# Variational Inference and Learning II

## Latent Variable Models and Variational Autoencoders

Michael U. Gutmann

Probabilistic Modelling and Reasoning (INFR11134)
School of Informatics, The University of Edinburgh

Spring Semester 2023

## Assumptions

- Model: $p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta})$
- Data: $\mathcal{D} = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$, $\mathbf{v}_i \overset{\text{iid}}{\sim} p_*$
- The model is a latent variable model: we have observations for all dimensions of $\mathbf{v}$ but no observations of the latents $\mathbf{h}$.
- For each observation $\mathbf{v}_i$, there is a latent $\mathbf{h}_i$.
- Because of iid assumption,

$$p(\mathbf{v}_1, \ldots, \mathbf{v}_n, \mathbf{h}_1, \ldots, \mathbf{h}_n; \boldsymbol{\theta}) = \prod_{i=1}^{n} p(\mathbf{v}_i, \mathbf{h}_i; \boldsymbol{\theta}) \qquad (1)$$

- We do not deal with the case of unobserved variables due to missing data, i.e. incomplete observations of $\mathbf{v}$. (Recent VI work on this topic: Simkus et al, *Variational Gibbs Inference for Statistical Model Estimation from Incomplete Data*, `https://arxiv.org/abs/2111.13180`)

# Program

1. Scalable generic variational learning of latent variable models

2. Deep latent variable models and variational autoencoders

# Program

1. Scalable generic variational learning of latent variable models
   - ELBO for iid data
   - Amortised variational inference
   - Reparametrisation and stochastic optimisation
2. Deep latent variable models and variational autoencoders

# Lower bound on the likelihood for iid data

- We had

$$\mathcal{L}_{\mathbf{x}}(q) = \mathbb{E}_{q(\mathbf{y}|\mathbf{x})}\left[\log \frac{p(\mathbf{x}, \mathbf{y})}{q(\mathbf{y}|\mathbf{x})}\right] \tag{2}$$

- Substitute

$$\mathbf{x} \to (\mathbf{v}_1, \ldots, \mathbf{v}_n) \qquad p(\mathbf{x}, \mathbf{y}) \to \prod_{i=1}^{n} p(\mathbf{v}_i, \mathbf{h}_i; \boldsymbol{\theta}) \tag{3}$$

$$\mathbf{y} \to (\mathbf{h}_1, \ldots, \mathbf{h}_n) \tag{4}$$

- Since the true conditional factorises, we use

$$q(\mathbf{h}_1, \ldots, \mathbf{h}_n|\mathbf{v}_1, \ldots, \mathbf{v}_n) = \prod_{i=1}^{n} q(\mathbf{h}_i|\mathbf{v}_i) \tag{5}$$

- We have one conditional variational distribution $q(\mathbf{h}|\mathbf{v})$.

# Lower bound on the likelihood for iid data

- The ELBO $\mathcal{L}_{\mathcal{D}}$ for iid data $\mathcal{D} = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ becomes a sum of per data-point ELBOs $\mathcal{L}_{\mathbf{v}_i}$, denoted by $\mathcal{L}_i$:

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \sum_{i=1}^{n} \mathcal{L}_i(\boldsymbol{\theta}, q) \tag{6}$$

$$\mathcal{L}_i(\boldsymbol{\theta}, q) = \mathbb{E}_{q(\mathbf{h}_i|\mathbf{v}_i)}\left[\log \frac{p(\mathbf{v}_i, \mathbf{h}_i; \boldsymbol{\theta})}{q(\mathbf{h}_i|\mathbf{v}_i)}\right] \tag{7}$$

- Technical detail: In $\mathcal{L}_i$, we can drop the index $i$ from $\mathbf{h}_i$ since it is just the random variable $\mathbf{h} \sim q(\mathbf{h}|\mathbf{v}_i)$. Hence:

$$\mathcal{L}_i(\boldsymbol{\theta}, q) = \mathbb{E}_{q(\mathbf{h}|\mathbf{v}_i)}\left[\log \frac{p(\mathbf{v}_i, \mathbf{h}; \boldsymbol{\theta})}{q(\mathbf{h}|\mathbf{v}_i)}\right] \tag{8}$$

# Lower bound on the likelihood for iid data

- From the basic properties of the ELBO, we have

$$\mathcal{L}_i(\boldsymbol{\theta}, q) = \log p(\mathbf{v}_i; \boldsymbol{\theta}) - \text{KL}(q(\mathbf{h}|\mathbf{v}_i)||p(\mathbf{h}|\mathbf{v}_i; \boldsymbol{\theta})) \tag{9}$$

- This gives

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \sum_{i=1}^{n} [\log p(\mathbf{v}_i; \boldsymbol{\theta}) - \text{KL}(q(\mathbf{h}|\mathbf{v}_i)||p(\mathbf{h}|\mathbf{v}_i; \boldsymbol{\theta}))] \tag{10}$$

- With $\ell(\boldsymbol{\theta}) = \sum_i \log p(\mathbf{v}_i; \boldsymbol{\theta})$ we obtain

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \ell(\boldsymbol{\theta}) - \sum_{i=1}^{n} \text{KL}(q(\mathbf{h}|\mathbf{v}_i)||p(\mathbf{h}|\mathbf{v}_i; \boldsymbol{\theta})) \tag{11}$$

- Maximum likelihood estimation

$$\max_{\boldsymbol{\theta}} \ell(\boldsymbol{\theta}) = \max_{\boldsymbol{\theta}, q} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) \tag{12}$$

# Properties of the ELBO for iid data

- For iid data, we have seen the connection between maximum likelihood estimation and minimisation of $\mathrm{KL}(p_*(\mathbf{v})||p(\mathbf{v};\boldsymbol{\theta}))$:

$$\underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, \ell(\boldsymbol{\theta}) \approx \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, \mathrm{KL}(p_*(\mathbf{v})||p(\mathbf{v};\boldsymbol{\theta})) \tag{13}$$

  Equality holds for large sample sizes $n$.
- Similar result can be shown for $\mathcal{L}_\mathcal{D}$:

$$\underset{\boldsymbol{\theta},q}{\operatorname{argmax}}\, \mathcal{L}_\mathcal{D}(\boldsymbol{\theta}, q) \approx \underset{\boldsymbol{\theta},q}{\operatorname{argmin}}\, \mathrm{KL}(p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v})||p(\mathbf{v},\mathbf{h};\boldsymbol{\theta})) \tag{14}$$

- Note: $\boldsymbol{\theta}$ and $q$ enter the KL divergence on different sides: $\boldsymbol{\theta}$ on the right; $q$ on the left.

