An introduction to the structured variational autoencoders (SVAE)

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UCSD

Variational inference

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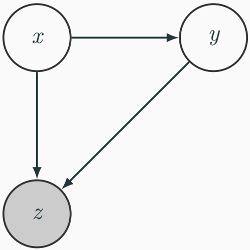

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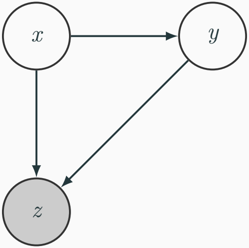

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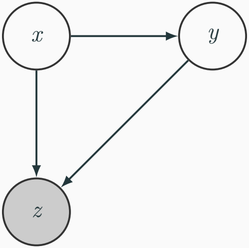

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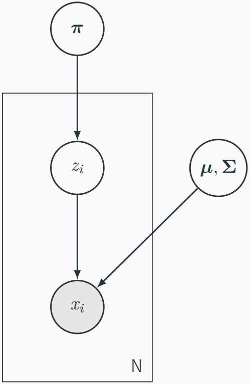
This can be computed via Bayes rule:

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

Example PGM

Latent variable model: Gaussian mixture model



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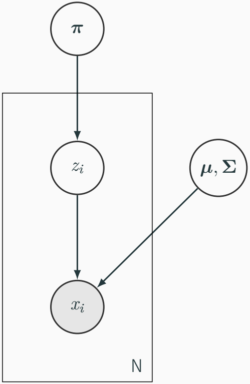

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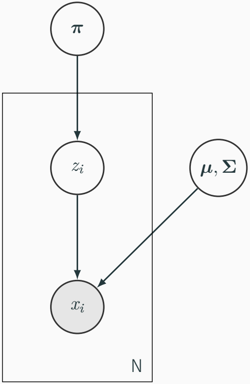

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Conjugacy

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- Dirichlet/multinomial

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Examples: Gaussian, Categorical, Dirichlet, inverse-Wishart

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

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For distributions $q(x)$ and $p(x)$,

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Properties:

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

Evidence lower bound

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\mathrm{KL}(q(\theta, z) \| p(\theta, z|x)) &= \int q(\theta, z) \log \frac{q(\theta, z)}{p(\theta, z|x)} \, d\theta, z \\
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and maximize the *evidence lower bound* (ELBO)

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

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Mean-field variational inference

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

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We are interested in the posterior $p(\mathbf{H}|\mathbf{V})$ and use variational distribution

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Mean-field variational inference (cont.)

The ELBO is now

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

where

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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 model 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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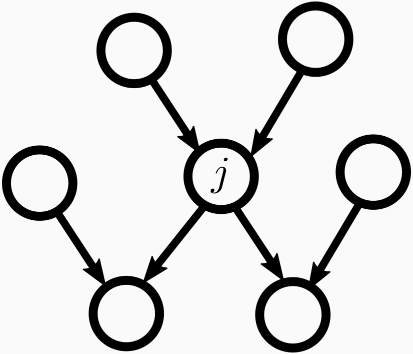
This gives rise to an efficient coordinate-ascent algorithm that can be extended with natural gradients (stochastic variational inference).

Variational message passing

An update for node j relies on only its Markov blanket.



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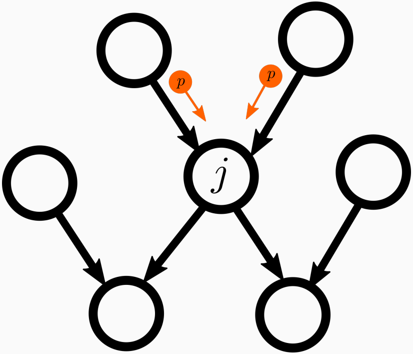

