# Probabilistic \& Unsupervised Learning 

## Parametric Variational Methods and Recognition Models

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## Variational methods

- Our treatment of variational methods has (except EP) emphasised 'natural' choices of variational family - often factorised using the same functional (ExpFam) form as joint.
- mostly restricted to joint exponential families - facilitates hierarchical and distributed models, but not non-linear/non-conjugate.


## Variational methods

- Our treatment of variational methods has (except EP) emphasised 'natural' choices of variational family - often factorised using the same functional (ExpFam) form as joint.
- mostly restricted to joint exponential families - facilitates hierarchical and distributed models, but not non-linear/non-conjugate.
- Consider parametric variational approximations using a constrained family $q(\mathcal{Z} ; \rho)$.

The constrained (approximate) variational E-step becomes:

$$
q(\mathcal{Z}):=\underset{q \in\{q(\mathcal{Z} ; \rho)\}}{\operatorname{argmax}} \mathcal{F}\left(q(\mathcal{Z}), \theta^{(k-1)}\right) \Rightarrow \rho^{(k)}:=\underset{\rho}{\operatorname{argmax}} \mathcal{F}\left(q(\mathcal{Z} ; \rho), \theta^{(k-1)}\right)
$$

and so we can replace constrained optimisation of $\mathcal{F}(q, \theta)$ with unconstrained optimisation of a constrained $\mathcal{F}(\rho, \theta)$ :

$$
\mathcal{F}(\rho, \theta)=\left\langle\log P\left(\mathcal{X}, \mathcal{Z} \mid \theta^{(k-1)}\right)\right\rangle_{q(\mathcal{Z} ; \rho)}+\mathbf{H}[\rho]
$$

It might still be valuable to use coordinate ascent in $\rho$ and $\theta$, although this is no longer necessary.

## Optimising the variational parameters

$$
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- In some special cases, the expectations of the log-joint under $q(\mathcal{Z} ; \rho)$ can be expressed in closed form, but these are rare.


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- "Score-based" gradient estimate, and Monte-Carlo (Ranganath et al. 2014).
- Recognition network trained in separate phase - not strictly variational (Dayan et al. 1995).
- Recognition network trained simultaneously with generative model using "frozen" samples (Kingma and Welling 2014; Rezende et al. 2014).


## Score-based gradient estimate

We have:

$$
\begin{aligned}
\nabla_{\rho} \mathcal{F}(\rho, \theta)= & \nabla_{\rho} \int d \mathcal{Z} q(\mathcal{Z} ; \rho)(\log P(\mathcal{X}, \mathcal{Z} \mid \theta)-\log q(\mathcal{Z} ; \rho)) \\
= & \int d \mathcal{Z}\left[\nabla_{\rho} q(\mathcal{Z} ; \rho)\right](\log P(\mathcal{X}, \mathcal{Z} \mid \theta)-\log q(\mathcal{Z} ; \rho)) \\
& +q(\mathcal{Z} ; \rho) \nabla_{\rho}[\log P(\mathcal{X}, \mathcal{Z} \mid \theta)-\log q(\mathcal{Z} ; \rho)]
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\end{aligned}
$$

Now,

$$
\begin{aligned}
& \nabla_{\rho} \log P(\mathcal{X}, \mathcal{Z} \mid \theta)=0 \\
& \int d \mathcal{Z} q(\mathcal{Z} ; \rho) \nabla_{\rho} \log q(\mathcal{Z} ; \rho)=\nabla_{\rho} \int d \mathcal{Z} q(\mathcal{Z} ; \rho)=0 \\
& \nabla_{\rho} q(\mathcal{Z} ; \rho)=q(\mathcal{Z} ; \rho) \nabla_{\rho} \log q(\mathcal{Z} ; \rho)
\end{aligned}
$$

So,

$$
\nabla_{\rho} \mathcal{F}(\rho, \theta)=\left\langle\left[\nabla_{\rho} \log q(\mathcal{Z} ; \rho)\right](\log P(\mathcal{X}, \mathcal{Z} \mid \theta)-\log q(\mathcal{Z} ; \rho))\right\rangle_{q(\mathcal{Z} ; \rho)}
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So,

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\nabla_{\rho} \mathcal{F}(\rho, \theta)=\left\langle\left[\nabla_{\rho} \log q(\mathcal{Z} ; \rho)\right](\log P(\mathcal{X}, \mathcal{Z} \mid \theta)-\log q(\mathcal{Z} ; \rho))\right\rangle_{q(\mathcal{Z} ; \rho)}
$$

Reduced gradient of expectation to expectation of gradient - easier to compute. Also called the REINFORCE trick.