# Properties of the ELBO for iid data

$$\text{argmax}_{\boldsymbol{\theta},q}\, \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) \approx \text{argmin}_{\boldsymbol{\theta},q}\, \mathsf{KL}(p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v})||p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta}))$$

- For fixed $q$, maximising the ELBO wrt $\boldsymbol{\theta}$ same as MLE for augmented data $(\mathbf{v}, \mathbf{h})$, with $\mathbf{v} \sim p_*$ and $\mathbf{h} \sim q(\mathbf{h}|\mathbf{v})$.
- For fixed $\boldsymbol{\theta}$, maximising the ELBO wrt $q$ may lead to mode seeking behaviour.
- By changing $q$, we change the training data / the target distribution $p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v})$ that we would like to approximate with the model $p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta})$.
- This explains some failure modes of training variational autoencoders (Zhao et al, *InfoVAE: Information Maximizing Variational Autoencoders*, AAAI 2019, `https://arxiv.org/abs/1706.02262`)

# Properties of the ELBO for iid data

$$\text{argmax}_{\boldsymbol{\theta},q}\, \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) \approx \text{argmin}_{\boldsymbol{\theta},q}\, \mathsf{KL}(p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v})||p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta}))$$

- An example is the learning of representations in **h** space.
- Because of mode-seeking property, $q(\mathbf{h}|\mathbf{v})$ may only cover a small space in **h** (for sake of argument, a single mode).
- It thus produces "reduced" training data for $p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta})$.
- If $p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta})$ is sufficiently flexible, the KL div can be minimised and we do have $p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v}) \approx p(\mathbf{v}, \mathbf{h}; \hat{\boldsymbol{\theta}})$ and hence

$$p_*(\mathbf{v}) \approx p(\mathbf{v}; \hat{\boldsymbol{\theta}}) = \int p(\mathbf{v}, \mathbf{h}; \hat{\boldsymbol{\theta}}) d\mathbf{h} \tag{15}$$

- This means that the marginal $p(\mathbf{v}; \hat{\boldsymbol{\theta}})$ is meaningful and approximates the distribution of the observed data.
- But the joint $p(\mathbf{v}, \mathbf{h}; \hat{\boldsymbol{\theta}})$ and learned $q$ may not be meaningful at all since trained with "reduced" **h** samples.

# Properties of the ELBO for iid data (proof)

For large sample sizes $n$ we have

$$\frac{1}{n}\ell(\boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \log p(\mathbf{v}_i; \boldsymbol{\theta}) \to \mathbb{E}_{p_*(\mathbf{v})}\left[\log p(\mathbf{v}; \boldsymbol{\theta})\right] \tag{16}$$

Similarly

$$\frac{1}{n}\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \frac{1}{n}\sum_{i=1}^{n} \mathcal{L}_{\mathbf{v}_i}(\boldsymbol{\theta}, q) \to \mathbb{E}_{p_*(\mathbf{v})}\mathcal{L}_{\mathbf{v}}(\boldsymbol{\theta}, q) \tag{17}$$

Dividing Equation (11) by $n$ thus gives:

$$\frac{1}{n}\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \frac{1}{n}\ell(\boldsymbol{\theta}) - \frac{1}{n}\sum_{i=1}^{n} \text{KL}(q(\mathbf{h}|\mathbf{v}_i)||p(\mathbf{h}|\mathbf{v}_i; \boldsymbol{\theta})) \tag{18}$$

$$\to \mathbb{E}_{p_*(\mathbf{v})}\mathcal{L}_{\mathbf{v}}(\boldsymbol{\theta}, q) = \mathbb{E}_{p_*(\mathbf{v})}\left[\log p(\mathbf{v}; \boldsymbol{\theta})\right] - \mathbb{E}_{p_*(\mathbf{v})}\left[\text{KL}(q(\mathbf{h}|\mathbf{v})||p(\mathbf{h}|\mathbf{v}; \boldsymbol{\theta}))\right] \tag{19}$$

# Properties of the ELBO for iid data (proof)

$$\mathbb{E}_{p_*(\mathbf{v})}\mathcal{L}_{\mathbf{v}}(\boldsymbol{\theta}, q) = \mathbb{E}_{p_*(\mathbf{v})}\left[\log p(\mathbf{v};\boldsymbol{\theta})\right] - \mathbb{E}_{p_*(\mathbf{v})}\left[\mathrm{KL}(q(\mathbf{h}|\mathbf{v})||p(\mathbf{h}|\mathbf{v};\boldsymbol{\theta}))\right] \quad (20)$$

$$= \mathbb{E}_{p_*(\mathbf{v})}\left[\log p(\mathbf{v};\boldsymbol{\theta})\right] - \mathbb{E}_{p_*(\mathbf{v})}\mathbb{E}_{q(\mathbf{h}|\mathbf{v})}\left[\log \frac{q(\mathbf{h}|\mathbf{v})}{p(\mathbf{h}|\mathbf{v};\boldsymbol{\theta})}\right] \quad (21)$$

$$= -\mathbb{E}_{p_*(\mathbf{v})}\mathbb{E}_{q(\mathbf{h}|\mathbf{v})}\left[\log \frac{q(\mathbf{h}|\mathbf{v})}{p(\mathbf{h}|\mathbf{v};\boldsymbol{\theta})p(\mathbf{v};\boldsymbol{\theta})}\right] \quad (22)$$

Subtract $\mathbb{E}_{p_*(\mathbf{v})}[\log p_*(\mathbf{v})]$ on both sides:

$$\mathbb{E}_{p_*(\mathbf{v})}\left[\mathcal{L}_{\mathbf{v}}(\boldsymbol{\theta}, q) - \log p_*(\mathbf{v})\right] = -\mathbb{E}_{p_*(\mathbf{v})}\mathbb{E}_{q(\mathbf{h}|\mathbf{v})}\left[\log \frac{q(\mathbf{h}|\mathbf{v})}{p(\mathbf{h}|\mathbf{v};\boldsymbol{\theta})p(\mathbf{v};\boldsymbol{\theta})}\right] - \mathbb{E}_{p_*(\mathbf{v})}\log p_*(\mathbf{v}) \quad (23)$$

$$= -\mathbb{E}_{p_*(\mathbf{v})}\mathbb{E}_{q(\mathbf{h}|\mathbf{v})}\left[\log \frac{p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v})}{p(\mathbf{h}|\mathbf{v};\boldsymbol{\theta})p(\mathbf{v};\boldsymbol{\theta})}\right] \quad (24)$$

$$= -\mathrm{KL}\left(p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v})||p(\mathbf{h}|\mathbf{v};\boldsymbol{\theta})p(\mathbf{v};\boldsymbol{\theta})\right) \quad (25)$$

$$= -\mathrm{KL}\left(p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v})||p(\mathbf{h},\mathbf{v};\boldsymbol{\theta})\right) \quad (26)$$

