Model learning with structured latent representations

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UCSD

Background

Probabilistic graphical models

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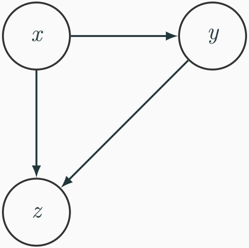

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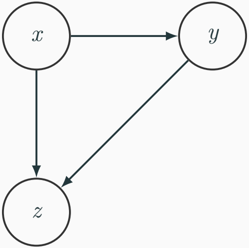

The joint distribution factorizes as

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

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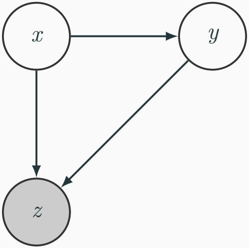

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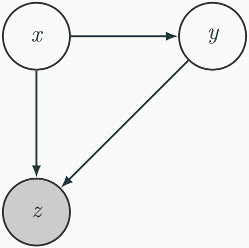

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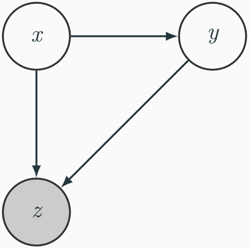

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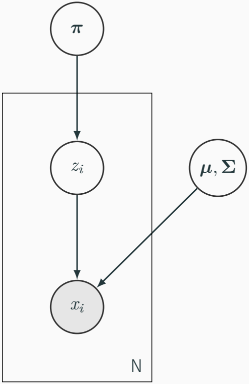
This can be computed via Bayes rule:

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

Example PGM

Latent variable model: Gaussian mixture model



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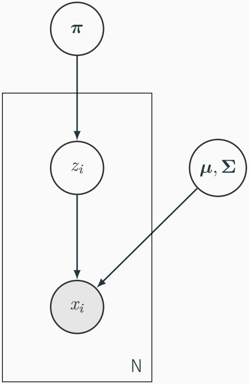

Local variables: $\{z_i\}_{i=1}^N$

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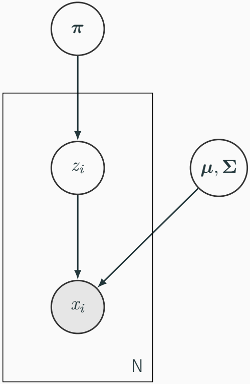

Local variables: $\{z_i\}_{i=1}^N$

Global variables: μ, π

Conjugacy

Conjugate

Two random variables x and y whose distribution is

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are said to be *conjugate* if the posterior $p(x|y)$ is in the same family of distributions as $p(x)$.

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- Dirichlet/multinomial

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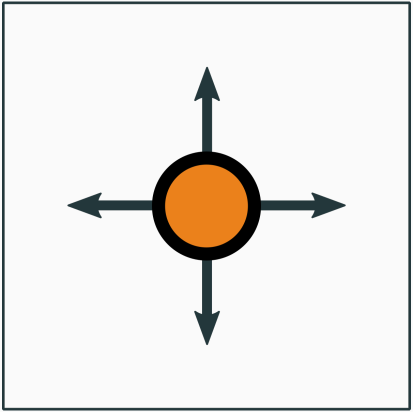
PGMs offer interpretability and quantifiable uncertainty, but often don't scale well with data and can be underexpressive.

Model learning

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



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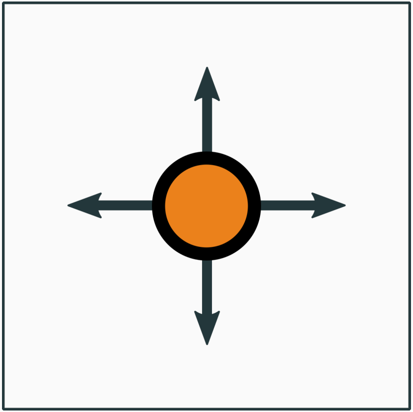

Model learning is the problem of estimating the dynamics of the system when we don't know it beforehand.

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

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

Bayesian linear dynamical system

A simple assumption: Bayesian linear dynamical system (LDS)

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

$$\mathbf{s}_0 \mid \mu_\rho, \Sigma_\rho \sim \mathcal{N}(\mu_\rho, \Sigma_\rho)\,, \qquad \mathbf{s}_{t+1} \mid \mathbf{s}_t, \mathbf{a}_t \sim \mathcal{N}\left(\mathbf{F}\begin{bmatrix}\mathbf{s}_t \\ \mathbf{a}_t\end{bmatrix}, \Sigma\right) \text{ for } t \in [0, \ldots, T]$$

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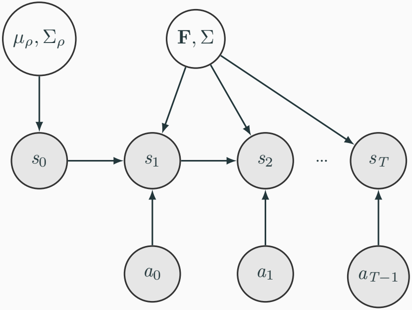