## Factorisation

$$
\nabla_{\rho} \mathcal{F}(\rho, \theta)=\left\langle\left[\nabla_{\rho} \log q(\mathcal{Z} ; \rho)\right](\log P(\mathcal{X}, \mathcal{Z} \mid \theta)-\log q(\mathcal{Z} ; \rho))\right\rangle_{q(\mathcal{Z} ; \rho)}
$$

- Still requires a high-dimensional expectation, but can now be evaluated by Monte-Carlo.
- Dimensionality reduced by factorisation (particularly where $P(\mathcal{X}, \mathcal{Z})$ is factorised). Let $q(\mathcal{Z})=\prod_{i} q\left(\mathcal{Z}_{i} \mid \rho_{i}\right)$ factor over disjoint cliques; let $\overline{\mathcal{Z}}_{i}$ be the minimal Markov blanket of $\mathcal{Z}_{i}$ in the joint; $P_{\overline{\mathcal{Z}}_{i}}$ be the product of joint factors that include any element of $\mathcal{Z}_{i}$ (so the union of their arguments is $\overline{\mathcal{Z}}_{i}$ ); and $P_{\neg \overline{\mathcal{Z}}_{i}}$ the remaining factors. Then,

$$
\begin{aligned}
\nabla_{\rho_{i}} \mathcal{F}\left(\left\{\rho_{j}\right\}, \theta\right)= & \left\langle\left[\nabla_{\rho_{i}} \sum_{j} \log q\left(\mathcal{Z}_{j} ; \rho_{j}\right)\right]\left(\log P(\mathcal{X}, \mathcal{Z} \mid \theta)-\sum_{j} \log q\left(\mathcal{Z}_{j} ; \rho_{j}\right)\right)\right\rangle_{q(\mathcal{Z})} \\
& =\left\langle\left[\nabla_{\rho_{i}} \log q\left(\mathcal{Z}_{i} ; \rho_{i}\right)\right]\left(\log P_{\overline{\mathcal{Z}}_{i}}\left(\mathcal{X}, \overline{\mathcal{Z}}_{i}\right)-\log q\left(\mathcal{Z}_{i} ; \rho_{i}\right)\right\rangle_{q\left(\overline{\mathcal{Z}}_{i}\right)}\right. \\
& +\langle\left[\nabla_{\rho_{i}} \log q\left(\mathcal{Z}_{i} ; \rho_{i}\right)\right] \underbrace{}_{\text {constant wrt }})
\end{aligned}
$$

So the second term is proportional to $\left\langle\nabla_{\rho_{i}} \log q\left(\mathcal{Z}_{i} ; \rho_{i}\right)\right\rangle_{q\left(\mathcal{Z}_{i}\right)}$, this $=0$ as before. So expectations are only needed wrt $q\left(\overline{\mathcal{Z}}_{i}\right) \rightarrow$ variational message passing!

## Sampling

So the "black-box" variational approach is as follows:

- Choose a parametric (factored) variational family $q(\mathcal{Z})=\prod_{i} q\left(\mathcal{Z}_{i} ; \rho_{i}\right)$.
- Initialise factors.
- Repeat to convergence:
- Stochastic VE-step. For each $i$ :
- Sample from $q\left(\overline{\mathcal{Z}}_{i}\right)$ and estimate expected gradient $\nabla_{\rho_{i}} \mathcal{F}$.
- Update $\rho_{i}$ along gradient.
- Stochastic M-step. For each $i$ :
- Sample from each $q\left(\overline{\mathcal{Z}}_{i}\right)$.
- Update corresponding parameters.
- Stochastic gradient steps may employ a Robbins-Munro step-size sequence to promote convergence.
- Variance of the gradient estimators can also be controlled by clever Monte-Carlo techniques (orginal authors used a "control variate" method that we have not studied).


## Recognition Models

We have not generally distinguished between multivariate models and iid data instances, grouping all variables together in $\mathcal{Z}$.

