

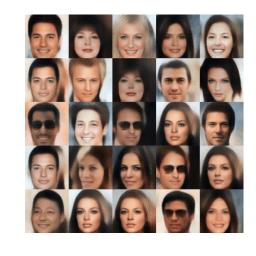
$$\nabla_{\phi} J(\phi) \approx \frac{1}{M} \sum_{j} \nabla_{\phi} r(x_i, \mu_{\phi}(x_i) + \epsilon_j \sigma_{\phi}(x_i))$$

Example Models

The variational autoencoder

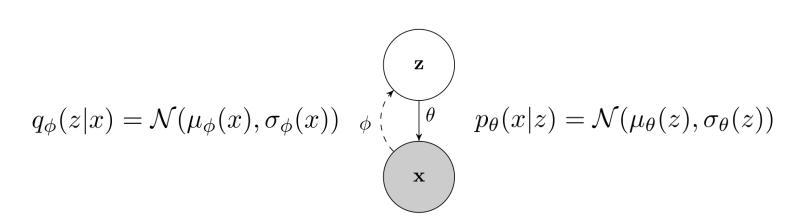


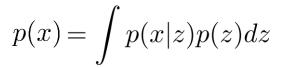




$$\max_{\theta,\phi} \frac{1}{N} \sum_{i} \log p_{\theta}(x_i | \mu_{\phi}(x_i) + \epsilon \sigma_{\phi}(x_i)) - D_{\mathrm{KL}}(q_{\phi}(z|x_i) || p(z))$$

Using the variational autoencoder





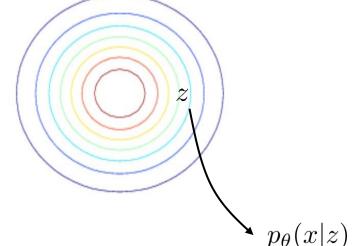
why does this work?

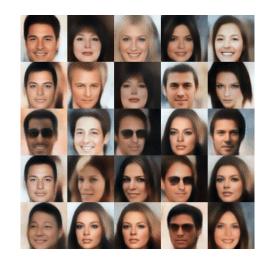
 $\mathcal{L}_i = E_{z \sim q_{\phi}(z|x_i)}[\log p_{\theta}(x_i|z)] - D_{\mathrm{KL}}(q_{\phi}(z|x_i)||p(z))$

sampling:

$$z \sim p(z)$$

$$x \sim p(x|z)$$





Conditional models

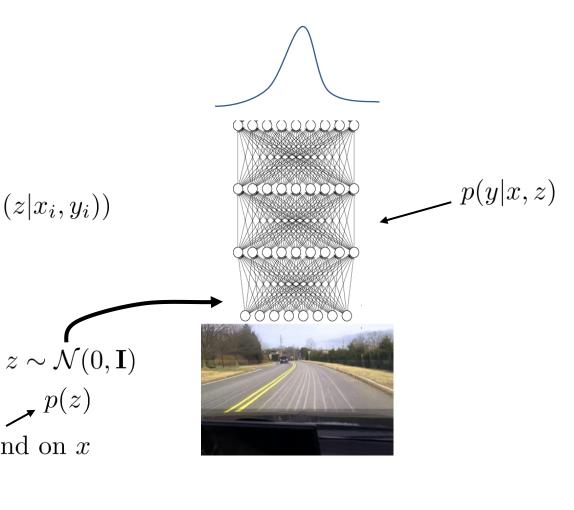
$$\mathcal{L}_i = E_{z \sim q_{\phi}(z|x_i, y_i)} [\log p_{\theta}(y_i|x_i, z) + \log p(z|x_i)] + \mathcal{H}(q_{\phi}(z|x_i, y_i))$$

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

at test time:

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

can optionally depend on x



Examples

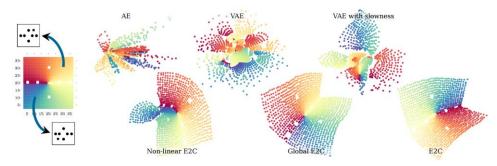
Embed to Control: A Locally Linear Latent Dynamics Model for Control from Raw Images