Hence: $\operatorname{argmax}_{\boldsymbol{\theta},q}\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) \approx \operatorname{argmin}_{\boldsymbol{\theta},q}\mathrm{KL}(p_*(\mathbf{v})q(\mathbf{h}|\mathbf{v})||p(\mathbf{v},\mathbf{h};\boldsymbol{\theta}))$

# Key technical difficulties

- Let us return to the case of finite samples.
- We have to maximise $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q) = \sum_i \mathcal{L}_i(\boldsymbol{\theta}, q)$ with respect to $\boldsymbol{\theta}$ and the conditional $q(\mathbf{h}|\mathbf{v})$.
- We had

$$\mathcal{L}_i(\boldsymbol{\theta}, q) = \mathbb{E}_{q(\mathbf{h}|\mathbf{v}_i)}\left[\log \frac{p(\mathbf{v}_i, \mathbf{h}; \boldsymbol{\theta})}{q(\mathbf{h}|\mathbf{v}_i)}\right] \tag{27}$$

  Analytical closed form expression only available in special cases.
- We do not want to restrict the model class but solve the optimisation problem for large $n$ and generic $p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta})$.
- Key technical difficulties are:
  1. Learning of conditional variational distribution $q(\mathbf{h}|\mathbf{v})$
  2. Maximisation when the objective involves the $\mathbb{E}_{q(\mathbf{h}|\mathbf{v}_i)}$

# Issue 1: Learning the conditional variational distribution

- Learning the conditional $q(\mathbf{h}|\mathbf{v})$ is hard since we have to effectively learn infinitely many pdfs/pmfs (one for each $\mathbf{v}$!).
- $\mathcal{L}_i$ only involves $q(\mathbf{h}|\mathbf{v}_i)$. Hence we could optimise $\mathcal{L}_\mathcal{D}$ by optimising each $\mathcal{L}_i$ with respect to $q_i(\mathbf{h}) = q(\mathbf{h}|\mathbf{v}_i)$

$$\max_q \mathcal{L}_\mathcal{D}(\boldsymbol{\theta}, q) \Leftrightarrow \max_{q_i} \mathcal{L}_i(\boldsymbol{\theta}, q_i) \quad \text{for } i = 1, \ldots, n \tag{28}$$

- We typically make some parametric assumptions. Let $q_i(\mathbf{h})$ be parametrised as $q_i(\mathbf{h}; \boldsymbol{\lambda}_i) \in \mathcal{Q}_i$.
- Different $q_i(\mathbf{h}; \boldsymbol{\lambda}_i)$ may belong to different parametric families.
- Optimisation with respect to $q_i$ then becomes optimisation with respect to $\boldsymbol{\lambda}_i$.

# Issue 1: Learning the conditional variational distribution

- Closed form solution typically not available. This means that we have to iteratively optimise $\mathcal{L}_i$ with respect to $\boldsymbol{\lambda}_i$ for all data points.
- We then have a nested loop: outer loop over data points $\mathbf{v}_i$ and the inner optimisation loop for $\boldsymbol{\lambda}_i$.
- Feasible if $n$ is very small. But too costly otherwise.

# Amortisation

- Let us parametrise the conditional distribution $q(\mathbf{h}|\mathbf{v})$ directly as
$$q(\mathbf{h}|\mathbf{v}) = q_{\phi}(\mathbf{h}|\mathbf{v}) = q(\mathbf{h}; \boldsymbol{\lambda}_{\phi}(\mathbf{v})) \tag{29}$$
where $\boldsymbol{\lambda}_{\phi}(\mathbf{v})$ is a nonlinear function parametrised by $\phi$. It is called inference or encoder network, or simply encoder.
- This means that we assume that each $q(\mathbf{h}|\mathbf{v}_i)$ belongs to the same parametric family $\mathcal{Q} = \{q(\mathbf{h}; \boldsymbol{\lambda})\}_{\boldsymbol{\lambda}}$.
- The function $\boldsymbol{\lambda}_{\phi}(\mathbf{v})$ maps each $\mathbf{v}$ to its corresponding parameter value $\boldsymbol{\lambda}$.
- Note: $\boldsymbol{\lambda}$ are the parameters of the variational distribution while $\phi$ are the parameters of the encoder network.
- Denote $\mathcal{L}_i(\boldsymbol{\theta}, q_{\phi})$ by $\mathcal{L}_i(\boldsymbol{\theta}, \phi)$ and $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, q_{\phi})$ by $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, \phi)$.
- We learn $\phi$ by maximising
$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, \phi) = \sum_{i=1}^{n} \mathcal{L}_i(\boldsymbol{\theta}, \phi) \tag{30}$$

# Amortisation (example)

- A popular choice for $q_\phi(\mathbf{h}|\mathbf{v})$ is

$$q_\phi(\mathbf{h}|\mathbf{v}) = \prod_k^H q_\phi(h_k|\mathbf{v}) \tag{31}$$

$$q_\phi(h_k|\mathbf{v}) = \mathcal{N}(h_k; \mu_k(\mathbf{v}; \phi_k^\mu), \sigma_k^2(\mathbf{v}; \phi_k^\sigma)) \tag{32}$$

  $\phi$ denotes parameters needed to parameterise all mean and var functions.
- Often used for variational autoencoders (see later).
- Makes both an independence and parametric assumption.
- This means that $\mathcal{Q} = \{q(\mathbf{h}; \boldsymbol{\lambda})\}_{\boldsymbol{\lambda}}$ equals the factorised Gaussian family with parameters

$$\boldsymbol{\lambda} = (\mu_1, \ldots, \mu_H, \sigma_1^2, \ldots, \sigma_H^2) \tag{33}$$