However, even for large models (such as HMMs), we often work with multiple data draws (e.g. multiple strings) and each instance requires a separate variational optimisation.

Suppose that we have fixed length vectors $\left\{\left(\mathbf{x}_{i}, \mathbf{z}_{i}\right)\right\}$ ( $\mathbf{z}$ is still latent).

- Optimal variational distribution $q^{*}\left(\mathbf{z}_{i}\right)$ depends on $\mathbf{x}_{i}$.
- Learn this mapping (in parametric form): $q\left(\mathbf{z}_{i} ; \rho=f\left(\mathbf{x}_{i} ; \phi\right)\right)$.
- Now $\rho$ is the output of a general function approximator $f$ (a GP, neural network or similar) parametrised by $\phi$, trained to map $\mathbf{x}_{i}$ to the variational parameters of $q\left(\mathbf{z}_{i}\right)$.
- The mapping function $f$ is called a recognition model.
- This is approach is now often called amortised inference.

How to learn $f$ ?

## The Helmholtz Machine

Dayan et al. (1995) originally studied binary sigmoid belief net, with parallel recognition model:


Two phase learning:

- Wake phase: given current $f$, estimate mean-field representation from data (mean sufficient stats for Bernoulli are just probabilities):

$$
q\left(\mathbf{z}_{i}\right)=\text { Bernoulli }\left[\hat{\mathbf{z}}_{i}\right] \quad \hat{\mathbf{z}}_{i}=f\left(\mathbf{x}_{i} ; \phi\right)
$$

Update generative parameters $\theta$ according to $\nabla_{\theta} \mathcal{F}\left(\left\{\hat{\mathbf{z}}_{i}\right\}, \theta\right)$.

- Sleep phase: sample $\left\{\mathbf{z}_{s}, \mathbf{x}_{s}\right\}_{s=1}^{S}$ from current generative model. Update recognition parameters $\phi$ to direct $f\left(\mathbf{x}_{s}\right)$ towards $\mathbf{z}_{s}$ (simple gradient learning).

$$
\Delta \phi \propto \sum_{s}\left(\mathbf{z}_{s}-f\left(\mathbf{x}_{s} ; \phi\right)\right) \nabla_{\phi} f\left(\mathbf{x}_{s} ; \phi\right)
$$

## The Helmholtz Machine

- Can sample $\mathbf{z}$ from recognition model rather than just evaluate means.
- Expectations in free-energy can be computed directly rather than by mean substitution.
- In hierarchical models, output of higher recognition layers then depends on samples at previous stages, which introduces correlations between samples at different layers.
- Recognition model structure need not exactly echo generative model.
- More general approach is to train $f$ to yield mean parameters of ExpFam $q(\mathbf{z})$ (later).
- Sleep phase learning minimises $\operatorname{KL}\left[p_{\theta}(\mathbf{z} \mid \mathbf{x}) \| q(\mathbf{z} ; f(\mathbf{x}, \phi))\right]$. Opposite to variational objective, but may not matter if divergence is small enough.


## Variational Autoencoders



- Fuses the wake and sleep phases.
- Generate recognition samples using deterministic transformations of external random variates (reparametrisation trick).
- E.g. if $\mathbf{f}$ gives marginal $\mu_{i}$ and $\sigma_{i}$ for latents $z_{i}$ and

$$
\epsilon_{i}^{s} \sim \mathcal{N}(0,1), \text { then } z_{i}^{s}=\mu_{i}+\sigma_{i} \epsilon_{i}^{s} .
$$

- Now generative and recognition parameters can be trained together by gradient descent (backprop), holding $\epsilon^{s}$ fixed.

$$
\begin{aligned}
\mathcal{F}_{i}(\theta, \phi) & =\sum_{s} \log P\left(\mathbf{x}_{i}, \mathbf{z}_{i}^{s} ; \theta\right)-\log q\left(\mathbf{z}_{i}^{s} ; \mathbf{f}\left(\mathbf{x}_{i}, \phi\right)\right) \\
\frac{\partial}{\partial \theta} \mathcal{F}_{i}= & \sum_{s} \nabla_{\theta} \log P\left(\mathbf{x}_{i}, \mathbf{z}_{i}^{s} ; \theta\right) \\
\frac{\partial}{\partial \phi} \mathcal{F}_{i}= & \sum_{s} \frac{\partial}{\partial \mathbf{z}_{i}^{s}}\left(\log P\left(\mathbf{x}_{i}, \mathbf{z}_{i}^{s} ; \theta\right)-\log q\left(\mathbf{z}_{i}^{s} ; \mathbf{f}\left(\mathbf{x}_{i}\right)\right)\right) \frac{d \mathbf{z}_{i}^{s}}{d \phi} \\
& +\frac{\partial}{\partial \mathbf{f}\left(\mathbf{x}_{i}\right)} \log q\left(\mathbf{z}_{i}^{s} ; \mathbf{f}\left(\mathbf{x}_{i}\right)\right) \frac{d \mathbf{f}\left(\mathbf{x}_{i}\right)}{d \phi}
\end{aligned}
$$

