Model learning with structured latent representations

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UCSD

Background

Background
- Probabilistic graphical models
- Model learning
- Variational inference

Structured variational autoencoder
- Model learning

Conclusion
- Applications
- Current work

Probabilistic graphical models

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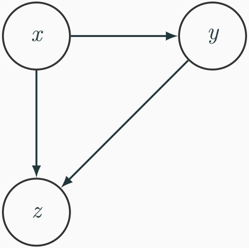

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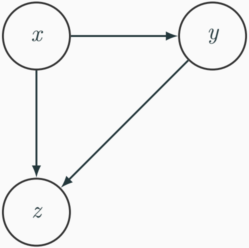

The joint distribution factorizes as

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

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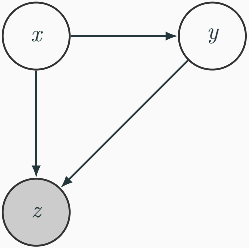

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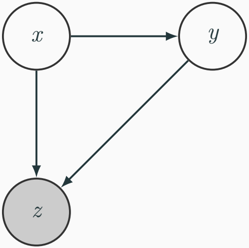

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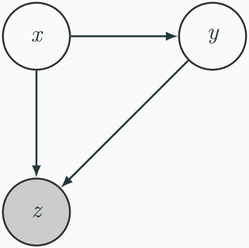

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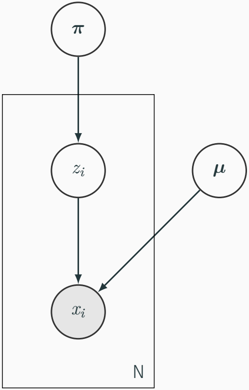
This can be computed via Bayes rule:

$$p(x, y|z) = \frac{p(x, y, z)}{p(z)} = \frac{p(x)p(y|x)p(z|x, y)}{\int p(x)p(y|x)p(z|x, y)\,dxdy}$$

Example PGM

Latent variable model: Gaussian mixture model



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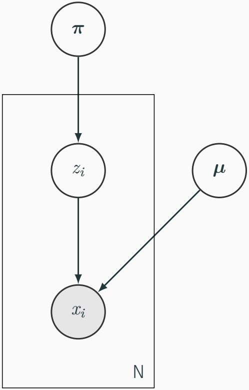

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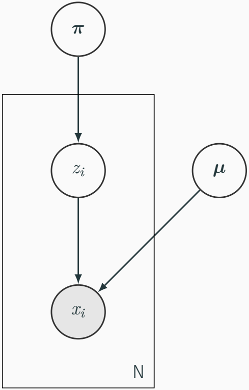

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Global variables: μ, π

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Two random variables x and y whose distribution is

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- Dirichlet/multinomial

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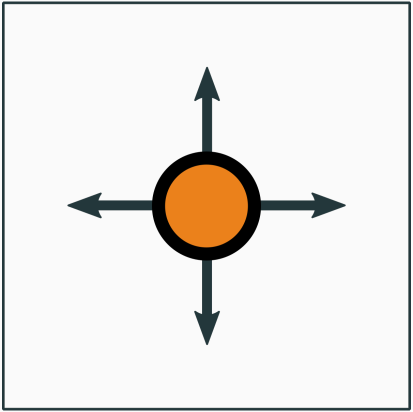
PGMs offer interpretability and quantifiable uncertainty, but often don't scale well with data and can be underexpressive.

Model learning

Consider an agent in a system, and a set of its possible actions.



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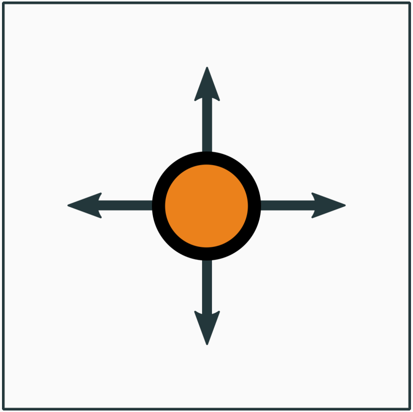

Model learning is the problem of estimating the dynamics of the system when we don't know it beforehand.