- The mapping $\boldsymbol{\lambda}_\phi(\mathbf{v})$ maps $\mathbf{v}$ to the means and variances,

$$(\mu_1, \ldots, \mu_H, \sigma_1^2, \ldots, \sigma_H^2) = \boldsymbol{\lambda}_\phi(\mathbf{v}) \tag{34}$$

# Amortisation gap

- $\mathcal{L}_\mathcal{D}$ is maximised if all individual per data-point $\mathcal{L}_i$ are maximised.
- When learning $\phi$, we hope that after learning

$$q(\mathbf{h}; \boldsymbol{\lambda}_{\hat{\phi}}(\mathbf{v}_i)) \approx \operatorname*{argmax}_{q_i \in \mathcal{Q}_i} \mathcal{L}_i(\boldsymbol{\theta}, q_i) \quad \text{for all } i \tag{35}$$

- The optimisation $\operatorname{argmax}_{q_i} \mathcal{L}_i$ maps $\mathbf{v}_i$ to the optimal $q_i$, and the idea of amortised inference is to approximate this mapping.
- However, the approximation will not be perfect because
  - $\boldsymbol{\lambda}_\phi(\mathbf{v})$ is learned by maximising the sum $\sum_i \mathcal{L}_i(\boldsymbol{\theta}, \phi)$ and not a single $\mathcal{L}_i(\boldsymbol{\theta}, \phi)$ for a given $\mathbf{v}_i$.
  - We assume that all $q(\mathbf{h}|\mathbf{v}_i)$ belong to the same parametric family, i.e. $\mathcal{Q} = \mathcal{Q}_i$ for all $i$, which may not be the case.
- The approximation will be better for some $\mathbf{v}_i$ than for others.

# Amortisation gap

- The approximation error due to amortisation is

$$q_i^*(\mathbf{h}|\mathbf{v}_i) - q(\mathbf{h}; \boldsymbol{\lambda}_{\hat{\phi}}(\mathbf{v}_i)), \quad q_i^*(\mathbf{h}|\mathbf{v}_i) = \underset{q_i \in \mathcal{Q}_i}{\operatorname{argmax}} \mathcal{L}_i(\boldsymbol{\theta}, q_i) \quad (36)$$

  (If $\mathcal{Q} = \mathcal{Q}_i$, we can also compare the amortised with the optimal parameter $\boldsymbol{\lambda}$)

- Difference between corresponding ELBOs is called the amortisation gap

$$\mathcal{L}_i(\boldsymbol{\theta}, q_i^*) - \mathcal{L}_i(\boldsymbol{\theta}, \hat{\phi}) \quad \text{with } \hat{\phi} = \underset{\phi}{\operatorname{argmax}} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, \phi) \quad (37)$$

- After learning, the encoder network $\boldsymbol{\lambda}_{\hat{\phi}}(\mathbf{v})$ can be applied to test inputs $\mathbf{v}_{\text{test}}$ thereby bypassing an optimisation of the ELBO $\mathcal{L}_{\mathbf{v}_{\text{test}}}$.
- The approximation error and amortisation gap will likely be larger for $\mathbf{v}_{\text{test}}$ than for the training data $\mathbf{v}_1, \ldots, \mathbf{v}_n$.

  For methods to reduce the amortisation gap, see e.g. Marino et al, *Iterative amortised inference*, ICML 2018, `https://arxiv.org/abs/1807.09356`

# Amortisation gap

- Example in two dimensions where $q_i$ is assumed Gaussian with parameters $\boldsymbol{\lambda} = (\mu_1, \mu_2)$.
- The contour plot shows $\mathcal{L}_i(\boldsymbol{\theta}, q_i)$ as a function of $\boldsymbol{\lambda}$
- The blue line shows the gradient ascent optimisation path when the ELBO is optimised without amortisation.
- The cyan diamond shows the amortised estimate $\boldsymbol{\lambda}_{\hat{\phi}}(\mathbf{v}_i)$.

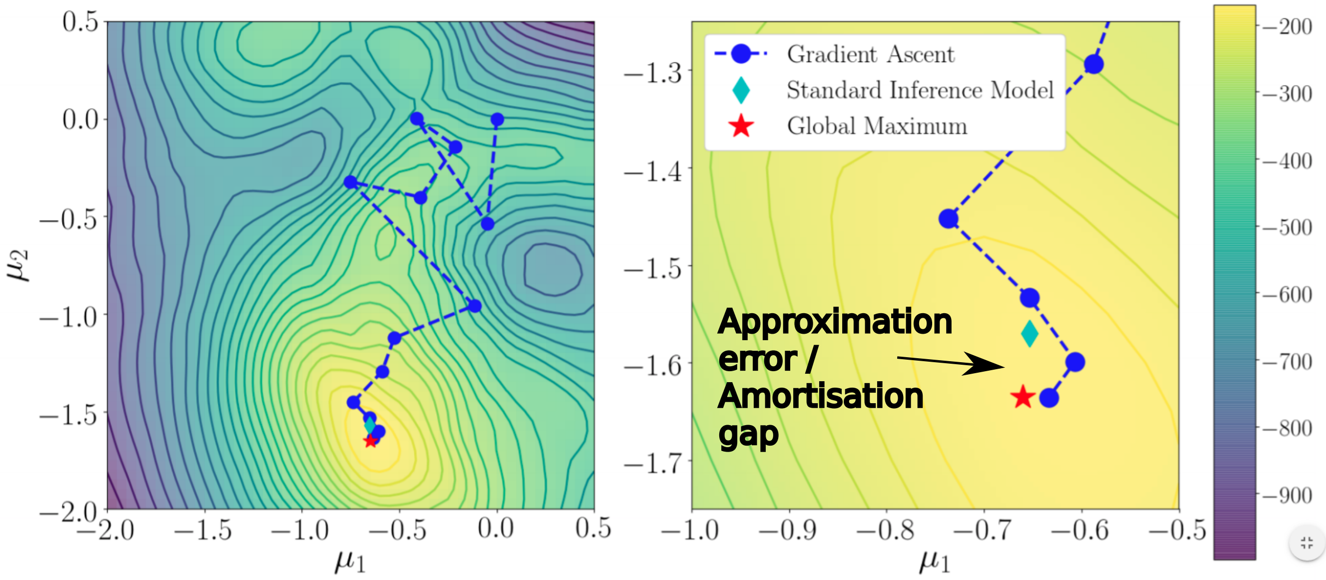



Figure 1 from Marino et al, ICML 2018.