## Variational Autoencoders

- Frozen samples $\epsilon^{s}$ can be redrawn to avoid overfitting.
- May be possible to evaluate entropy and $\log P(\mathbf{z})$ without sampling, reducing variance.
- Differentiable reparametrisations are available for a number of different distributions.
- Conditional $P(\mathbf{x} \mid \mathbf{z}, \theta)$ is often implemented as a neural network with additive noise at output, or at transitions. If at transitions recognition network must estimate each noise input.
- In practice, hierarchical models appear difficult to learn.


## More recent work

- Changing the variational cost function (tightening the bound):
- Importance-Weighted autoencoder (IWAE)
- Filtering variational objective (FIVO)
- Thermodynamic variational objective (TVO)
- Flexible variational distributions
- Normalising flows
- DDC-Helmholtz machine
- Structured generative models
- "standard" VAE generative model both too powerful and too simple for learning
- local conjugate inference - structured VAEs
- DDC message passing

Far from exhaustive . . . these are all areas of active research. We'll survey a few ideas.

## Importance-weighted free energy

Another interpretation of the free energy:

$$
\mathcal{F}(q, \theta)=\left\langle\log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}\right\rangle_{q}=\underset{\mathbf{E} \sim q}{\substack{\text { proposal } \\ \downarrow}}\left[\log p(\mathbf{x}) \frac{p(\mathbf{z} \mid \mathbf{x})}{q(\mathbf{z})}\right]
$$

Jensen bound on importance sampled estimate:

$$
\ell(\theta)=\log \mathbb{E}_{\mathbf{z} \sim q}\left[\frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}\right] \geq \mathbb{E}_{\mathbf{z} \sim q}\left[\log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}\right]
$$

Suggests more accurate importance sampling:

$$
\ell(\theta)=\log \mathbb{E}_{\mathbf{z}_{1} \ldots \mathbf{z}_{K} \sim} \mathrm{iid}_{\sim}\left[\frac{1}{K} \sum_{k} \frac{p\left(\mathbf{x}, \mathbf{z}_{k}\right)}{q\left(\mathbf{z}_{k}\right)}\right] \geq \mathbb{E}_{\mathbf{z}_{1} \ldots \mathbf{z}_{K} \sim q} \underset{\sim}{\mathrm{iid}}\left[\log \frac{1}{K} \sum_{k} \frac{p\left(\mathbf{x}, \mathbf{z}_{k}\right)}{q\left(\mathbf{z}_{k}\right)}\right]
$$

Tighter bound, and reparametrisation friendly, but as $K \rightarrow \infty$ the signal for learning amortised $q$ grows weaker so VAE learning doesn't always improve.

## Normalising flows

$$
\mathcal{F}(q, \theta)=\langle\log p(\mathbf{x}, \mathbf{z} \mid \theta)\rangle_{q}-\langle\log q(\mathbf{z})\rangle_{q}
$$

To evaluate $\mathcal{F}$ (or its gradients) we need to be able to find expectations wrt $q$ (e.g. by Monte Carlo) and evaluate the log-density - usually restricts us to tractable inferential families.