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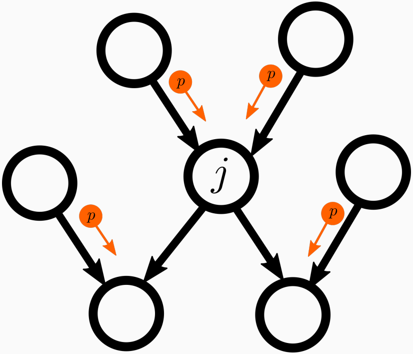

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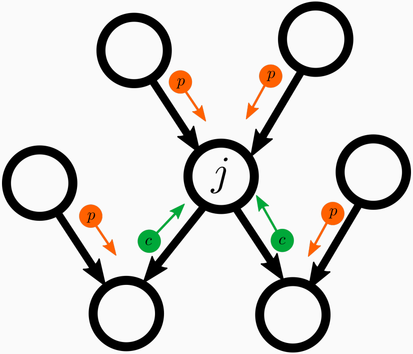

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Drawbacks: can be underexpressive (conjugate-exponential requirement)

Demo

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Perform Monte-Carlo estimate:

$$\hat{\mathcal{L}}[q(\theta, z)] = \sum_{l=1}^{L} q(\theta^{(l)}, z^{(l)})\left[\log \frac{p(x, \theta^{(l)}, z^{(l)})}{q(\theta^{(l)}, z^{(l)})}\right]$$

Gradient-based approaches

1. Start with Monte-Carlo loss

$$\hat{\mathcal{L}}[q(\theta, z)] = \frac{1}{S} \sum_{s=1}^{S} q(\theta^{(s)}, z^{(s)}) \left[\log \frac{p(x, \theta^{(s)}, z^{(s)})}{q(\theta^{(s)}, z^{(s)})} \right]$$

2. Compute gradient

$$\nabla_\phi \hat{\mathcal{L}}[q_\phi(\theta, z)] = \frac{1}{S} \sum_{s=1}^{S} \nabla_\phi q(\theta^{(s)}, z^{(s)}) \left[\log \frac{p(x, \theta^{(s)}, z^{(s)})}{q(\theta^{(s)}, z^{(s)})} \right]$$

3. Perform gradient ascent

Issues with gradient-based approaches

Core problem: high-variance gradients

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How do we address this?

- Rao-Blackwellization (replace $\mathbb{E}[f(X, Y)]$ with $\mathbb{E}[f(X, Y)|X]$)[1]
- Reparametrization trick [2]

Variational autoencoder

The VAE is a generative model for data [2].

$$z_i \sim \mathcal{N}(0, I)$$
$$x_i \sim \mathcal{N}(\mu_\gamma(z_i), \Sigma_\gamma(z_i))$$

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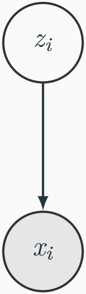

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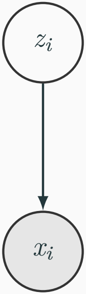

How do we do inference?

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Reparametrization trick

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What is the reparametrization trick? We want to sample $z \sim q(z|x)$ and do so it in a roundabout way.

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This is very effective at decreasing the variance of the gradient.

Structured variational autoencoder

What is an SVAE?

There are two ways of thinking about it

- A conjugate-exponential graphical model augmented with a neural network observation model
- A VAE augmented with also a graphical because of a neural-network observation model

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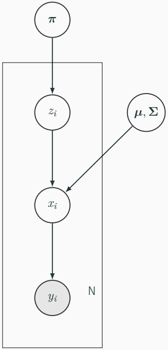
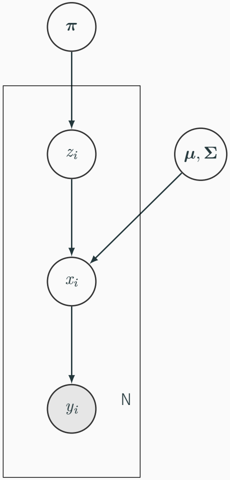