# Issue 2: Maximisation

- The optimisation problem is

$$\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\phi}} = \underset{\boldsymbol{\theta}, \boldsymbol{\phi}}{\operatorname{argmax}} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, \boldsymbol{\phi}) \tag{38}$$

where

$$\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, \boldsymbol{\phi}) = \sum_{i=1}^{n} \mathcal{L}_i(\boldsymbol{\theta}, \boldsymbol{\phi}) \tag{39}$$

$$= \sum_{i=1}^{n} \mathbb{E}_{q_{\boldsymbol{\phi}}(\mathbf{h}|\mathbf{v}_i)} \left[ \log \frac{p(\mathbf{v}_i, \mathbf{h}; \boldsymbol{\theta})}{q_{\boldsymbol{\phi}}(\mathbf{h}|\mathbf{v}_i)} \right] \tag{40}$$

- We would like to solve it using gradient ascent.
- Difficulties:
  1. We generally cannot compute the expectations in closed form.
  2. The parameter $\boldsymbol{\phi}$ occurs in the expectation so that we cannot pull $\nabla_{\boldsymbol{\phi}}$ inside.

# Important special case

- For some $q_\phi$, part of the ELBO is available in closed form.
- From the basic properties of the ELBO

$$\mathcal{L}_i(\boldsymbol{\theta}, \phi) = \mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)} [\log p(\mathbf{v}_i, \mathbf{h}; \boldsymbol{\theta})] + \mathcal{H}(q_\phi) \tag{41}$$

  where $\mathcal{H}(q_\phi)$ is the entropy of $q_\phi$.
- The entropy can sometimes be computed in closed form.
- For factorised Gaussian:

$$\mathcal{H}(q_\phi) = \sum_{k=1}^{H} \frac{1}{2} \left(1 + \log(2\pi\sigma_k^2(\mathbf{v}))\right) \tag{42}$$

- However, the $\mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}$ issue remains for the first term.

# Reparametrisation

- Consider again the general case.
- We can approximate the expectation as a sample average, but we have to keep track of the $\phi$-dependency of the samples.
- For that, let us consider variational distributions $q_\phi(\mathbf{h}|\mathbf{v})$ that can be obtained via a transformation of a random variable $\boldsymbol{\epsilon}$ that we can sample from.

$$\mathbf{h} \sim q_\phi(\mathbf{h}|\mathbf{v}) \qquad \Longleftrightarrow \qquad \mathbf{h} = \mathbf{t}_\phi(\boldsymbol{\epsilon}, \mathbf{v}), \quad \boldsymbol{\epsilon} \sim p(\boldsymbol{\epsilon}) \qquad (43)$$

- Examples:
  - $h \sim \mathcal{N}(h; \mu(\mathbf{v}), \sigma^2(\mathbf{v})) \Leftrightarrow h = \mu(\mathbf{v}) + \sigma(\mathbf{v})\epsilon$ with $\epsilon \sim \mathcal{N}(\epsilon, 0, 1)$.
  - Inverse transform sampling
  - Factor analysis or ICA model where factor or mixing matrix depends on $\mathbf{v}$.
  - ...

# Reparametrisation

- By the law of the unconscious statistician, we then obtain

$$\mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}\left[\log \frac{p(\mathbf{v}_i, \mathbf{h}; \boldsymbol{\theta})}{q_\phi(\mathbf{h}|\mathbf{v}_i)}\right] = \mathbb{E}_{p(\epsilon)}\left[\log \frac{p(\mathbf{v}_i, \mathbf{t}_\phi(\epsilon, \mathbf{v}_i); \boldsymbol{\theta})}{q_\phi(\mathbf{t}_\phi(\epsilon, \mathbf{v}_i)|\mathbf{v}_i)}\right] \quad (44)$$

- We can now pull the gradients inside

$$\nabla_{\boldsymbol{\theta},\phi}\mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}[\cdots] = \nabla_{\boldsymbol{\theta},\phi}\mathbb{E}_{p(\epsilon)}[\cdots] = \mathbb{E}_{p(\epsilon)}[\nabla_{\boldsymbol{\theta},\phi}\cdots]$$

- The gradient can then be computed via auto-differentiation.
- Note: Alternative to reparametrisation is to use an approach called score function gradient estimation (not examinable).

# Stochastic optimisation

- The gradient of $\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, \phi)$ thus becomes

$$\nabla_{\boldsymbol{\theta},\phi}\mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta}, \phi) = \sum_{i=1}^{n} \mathbb{E}_{p(\epsilon_i)}\left[\nabla_{\boldsymbol{\theta},\phi} \log \frac{p(\mathbf{v}_i, \mathbf{t}_\phi(\epsilon_i, \mathbf{v}_i); \boldsymbol{\theta})}{q_\phi(\mathbf{t}_\phi(\epsilon_i, \mathbf{v}_i)|\mathbf{v}_i)}\right] \tag{45}$$

- We can approximate $\mathbb{E}_{p(\epsilon_i)}$ with a sample average (Monte Carlo integration) with $S$ samples.
- For large $n$ and $S$, evaluation of the gradient is expensive.
- Computing the gradient for all $\mathbf{v}_i$ and using a large $S$ is not necessary. We can use stochastic optimisation instead.
- This means we only evaluate the gradient for a random subset (minibatch) of the $\mathbf{v}_i$ and set $S$ to a small number (e.g. 1!).

We gloss over technical details here; for an introduction to stochastic optimisation, see *Introduction to Stochastic Search and Optimization* by James Spall.

Eq (45) can be manipulated to reduce the variance of the stochastic gradient, see Roeder et al, *Sticking the Landing: Simple, Lower-Variance Gradient Estimators for Variational Inference*, NeuRIPS 2017.