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Consider defining a recognition model $q(\mathbf{z})$ implicitly by:

$$
\begin{aligned}
\mathbf{z}_{0} & \sim q_{0}(\cdot ; \mathbf{x}) \\
\mathbf{z} & =f_{K}\left(f_{K-1}\left(\ldots f_{1}\left(\mathbf{z}_{0}\right)\right)\right)
\end{aligned}
$$

$\leftarrow$ fixed, tractable, e.g. $\mathcal{N}(\mathbf{x}, I)$
$\leftarrow f_{k}$ smooth, invertible, parametrised by $\phi$

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Then

$$
\begin{aligned}
\langle F(\mathbf{z})\rangle_{q} & =\left\langle F\left(f_{K}\left(f_{K-1}\left(\ldots f_{1}\left(\mathbf{z}_{0}\right)\right)\right)\right)\right\rangle_{q_{0}} \\
\log q(\mathbf{z}) & =\log q_{0}\left(f_{1}^{-1}\left(f_{2}^{-1}\left(\ldots f_{K}^{-1}(\mathbf{z})\right)\right)\right)-\sum_{k} \log \left|\nabla f_{k}\right|
\end{aligned}
$$

where the second result applies from repeated transformations of variables

$$
\mathbf{z}_{k}=f_{k}\left(\mathbf{z}_{k-1}\right) \Rightarrow q\left(\mathbf{z}_{k}\right)=q\left(f_{k}^{-1}\left(\mathbf{z}_{k}\right)\right)\left|\frac{\partial \mathbf{z}_{k-1}}{\partial \mathbf{z}_{k}}\right|=q\left(f_{k}^{-1}\left(\mathbf{z}_{k}\right)\right)\left|\nabla f_{k}\left(\mathbf{z}_{k-1}\right)\right|^{-1}
$$

## Normalising flows

So, given a sample $\mathbf{z}_{0}^{\text {sid }} \stackrel{\text { iid }}{\sim} q_{0}(\cdot ; \mathbf{x})$ :

$$
\left.\mathcal{F}(q, \theta) \approx \frac{1}{S} \sum_{s} \log p\left(\mathbf{x}, f_{k}\left(\ldots f_{1}\left(\mathbf{z}_{0}^{s}\right)\right)\right)\right)+\mathbf{H}\left[q_{0}\right]+\frac{1}{S} \sum_{s} \sum_{k}\left|\nabla f_{k}\left(f_{k-1}\left(\ldots f_{1}\left(\mathbf{z}_{0}^{s}\right)\right)\right)\right|
$$

and we can compute gradients of this expression wrt $\theta$ and $\phi$.

Useful fs (from Rezende \& Mohammed 2015):

$$
\begin{aligned}
f(\mathbf{z})=\mathbf{z}+\mathbf{u} h\left(\mathbf{w}^{\top} \mathbf{z}+b\right) & \Rightarrow \\
\left.f(\mathbf{z})=\mathbf{z}+\frac{\beta}{\alpha+\mid \mathbf{z -}} \mathbf{\mathbf { z } _ { 0 } |} \right\rvert\, & \Rightarrow\left|1+\mathbf{u}^{\top} \psi(\mathbf{z})\right| \quad \psi(\mathbf{z})=h^{\prime}\left(\mathbf{w}^{\top} \mathbf{z}+b\right) \mathbf{w} \\
& r=\left|\mathbf{z}-\mathbf{z}_{0}\right|, h=\frac{1}{\alpha+r}
\end{aligned}
$$

Both can be cascaded to give a flexible variational family.

## DDC Helmholtz machine

A (loosely) neurally inspired idea. Define $q$ as an unnormalisable exponential family with a large set of sufficient statistics

$$
q(\mathbf{z}) \propto e^{\sum_{i} \eta_{i} \psi_{i}(\mathbf{z})}
$$

and parametrise by mean parameters $\mu=\langle\phi(\mathbf{z})\rangle$ : Distributed distributional code (DDC). Train recognition model using sleep samples:

$$
\begin{aligned}
& \boldsymbol{\mu}=\langle\boldsymbol{\psi}(\mathbf{z})\rangle_{q}=f(\mathbf{x} ; \phi) \\
& \Delta \phi \propto \sum_{s}\left(\boldsymbol{\psi}\left(\mathbf{z}_{s}\right)-f\left(\mathbf{x}_{s} ; \phi\right)\right) \nabla_{\phi} f\left(\mathbf{x}_{s} ; \phi\right)
\end{aligned}
$$

Also learn linear approximation $\nabla \log p(\mathbf{x}, \mathbf{z} \mid \theta) \approx A \psi(\mathbf{z})$

$$
A=\left(\sum_{s} \nabla \log p\left(\mathbf{x}_{s}, \mathbf{z}_{s} \mid \theta\right) \boldsymbol{\psi}\left(\mathbf{z}_{s}\right)\right)^{\top}\left(\sum_{s} \boldsymbol{\psi}\left(\mathbf{z}_{s}\right) \psi\left(\mathbf{z}_{s}\right)^{\top}\right)^{-1}
$$

Then

$$
\langle\nabla \log p(\mathbf{x}, \mathbf{z})\rangle_{q} \approx A\langle\boldsymbol{\psi}(\mathbf{z})\rangle_{q} \approx A f(\mathbf{x}, \phi)
$$

Approach can be generalised to an infinite dimensional $\psi$ using the kernel trick.