SVAE GMM



$$
\begin{aligned}
\pi &\sim \mathrm{Dir}(\alpha) \\
\mu_k, \Sigma_k &\sim \mathcal{NIW}(\psi, \mu_0, \kappa, \nu) \\
z_i | \pi &\sim \mathrm{Cat}(\pi) \\
x_i | z_i, \boldsymbol{\mu}, \boldsymbol{\Sigma} &\sim \mathcal{N}(\mu_{z_i}, \Sigma_{z_i}) \\
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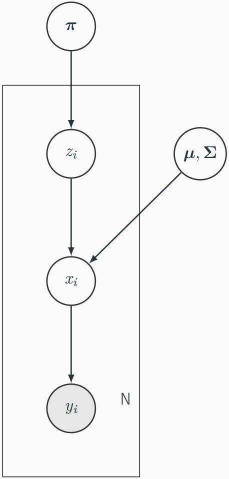

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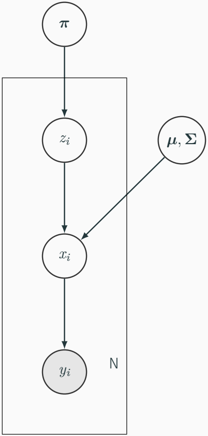

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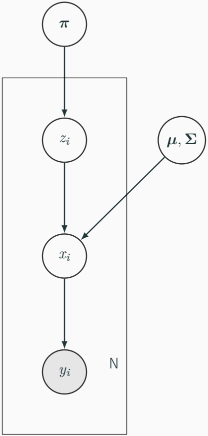

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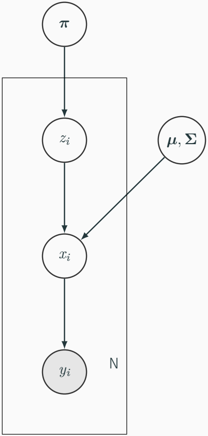

- Learn $q(z_i), q(x_i), q(\pi), q(\mu, \Sigma)$ with stochastic VMP using a neural network $r_\phi(y) = m_{y_i \to x_i}$
- Learn weights of neural networks $(\mu_\gamma, \Sigma_\gamma), r_\phi$ using the gradient of the ELBO

Conclusion

Why SVAE?

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

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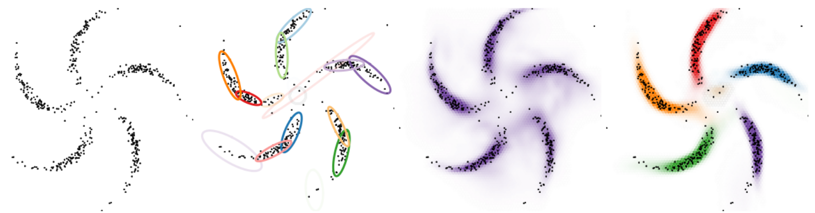

(a) Data (b) GMM (c) Density net (VAE) (d) GMM SVAE

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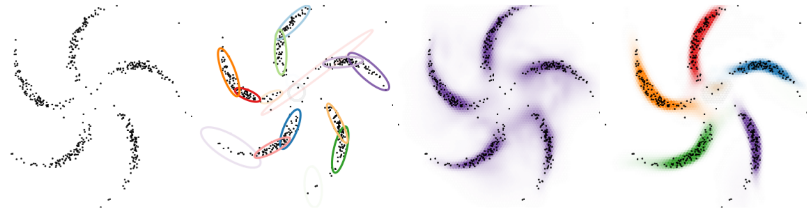

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In this scenario, the SVAE enables modeling non-Gaussian cluster shapes [3].

Current work

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Demo

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Questions?

References

[1] Rajesh Ranganath, Sean Gerrish, and David M. Blei. Black Box Variational Inference. dec 2013.

[2] Diederik P Kingma and Max Welling. Auto-Encoding Variational Bayes. dec 2013.

[3] 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.