# Program

1. Scalable generic variational learning of latent variable models
   - ELBO for iid data
   - Amortised variational inference
   - Reparametrisation and stochastic optimisation
2. Deep latent variable models and variational autoencoders

# Program

1. Scalable generic variational learning of latent variable models

2. Deep latent variable models and variational autoencoders
   - Deep latent variable model
   - Variational autoencoder (VAE)
   - Gaussian and Bernoulli VAE

# Deep directed graphical models

- Parametric directed graphical models are sets of pdfs/pmfs that factorise as

$$p(\mathbf{x}; \boldsymbol{\theta}) = \prod_{k=1}^{d} p(x_k | \mathrm{pa}_k; \boldsymbol{\theta}) \tag{46}$$

  where $\mathrm{pa}_k$ denotes the parents of $x_k$ in a given directed acyclic graph (DAG).
- We say that the model is a deep directed graphical model if

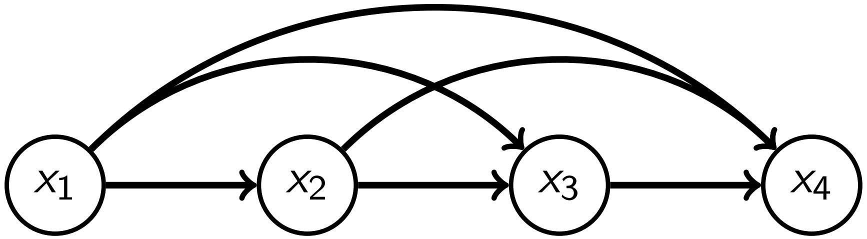
$$p(x_k | \mathrm{pa}_k; \boldsymbol{\theta}) = p(x_k; \boldsymbol{\eta}_k) \quad \text{with} \quad \boldsymbol{\eta}_k = \boldsymbol{\eta}^k_{\boldsymbol{\theta}}(\mathrm{pa}_k) \tag{47}$$

  where $p(x_k; \boldsymbol{\eta})$ is a parametric model and $\boldsymbol{\eta}^k_{\boldsymbol{\theta}}(\mathrm{pa}_k)$ a parametrised nonlinear function (deep neural network) that maps the parents $\mathrm{pa}_k$ to the model-parameters $\boldsymbol{\eta}_k$.

# Example

- Chain rule $p(\mathbf{x};\boldsymbol{\theta}) = \prod_{k=1}^{d} p(x_k|\mathrm{pre}_k;\boldsymbol{\theta})$ with

$$p(x_k|\mathrm{pre}_k;\boldsymbol{\theta}) = \mathcal{N}(x_k;\mu_k,\sigma_k^2), \qquad (\mu_k,\sigma_k^2) = \boldsymbol{\eta}_{\boldsymbol{\theta}}^k(\mathrm{pre}_k)$$




- Markov chain $p(\mathbf{x};\boldsymbol{\theta}) = \prod_{k=1}^{d} p(x_k|x_{k-1};\boldsymbol{\theta})$ with

$$p(x_k|x_{k-1};\boldsymbol{\theta}) = \mathcal{N}(x_k;\mu_k,\sigma_k^2), \qquad (\mu_k,\sigma_k^2) = \boldsymbol{\eta}_{\boldsymbol{\theta}}^k(x_{k-1})$$

# Deep latent variable model

- A deep (directed) latent variable model is a deep directed graphical model with latent variables.
- Often, they are models of the form

$$p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta}) = p(\mathbf{v}|\mathbf{h}; \boldsymbol{\theta})p(\mathbf{h}) \tag{48}$$

where $p(\mathbf{h})$ does not depend on $\boldsymbol{\theta}$ and $p(\mathbf{v}|\mathbf{h}; \boldsymbol{\theta})$ is

$$p(\mathbf{v}|\mathbf{h}; \boldsymbol{\theta}) = \prod_{k=1}^{d} p(v_k|\mathrm{pa}_k, \mathbf{h}; \boldsymbol{\theta}) \tag{49}$$

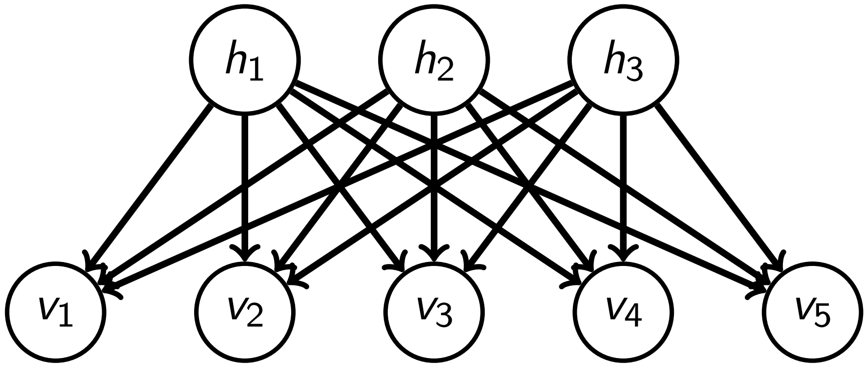
with

$$p(v_k|\mathrm{pa}_k, \mathbf{h}; \boldsymbol{\theta}) = p(v_k; \boldsymbol{\eta}_k) \qquad \boldsymbol{\eta}_k = \boldsymbol{\eta}_{\boldsymbol{\theta}}^k(\mathrm{pa}_k, \mathbf{h}) \tag{50}$$

- The latents $\mathbf{h}$ affect the distribution of all the visibles; $\mathrm{pa}_k$ are here the parents of $v_k$ without the $\mathbf{h}$.
- Note: Parametrised models $p(\mathbf{h}; \boldsymbol{\theta})$ may also be used.

# Graphical model for variational autoencoders

Reconsider the directed acyclic graph for FA and ICA:



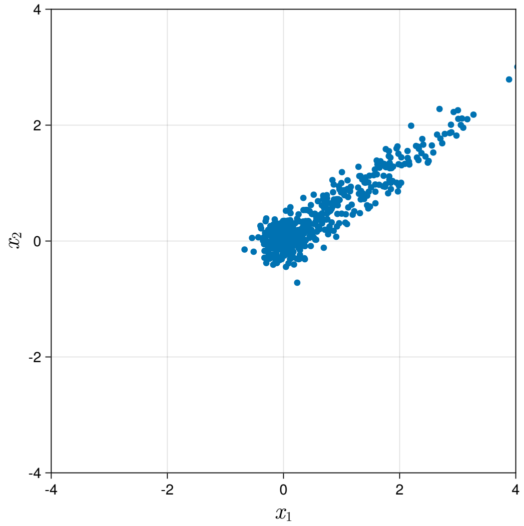

- The visibles $\mathbf{v} = (v_1, \ldots, v_d)$ are independent from each other given the latents $\mathbf{h} = (h_1, \ldots, h_H)$.
- Different assumptions on $p(v_k|\mathbf{h})$ and $p(\mathbf{h})$ give different methods, e.g. FA and ICA.
- Working with $H < d$ and $p(v_k|\mathbf{h}; \boldsymbol{\theta}) = p(v_k; \boldsymbol{\eta}_k)$ where $\boldsymbol{\eta}_k = \boldsymbol{\eta}_{\boldsymbol{\theta}}^k(\mathbf{h})$ gives variational autoencoders (VAE).
- The function $\boldsymbol{\eta}_k = \boldsymbol{\eta}_{\boldsymbol{\theta}}^k(\mathbf{h})$ is called the decoder or decoder network.