Model learning

Formally, consider an agent in a system with state space $\mathcal{S}$ with action space $\mathcal{A}$ with underlying dynamics function $p(s_{t+1}|s_t, a_t)$.

We are interested in learning an approximate dynamics function

$$\hat{p}(s_{t+1}|s_t, a_t)$$

from a dataset of trajectories

$$\boldsymbol{\tau} = \{(s_0^{(i)}, a_0^{(i)}, s_1^{(i)}, a_1^{(i)}, \dots, s_T^{(i)})\}_{i=1}^{N}$$

Bayesian linear dynamical system

A simple assumption: **Bayesian linear dynamical system** (LDS)

$$\mu_\rho, \Sigma_\rho \sim \mathcal{NIW}(\Psi, \nu, \mu_0, \kappa)\,, \quad \mathbf{F}, \Sigma \;\sim \mathcal{MNIW}(\Psi, \nu, \boldsymbol{M}_0,\, \boldsymbol{V})\,,$$

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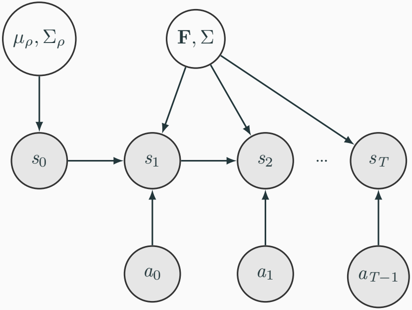

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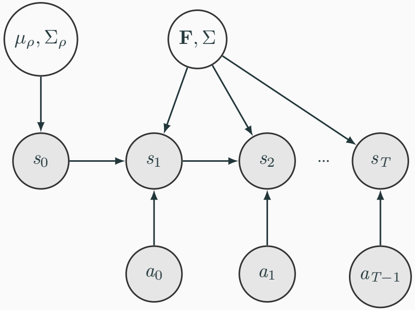

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If $q(\theta, z)$ is sufficiently expressive, it can approximate $p(\theta, z|x)$ quite well.

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Properties:

- $\mathrm{KL}(q(x) \| p(x)) = 0$ if $q(x) = p(x)$.
- Asymmetric

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and maximize the *evidence lower bound* (ELBO)

$$\mathcal{L}[q(\theta, z)] = \mathbb{E}_{q(\theta, z)} \left[\log \frac{p(x, \theta, z)}{q(\theta, z)} \right]$$

Variational inference for PGMs

For a general graphical model with variable set $\mathbf{X} = \{x_1, x_2, \ldots\}$ we have joint distribution

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This is called the *mean-field* assumption.

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Mean-field variational inference

Until converged, for each factor $q(\mathbf{H}_j)$, hold factors $q(\mathbf{H}_{i \neq j})$ constant and set $q(\mathbf{H}_j) = \tilde{q}(\mathbf{H}_j, \mathbf{V})$.

Conjugate-exponential graphical models

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- $\log Z(\eta_x(\theta))$: log-partition function

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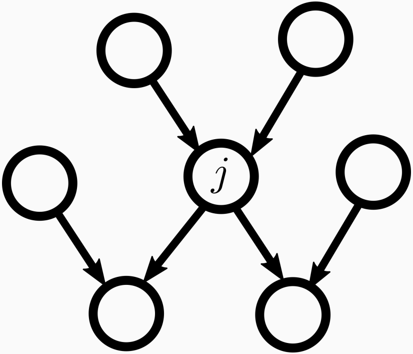
We now return to graphs! If we assume a mean-field variational distribution and our PGM is conjugate-exponential, we get a very elegant graph algorithm, called *variational message passing* (VMP) [1].



