Variational Auto-Encoders

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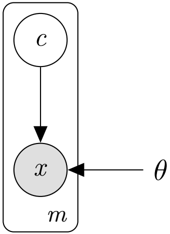
Generative models with neural networks

Mixture model



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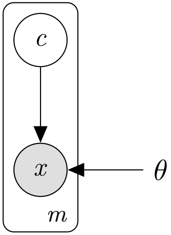

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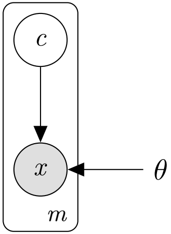

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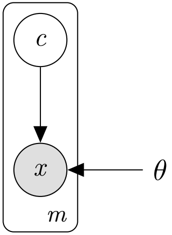

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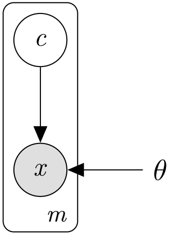

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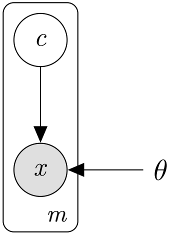

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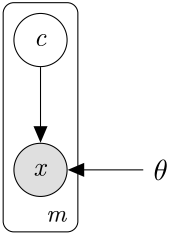

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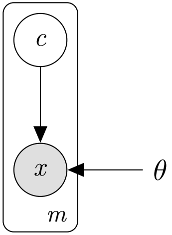

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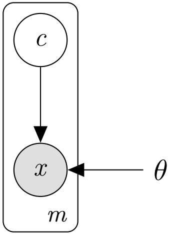

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$$P(x) = \underbrace{\sum_{c=1}^{K} \underbrace{P(c)P(x|c)}_{\text{differentiable function of } \theta}}_{\text{tractable for small } K}$$

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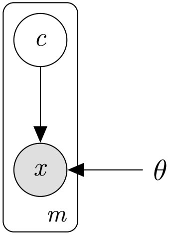

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Gradient-based optimisation! $\nabla_\theta \log P_\theta(x)$

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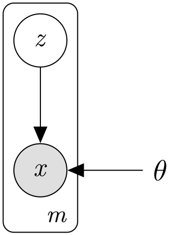
Continuous mixture model



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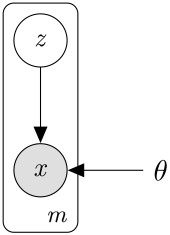

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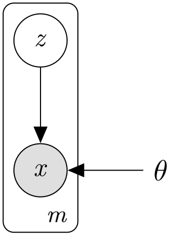

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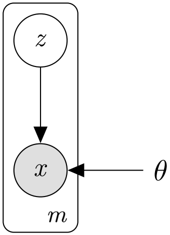

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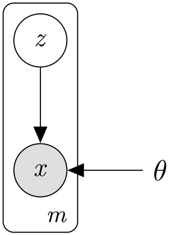

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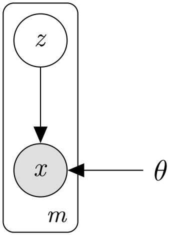

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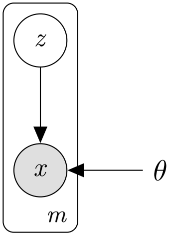

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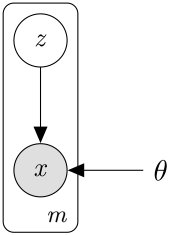

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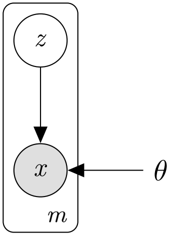

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- Intractability
  - $P(x) = \int p(z) P(x|z) \mathrm{d}z$
  - $P(z|x) = \frac{p(z)P(x|z)}{\int p(z')P(x|z')\mathrm{d}z'}$

Variational inference

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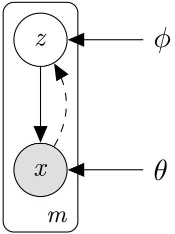

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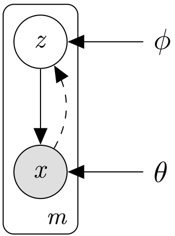

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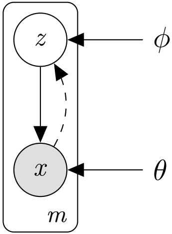