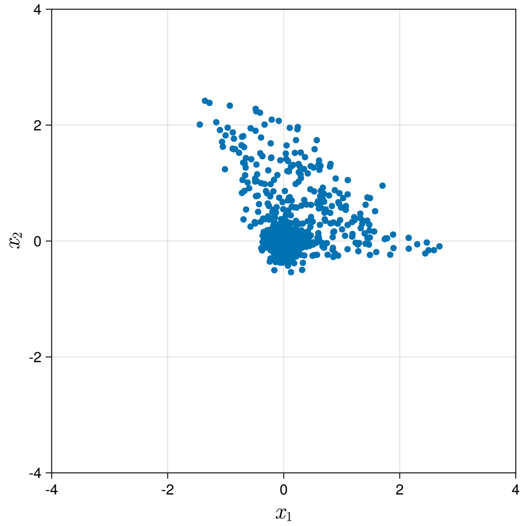
# VAE: overview

- Depending on the data, different parametric families are chosen for the univariate distributions $p(v_k; \boldsymbol{\eta}_k)$
- For example:
  - Gaussian pdf for $v_k \in \mathbb{R}$: Here $\boldsymbol{\eta}_k = (m_k, v_k^2)$ are the mean and variance.
  - Bernoulli pmf for $v_k \in \{0, 1\}$: Here $\boldsymbol{\eta}_k = p_k$ is the probability for $v_k = 1$.
- Note: The parametric families may be simple but the parameter $\boldsymbol{\eta}_k$ is a nonlinear transformation of $\mathbf{h}$: $\boldsymbol{\eta}_k = \boldsymbol{\eta}_{\boldsymbol{\theta}}^k(\mathbf{h})$

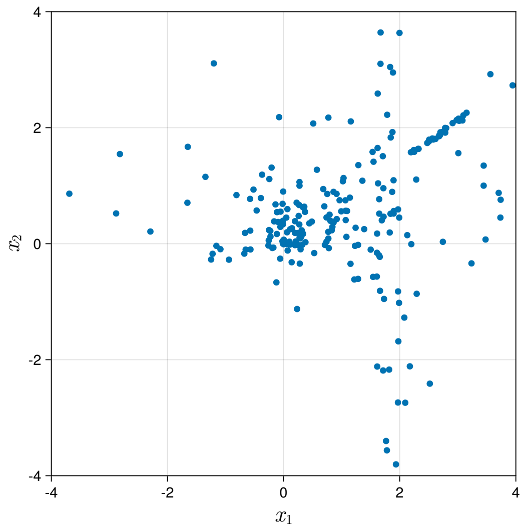
# Example: Gaussian VAE

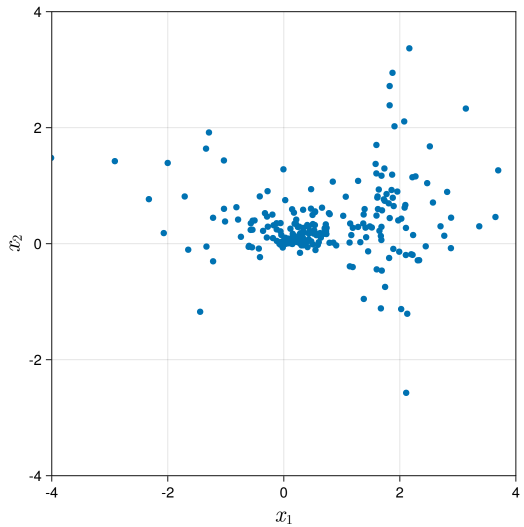
Nonlinear mean function (NN with random weights and ReLu), constant variance:




Nonlinear mean and variance functions:



# VAE: overview

- The variational distribution $q_\phi(\mathbf{h}|\mathbf{v})$ is often assumed to be a factorised Gaussian.
- Variational distribution $q_\phi(\mathbf{h}|\mathbf{v})$ goes under several names: encoder, inference model, or recognition model are used; the model $p(\mathbf{v}|\mathbf{h};\boldsymbol{\theta})$ is called the decoder or generative model.
- Note: the encoder/decoder names may refer to the distribution or the mapping to their parameters.

# VAE: learning

- We now derive the ELBO for the VAE using that:
  - $p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta}) = p(\mathbf{v}|\mathbf{h}; \boldsymbol{\theta})p(\mathbf{h})$ with $p(\mathbf{h}) = \mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{I})$
  - Factorised Gaussian for the variational distribution $q_\phi(\mathbf{h}|\mathbf{v})$
- As before:

$$q_\phi(\mathbf{h}|\mathbf{v}) = \prod_k^H q(h_k|\mathbf{v}) \tag{51}$$

$$q_\phi(h_k|\mathbf{v}) = \mathcal{N}(h_k; \mu_k(\mathbf{v}), \sigma_k^2(\mathbf{v})) \tag{52}$$

  That is, $\boldsymbol{\lambda}_\phi(\mathbf{v})$ maps $\mathbf{v}$ to $(\mu_1, \ldots, \mu_H, \sigma_1^2, \ldots, \sigma_H^2)$.

  ($\phi$-dependency of $\mu_k(\mathbf{v}), \sigma_k^2(\mathbf{v})$ is suppressed.)
- With the Gaussianity assumption on $p(\mathbf{h})$ and $q_\phi(\mathbf{h}|\mathbf{v})$, part of the ELBO can be computed in closed form.