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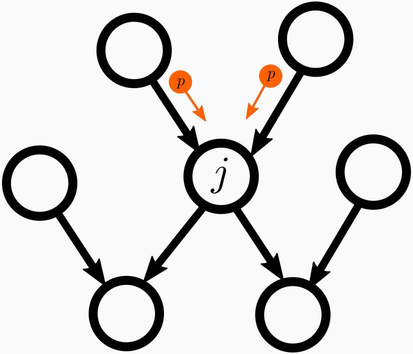

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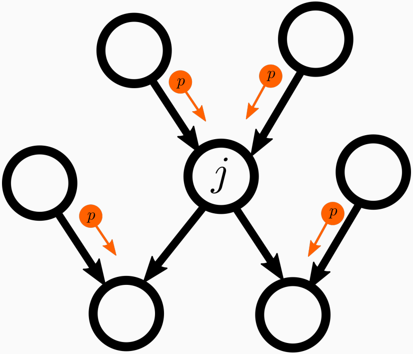

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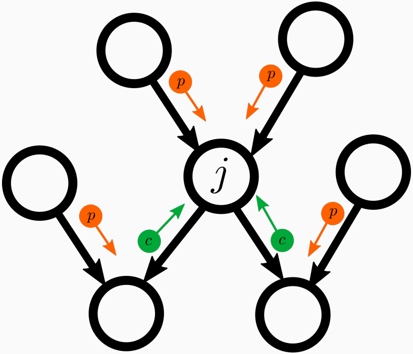

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In conjugate-exponential PGMs, messages can be computed in closed-form.

Summary of VMP

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Problem: Compute posterior $p(\mathbf{H}|\mathbf{V})$, approximated with $q(\mathbf{H}) = \prod_j q(\mathbf{H}_j)$

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Drawbacks: can be underexpressive (conjugate-exponential requirement)

Structured variational autoencoder

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Model learning

Recall the model learning problem.

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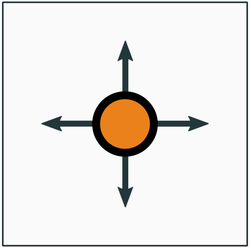

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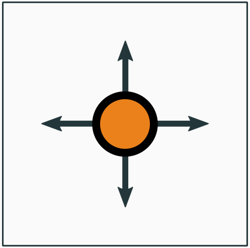

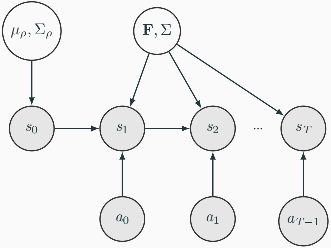

Adding expressivity

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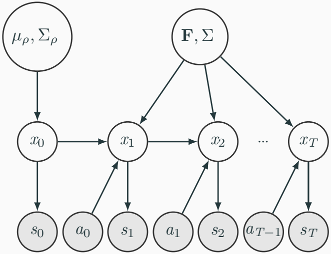

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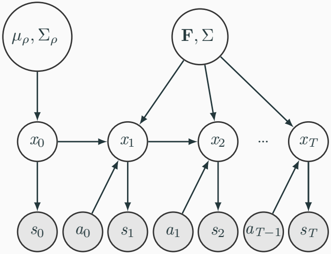

What if this observation model was a neural network?

Structured variational autoencoder

We augment the Bayesian LDS with a neural network observation model.

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$$\mu_\rho, \Sigma_\rho \sim \mathcal{NIW}(\Psi, \nu, \mu_0, \kappa)\,, \quad \mathbf{F}, \Sigma \sim \mathcal{MNIW}(\Psi, \nu, \boldsymbol{M}_0, \boldsymbol{V})\,,$$

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But what does it do?