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  - $\sigma^2_\phi(x) = \exp(W^{(\sigma)} v(x) + b^{(\sigma)})$
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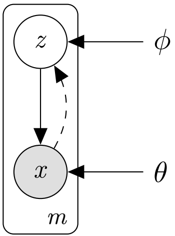

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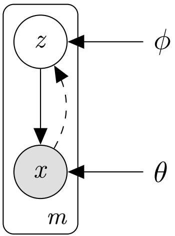

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Mean field assumption

- $q_{\phi_i}(Z|x_i)$ is specified for each observation x_i by locally predicting its mean and variance

Approximate inference by optimisation

Maximise ELBO

$$\log P_\theta(x) \geq \underbrace{\mathbb{E}_{q_\phi(Z|x)}\left[\log \frac{q_\phi(Z|x)}{p_\theta(Z)}\right]}_{-\mathrm{KL}(q_\theta(Z|x)||p_\theta(Z))} + \underbrace{\mathbb{E}_{q_\phi(Z|x)}\left[\log P_\theta(X = x|Z)\right]}_{\text{intractable!}}$$

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Prior term

$$\mathrm{KL}(q_\phi(Z|x)||p_\theta(Z)) = -\frac{1}{2}\sum_{j=1}^{d}(1 + \log\sigma_\phi^2(x)_j - \mu_\phi^2(x)_j - \sigma_\phi^2(x)_j)$$

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Likelihood term is intractable

- the Categorical likelihood is not conjugate with the Normal approximate posterior

Change of variable for location-scale distributions

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- $Z = \mu + \sigma E$

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back to the ELBO

$$\mathbb{E}_{q_\phi(Z|x)}\left[\log P(x|Z)\right] = \mathbb{E}_{\epsilon \sim N(0,I)}\left[\log P(x|Z = \mu_\phi(x) + \sigma_\phi(x)\epsilon)\right]$$

Monte Carlo estimate

$$
\begin{aligned}
\mathbb{E}_{q_\phi(Z|x)}\left[\log P(x|Z)\right] &= \mathbb{E}_{\epsilon \sim N(0,I)}\left[\log P(x|Z = \mu_\phi(x) + \sigma_\phi(x)\epsilon))\right] \\
&\approx \frac{1}{N}\sum_{n=1}^{N} \log P\left(x|\mu_\phi(x) + \sigma_\phi(x)\epsilon^{(n)}\right)
\end{aligned}
$$

MC estimate of the ELBO

$$\log P_\theta(x) \geq \underbrace{\mathbb{E}_{q_\phi(Z|x)}\left[\log \frac{q_\phi(Z|x)}{p_\theta(Z)}\right]}_{-\,\mathrm{KL}(q_\theta(Z|x)||p_\theta(Z))} + \underbrace{\mathbb{E}_{q_\phi(Z|x)}\left[\log P_\theta(X = x|Z)\right]}_{\text{intractable!}}$$

$$\approx \underbrace{\frac{1}{2}\sum_{j=1}^{d}\Big(1 + \log \sigma_\phi^2(x)_j - \mu_\phi^2(x)_j - \sigma_\phi^2(x)_j\Big)}_{-\,\mathrm{KL}(q_\theta(Z|x)||p_\theta(Z))}$$

$$+ \underbrace{\log P_\theta\left(x|\mu_\phi(x) + \sigma_\phi(x)\epsilon\right)}_{\text{single-sample estimate}}$$

Gradient-based optimisation

Let $\mathcal{L}(\theta, \phi | x)$ be our objective function

$$\mathcal{L}(\theta, \phi | x) = \underbrace{\frac{1}{2} \sum_{j=1}^{d} \Big(1 + \log \sigma_\phi^2(x)_j - \mu_\phi^2(x)_j - \sigma_\phi^2(x)_j\Big)}_{\text{differentiable function of } \phi}$$

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We can update θ and ϕ using stochastic gradient steps

- we know chain rule (thus we can get a gradient)
- we have a noisy though unbiased estimate
- guaranteed convergence to a local optimum of $\mathcal{L}$ (with appropriate learning rate schedule)

Further reading

- Auto-Encoding variational Bayes [Kingma and Welling, 2014]

References I

Diederik P. Kingma and Max Welling. Auto-encoding variational bayes. In *International Conference on Learning Representations*, 2014.