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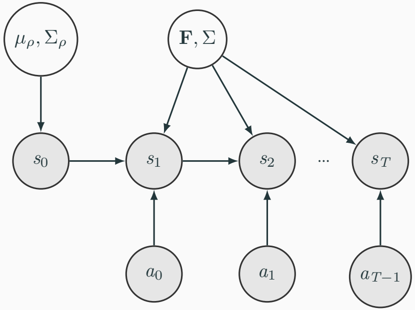

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If $q(\theta, z)$ is sufficiently expressive, it can approximate $p(\theta, z|x)$ quite well.

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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.

Variational inference for PGMs (cont.)

The ELBO is now

$$\begin{aligned}
\mathcal{L}[q(\mathbf{H})] &= \mathbb{E}_{q(\mathbf{H})}\left[\log \frac{p(\mathbf{H},\mathbf{V})}{q(\mathbf{H})}\right] \\
&= \int \prod_i q(\mathbf{H}_i)\left(\log p(\mathbf{H},\mathbf{V}) - \log \prod_i q(\mathbf{H}_i)\right) d\mathbf{H} \\
&= \int q(\mathbf{H}_j)\left(\int \log p(\mathbf{H},\mathbf{V}) \prod_{i\neq j} q(\mathbf{H}_i)\, d\mathbf{H}_i\right) d\mathbf{H}_j \\
&\quad - \int q(\mathbf{H}_j) \log q(\mathbf{H}_j)\, d\mathbf{H}_j + \text{const.} \\
&= \int q(\mathbf{H}_j) \log \tilde{q}(\mathbf{H}_j,\mathbf{V})\, d\mathbf{H}_j - \int q(\mathbf{H}_j)\log q(\mathbf{H}_j)\, d\mathbf{H}_j + \text{const.} \\
&= -\mathrm{KL}(q(\mathbf{H}_j) \| \tilde{q}(\mathbf{H}_j,\mathbf{V})) + \text{const.}
\end{aligned}$$

where

$$\log \tilde{q}(\mathbf{H}_j,\mathbf{V}) = \mathbb{E}_{i\neq j}\left[\log p(\mathbf{H},\mathbf{V})\right] + \text{const.}$$

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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

If our PGM is *conjugate-exponential*, where every node belongs in the exponential family of distributions, and is conjugate w.r.t. its parents,

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An exponential family distribution is one that can be written in the following form:

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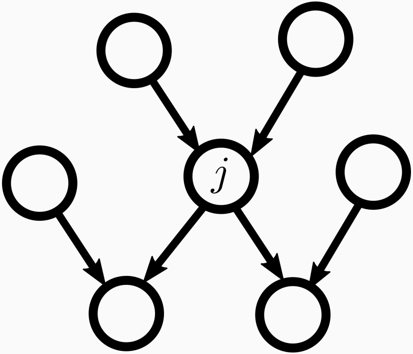
- $t_x(x)$: sufficient statistic
- $\log Z(\eta_x(\theta))$: log-partition function

Variational message passing

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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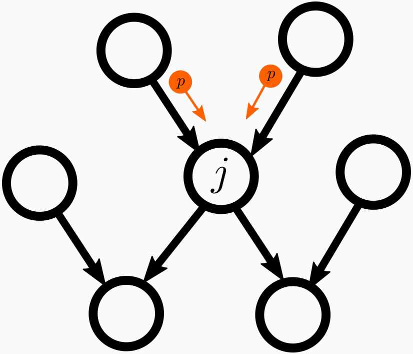

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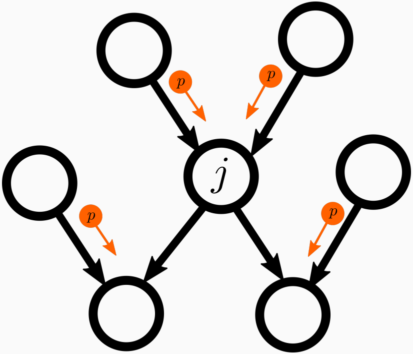

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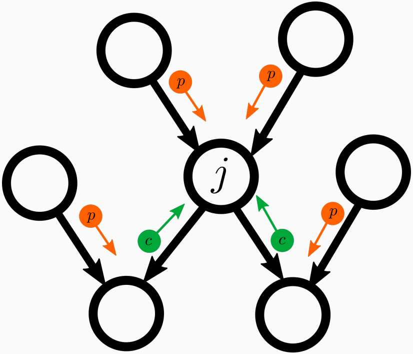

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Messages

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The message from a parent Y to a child X is

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

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Structured variational autoencoder

Model learning

Recall the model learning problem.