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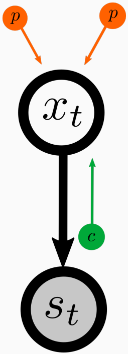

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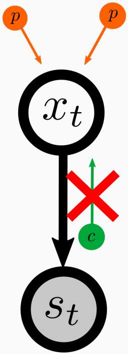

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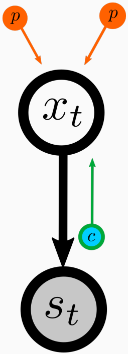

Messages in SVAE

The message from a **non-conjugate, non-exponential family** observation X to a parent Y is

$$m_{X \to Y} = r_\xi(t_X(X))$$

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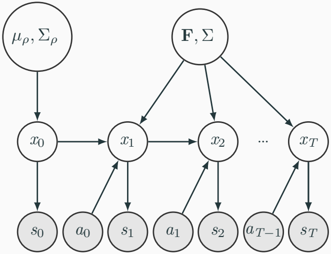
Inference in a SVAE

1. For a data $\tau = \{s_0, a_0, s_1, a_1, \ldots, s_T\}$, perform VMP using SVAE messages
2. Compute the ELBO $\mathcal{L}[q(\{x_i\}_{i=1}^{T}, \mu_\rho, \Sigma_\rho, \mathbf{F}, \Sigma)]$
3. Update neural networks with $\nabla_{\gamma,\xi}\mathcal{L}[q(\{x_i\}_{i=1}^{T}, \mu_\rho, \Sigma_\rho, \mathbf{F}, \Sigma)]$
4. Update global parameters $(\mu_\rho, \Sigma_\rho, \mathbf{F}, \Sigma)$ with natural gradients

Autoencoding

How is a SVAE an *autoencoder*?



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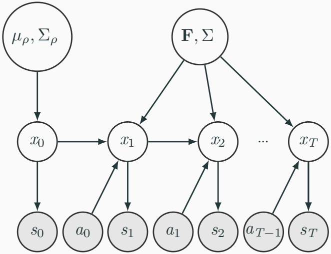

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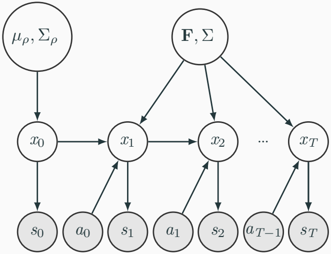

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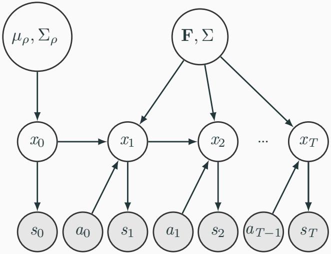

We have two neural networks:

1. $r_\xi(s)$: recognition network, takes real data and "encodes" it
2. $\mu_\gamma(x), \Sigma_\gamma(x)$: observation network, takes latent data and "decodes" it

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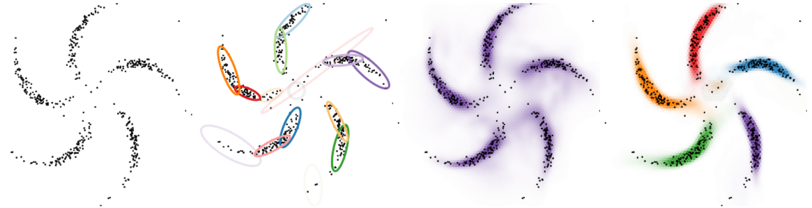

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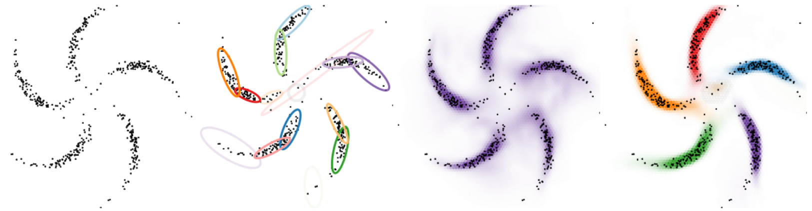

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In this scenario, the SVAE enables modeling non-Gaussian cluster shapes [2].

Current work

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Demo

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Questions?

References

[1] J. Winn and C. Bishop. Variational message passing. *JMLR*, 2005.

[2] M. Johnson, D. Duvenaud, A. Wiltschko, S. Datta, and R. Adams. Composing graphical models with neural networks for structured representations and fast inference. In *NIPS*, 2016.