# VAE: learning

- We have seen that if $q_\phi(\mathbf{h}|\mathbf{v})$ is a factorised Gaussian

$$\mathcal{L}_i = \mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}\left[\log p(\mathbf{v}_i, \mathbf{h}; \boldsymbol{\theta})\right] + \sum_{k=1}^{H} \frac{1}{2}\left(1 + \log(2\pi\sigma_k^2(\mathbf{v}_i))\right)$$

- Inserting further that $p(\mathbf{v}, \mathbf{h}; \boldsymbol{\theta}) = p(\mathbf{v}|\mathbf{h}; \boldsymbol{\theta})\mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{I})$, we have

$$\begin{aligned}\mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)} \log p(\mathbf{v}_i, \mathbf{h}; \boldsymbol{\theta}) = \mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}&[\log p(\mathbf{v}_i|\mathbf{h}; \boldsymbol{\theta})] + \\ &\mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}[\log \mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{I})]\end{aligned}$$

- We can compute the second term in closed form

$$\begin{aligned}\mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}[\log \mathcal{N}(\mathbf{h}; \mathbf{0}, \mathbf{I})] &= -\frac{H}{2}\log(2\pi) - \frac{1}{2}\mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}\left[\sum_{k=1}^{H} h_k^2\right] \\ &= -\frac{H}{2}\log(2\pi) - \frac{1}{2}\sum_{k=1}^{H}\left[\sigma_k^2(\mathbf{v}_i) + \mu_k^2(\mathbf{v}_i)\right]\end{aligned}$$

# VAE: learning

- Hence

$$
\begin{aligned}
\mathcal{L}_i &= \mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i))}\left[\log p(\mathbf{v}_i|\mathbf{h};\boldsymbol{\theta})\right] - \frac{H}{2}\log(2\pi) \\
&\quad - \frac{1}{2}\sum_{k=1}^{H}\left[\sigma_k^2(\mathbf{v}_i) + \mu_k^2(\mathbf{v}_i)\right] + \sum_{k=1}^{H}\frac{1}{2}\left(1 + \log(2\pi\sigma_k^2(\mathbf{v}_i))\right) \\
&= \mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}\left[\log p(\mathbf{v}_i|\mathbf{h};\boldsymbol{\theta})\right] \\
&\quad + \frac{1}{2}\sum_{k=1}^{H}\left(1 + \log(\sigma_k^2(\mathbf{v}_i)) - \sigma_k^2(\mathbf{v}_i) - \mu_k^2(\mathbf{v}_i)\right)
\end{aligned}
$$

- Same expression can be obtained from

$$
\mathcal{L}_i = \mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}\left[\log p(\mathbf{v}_i|\mathbf{h};\boldsymbol{\theta})\right] - \mathrm{KL}(q_\phi(\mathbf{h}|\mathbf{v}_i)||\mathcal{N}(\mathbf{h};\mathbf{0},\mathbf{I}))
$$

  and using the closed-form expression for the KL divergence.
- First term: reconstruction/fit; second term: regularisation

# VAE: learning

- With the conditional independence assumption for $p(\mathbf{v}_i|\mathbf{h};\boldsymbol{\theta})$:

$$\mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}[\log p(\mathbf{v}_i|\mathbf{h};\boldsymbol{\theta})] = \sum_{k=1}^{d} \mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}\left[\log p(v_{ik};\boldsymbol{\eta}_\theta^k(\mathbf{h}))\right]$$

  where $v_{ik}$ denotes the $k$-th element of $\mathbf{v}_i$.

- We thus have for the VAE:

$$\mathcal{L}_i(\boldsymbol{\theta},\boldsymbol{\phi}) = \sum_{k=1}^{d} \mathbb{E}_{q_\phi(\mathbf{h}|\mathbf{v}_i)}\left[\log p(v_{ik};\boldsymbol{\eta}_\theta^k(\mathbf{h}))\right] + \\ + \frac{1}{2}\sum_{k=1}^{H}\left(1+\log(\sigma_k^2(\mathbf{v}_i)) - \sigma_k^2(\mathbf{v}_i) - \mu_k^2(\mathbf{v}_i)\right) \quad (53)$$

- Optimisation problem

$$\hat{\boldsymbol{\theta}},\hat{\boldsymbol{\phi}} = \operatorname*{argmax}_{\boldsymbol{\theta},\boldsymbol{\phi}} \mathcal{L}_{\mathcal{D}}(\boldsymbol{\theta},\boldsymbol{\phi}) = \operatorname*{argmax}_{\boldsymbol{\theta},\boldsymbol{\phi}} \sum_{i=1}^{n} \mathcal{L}_i(\boldsymbol{\theta},\boldsymbol{\phi}) \quad (54)$$

- Solved using stochastic gradient ascent.

# Gaussian VAE

- The Gaussian VAE is obtained for

$$p(v_k|\mathbf{h};\boldsymbol{\theta}) = \mathcal{N}(v_k; m_k, s_k^2) \qquad (m_k, s_k^2) = \boldsymbol{\eta}_{\boldsymbol{\theta}}^k(\mathbf{h}) \qquad (55)$$

- Generative model $p(\mathbf{v}|\mathbf{h};\boldsymbol{\theta})$ equivalent to

$$\mathbf{v} = \begin{pmatrix} m_1(\mathbf{h}) \\ \vdots \\ m_D(\mathbf{h}) \end{pmatrix} + \begin{pmatrix} s_1(\mathbf{h}) & & \\ & \ddots & \\ & & s_D(\mathbf{h}) \end{pmatrix} \mathbf{n}, \quad \mathbf{n} \sim \mathcal{N}(\mathbf{n}; \mathbf{0}, \mathbf{I})$$

- FA obtained for $\mathbf{m} = (m_1, \ldots, m_D)^\top = \mathbf{F}\mathbf{h} + \mathbf{c}$ and $s_k^2 = \Psi_k$.
- Gaussian VAE is a nonlinear generalisation of FA.

# Bernoulli VAE

- The Bernoulli VAE with $v_k \in \{0, 1\}$ is obtained for

$$p(v_k|\mathbf{h}; \boldsymbol{\theta}) = p_k^{v_k}(1 - p_k)^{(1-v_k)} \qquad p_k = \eta_{\boldsymbol{\theta}}^k(\mathbf{h}) \tag{56}$$

- This is often also used for $v_k \in [0, 1]$. While the ELBO can be evaluated, it is formally wrong since $v_k$ is not binary.
- Use the so-called continuous Bernoulli distribution or the beta distribution instead.

  (see Loaiza-Ganem and Cunningham, *The continuous Bernoulli: fixing a pervasive error in variational autoencoders*, NeuRIPS 2019)

# Program recap

1. Scalable generic variational learning of latent variable models
   - ELBO for iid data
   - Amortised variational inference
   - Reparametrisation and stochastic optimisation

2. Deep latent variable models and variational autoencoders
   - Deep latent variable model
   - Variational autoencoder (VAE)
   - Gaussian and Bernoulli VAE