## Generative models

In practice, much of the VAE and related work has used a common generative model:

$$
\begin{aligned}
& \mathbf{z} \sim \mathcal{N}(\mathbf{0}, I) \\
& \mathbf{x} \sim \mathcal{N}(\mathbf{g}(\mathbf{z} ; \boldsymbol{\theta}), \psi I)
\end{aligned}
$$

where $g$ is a neural network.

- Overcomplicated: if $\operatorname{dim}(\mathbf{z})$ is large enough the optimal solution has $\psi \rightarrow 0$, $q(\mathbf{z} ; \mathbf{x}) \rightarrow \delta(\mathbf{z}-f(\mathbf{x}, \phi))$. In effect, the generative model learns a flow to transform a normal density to the target.
- Oversimplified: if $\operatorname{dim}(\mathbf{z})$ is small, this is just non-linear PCA!

Interesting latent representations are likely to require more structured generative models. Recent work has approached such models in both VAE and DDC frameworks.

## Structured VAEs

Consider a model where $p(\mathcal{Z} \mid \theta)$ has tractable joint exponential-family potentials and

$$
p(\mathcal{X} \mid \mathcal{Z}, \Gamma)=\prod_{i} p\left(\mathbf{x}_{i} \mid \mathbf{z}_{i}, \gamma_{i}\right)
$$

are intractable (say neural net + normal) cond ind observations. $\gamma_{i}$ might be the same for all $i$.

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are intractable (say neural net + normal) cond ind observations. $\gamma_{i}$ might be the same for all $i$. Consider factored variational inference $q(\mathcal{Z})=\prod_{i} q_{i}\left(\mathbf{z}_{i}\right)$. With no further constraint,

$$
\begin{aligned}
\log q_{i}^{*}\left(\mathbf{z}_{i}\right) & = \\
= & \langle\log p(\mathcal{Z}, \mathcal{X})\rangle_{q_{\neg i}}=\left\langle\log p\left(\mathbf{z}_{i} \mid \mathcal{Z}_{\neg i}\right)+\log p\left(\mathbf{x}_{i} \mid \mathbf{z}_{i}\right)\right\rangle_{q_{\neg i}} \\
& =\left\langle\boldsymbol{\eta}_{\neg i}\right\rangle_{q_{\neg i}}^{\top} \psi_{i}\left(\mathbf{z}_{i}\right)+\log p\left(\mathbf{x}_{i} \mid \mathbf{z}_{i}\right)
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where we have exploited the exponential-family form of $p(\mathcal{Z}) . \boldsymbol{\psi}_{i}$ are effective suff stats including $\log$ normalisers of children in a DAG; $\boldsymbol{\eta}_{\neg i}$ is a function of $\mathcal{Z}_{\neg i}$.

## Structured VAEs

Consider a model where $p(\mathcal{Z} \mid \theta)$ has tractable joint exponential-family potentials and

$$
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where we have exploited the exponential-family form of $p(\mathcal{Z}) . \boldsymbol{\psi}_{i}$ are effective suff stats including log normalisers of children in a DAG; $\boldsymbol{\eta}_{\neg i}$ is a function of $\mathcal{Z}_{\neg i}$.
Now, choose the parametric form $q_{i}\left(\mathbf{z}_{i}\right)=e^{\tilde{\boldsymbol{\eta}}_{i}^{\top} \psi_{i}\left(\mathbf{z}_{i}\right)-\Phi_{i}\left(\tilde{\eta}_{i}\right)}$. Constrained optimum has form

$$
\log q_{i}^{*}\left(\mathbf{z}_{i}\right) \underset{+C}{=}\left\langle\boldsymbol{\eta}_{\neg i}\right\rangle_{q_{\neg i}}^{\top} \boldsymbol{\psi}_{i}\left(\mathbf{z}_{i}\right)+\boldsymbol{\rho}\left(\mathbf{x}_{i}\right)^{\top} \boldsymbol{\psi}_{i}\left(\mathbf{z}_{i}\right)
$$

for some $\mathbf{x}_{i}$-dependent natural parameter. Introduce recognition models:

$$
\rho\left(\mathbf{x}_{i}\right)=f_{i}\left(\mathbf{x}_{i}, \phi_{i}\right)
$$

Recognition function $f_{i}$ might be same for all $i$ if all likelihoods are the same (e.g. HMM).