Manuel Watter* Jost Tobias Springenberg* Joschka Boedecker

University of Freiburg, Germany

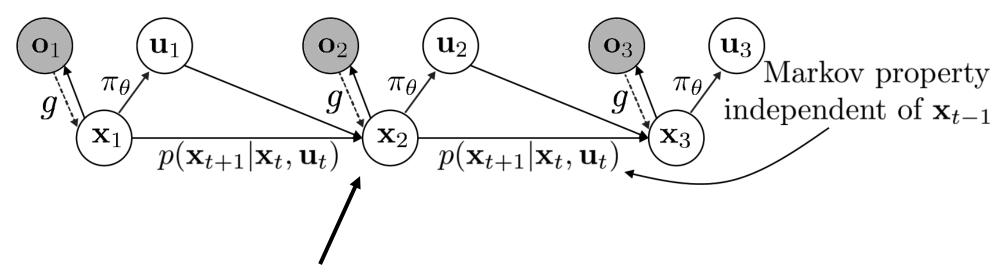
{watterm, springj, jboedeck}@cs.uni-freiburg.de

Martin Riedmiller
Google DeepMind
London, UK
riedmiller@google.com



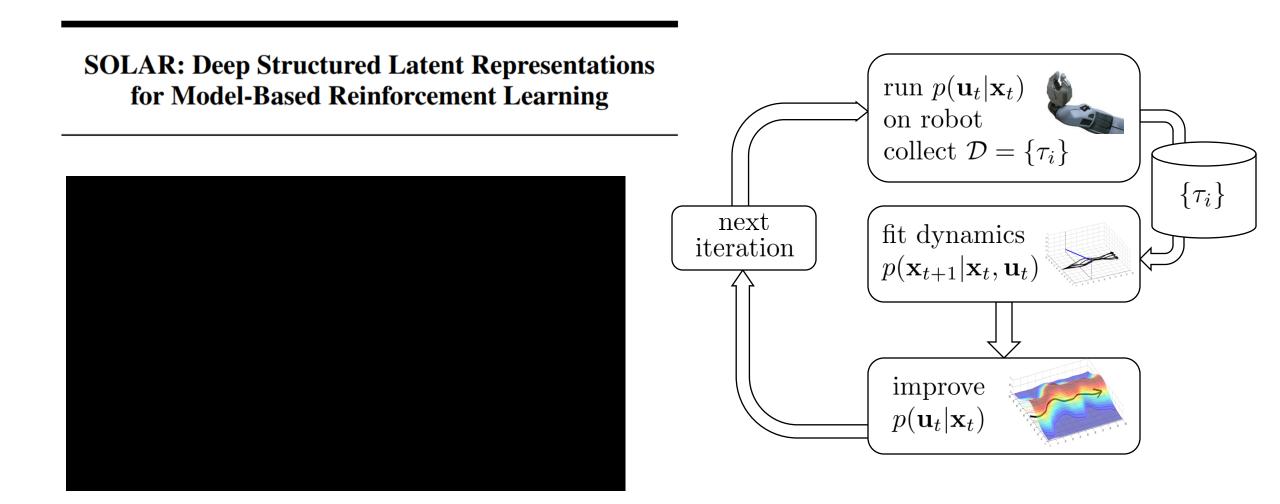
Swing-up with the E2C algorithm

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

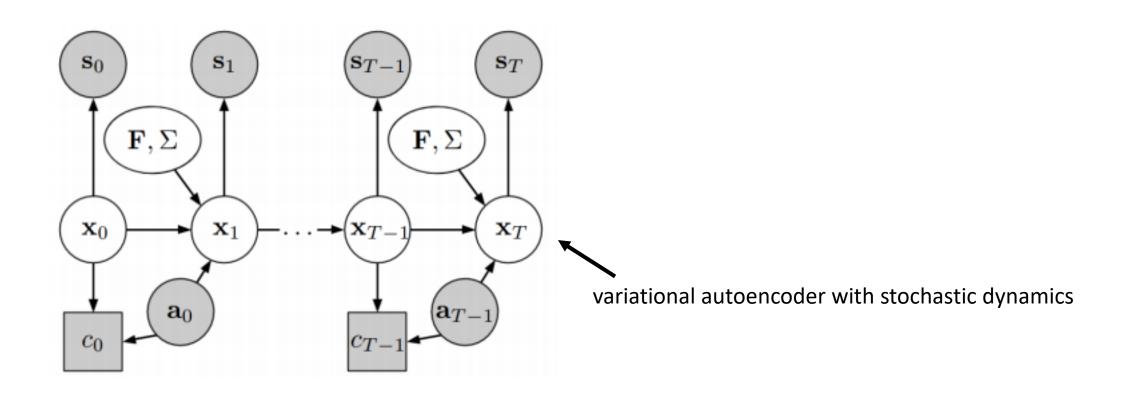


a type of variational autoencoder with temporally decomposed latent state!

Local models with images

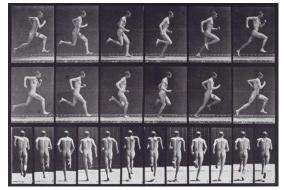


Local models with images



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



Using generative models and variational inference for exploration