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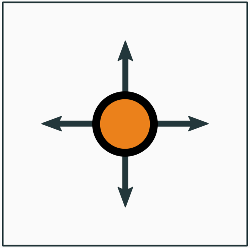

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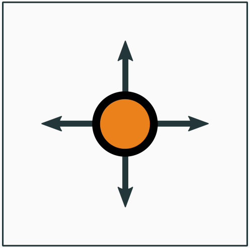

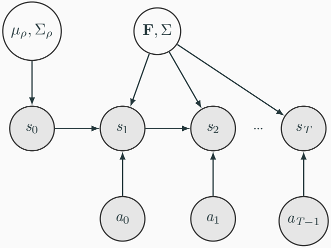

Adding expressivity

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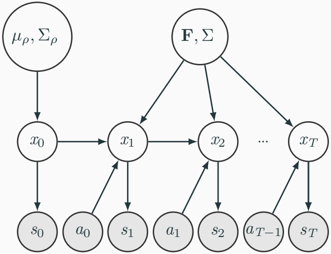

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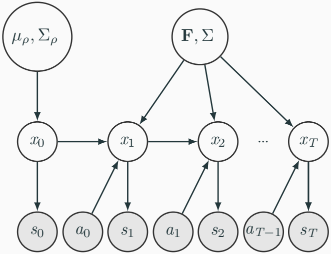

What if this observation model was a neural network?

Structured variational autoencoder

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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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where $\mu_\gamma(\mathbf{x}_t)$ and $\Sigma_\gamma(\mathbf{x}_t)$ are both neural networks parametrized by γ. This model is called a structured variational autoencoder (SVAE) [2].

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But what does it do?

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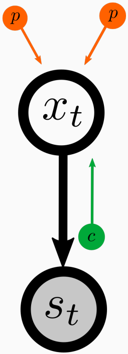

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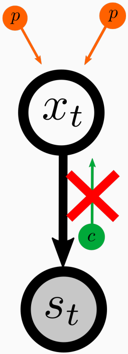

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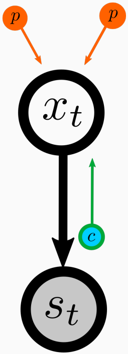

Messages in SVAE

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

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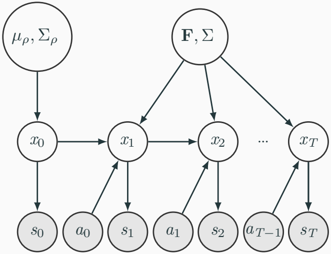
Inference in a SVAE

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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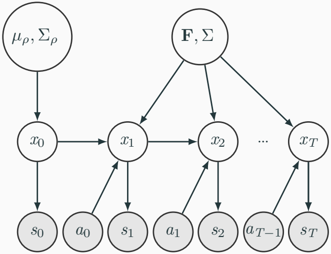

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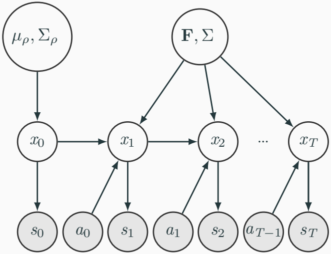

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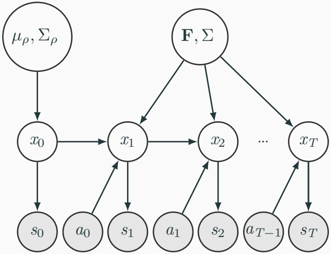

We have two neural networks:

1. $r_\xi(s)$: recognition network, takes real data and "encodes" it
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Conclusion

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The SVAE naturally applies to scenarios where there is already a tractable PGM.

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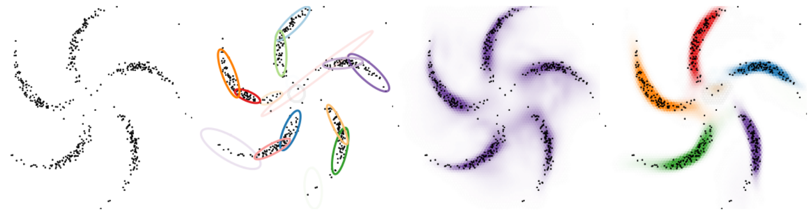

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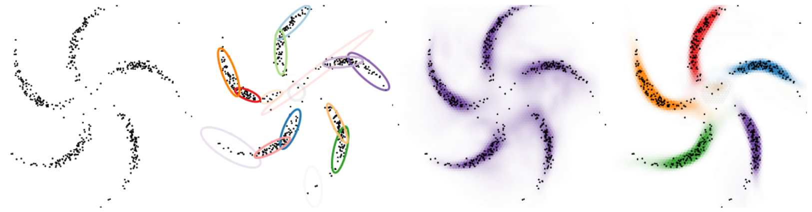

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In this scenario, the SVAE enables modeling non-Gaussian cluster shapes [2].

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.