## Structured VAE learning

Now, the free-energy can be written as a function of parameters and recognition parameters:

$$
\mathcal{F}\left(\theta, \Gamma,\left\{\phi_{i}\right\}\right)=\left\langle\sum_{i} \log p\left(\mathbf{x}_{i} \mid \mathbf{z}_{i}, \gamma_{i}\right)+\log p(\mathcal{Z} \mid \theta)\right\rangle_{q\left(\mathcal{Z} ; \theta,\left\{\phi_{i}\right\}\right)}+\sum_{i} \mathbf{H}\left[q_{i}\right]
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To update each $\phi_{i}$ and $\gamma_{i}$, find $\left\langle\boldsymbol{\eta}_{\neg i}\right\rangle_{q_{\neg i}}$ to give the "prior". Generate reparametrised samples $\mathbf{z}_{i}^{s} \sim q_{i}$. Then

$$
\begin{aligned}
\frac{\partial}{\partial \gamma_{i}} \mathcal{F}_{i} & =\sum_{s} \nabla_{\gamma_{i}} \log p\left(\mathbf{x}_{i}, \mathbf{z}_{i}^{s} ; \gamma_{i}\right) \\
\frac{\partial}{\partial \phi_{i}} \mathcal{F}_{i} & =\sum_{s} \frac{\partial}{\partial \mathbf{z}_{i}^{s}}\left(\log p\left(\mathbf{x}_{i}, \mathbf{z}_{i}^{s} ; \gamma_{i}\right)-\log q\left(\mathbf{z}_{i}^{s} ; \mathbf{f}\left(\mathbf{x}_{i}\right)\right)\right) \frac{d \mathbf{z}_{i}^{s}}{d \phi}+\frac{\partial}{\partial \mathbf{f}\left(\mathbf{x}_{i}\right)} \log q\left(\mathbf{z}_{i}^{s} ; \mathbf{f}\left(\mathbf{x}_{i}\right)\right) \frac{d \mathbf{f}\left(\mathbf{x}_{i}\right)}{d \phi}
\end{aligned}
$$

as for the standard VAE.

## DDC message passing

Consider simple chain inference:


$$
p\left(\mathbf{z}_{2} \mid \mathbf{x}\right)=\int d z_{1} p\left(\mathbf{z}_{2} \mid \mathbf{z}_{1}\right) p\left(\mathbf{z}_{1} \mid \mathbf{x}\right) .
$$

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- Connections $A_{i j}$ such that

$$
f_{i}\left(\mathbf{z}_{1}\right)=\int d \mathbf{z}_{2} \psi_{i}^{2}\left(\mathbf{z}_{2}\right) p\left(\mathbf{z}_{2} \mid \mathbf{z}_{1}\right) \approx \sum_{j} A_{j i} \psi_{j}^{1}\left(\mathbf{z}_{1}\right)
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$$
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$$

Convergent messages


$$
p\left(\mathbf{z}_{3} \mid \mathbf{x}\right)=\int d \mathbf{z}_{1} d \mathbf{z}_{2} p\left(\mathbf{z}_{3} \mid \mathbf{z}_{1}, \mathbf{z}_{2}\right) p\left(\mathbf{z}_{2} \mid \mathbf{x}_{2}\right) p\left(\mathbf{z}_{1} \mid \mathbf{x}_{1}\right)
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- Multilinear combination. Connections $A_{i j k}$ such that

$$
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$$

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$$
r_{k}^{3}=\sum_{j k} A_{j i k} r_{i}^{1} r_{j}^{2}=\left\langle\psi^{3}\left(\mathbf{z}_{3}\right)\right\rangle_{p\left(\mathbf{z}_{3} \mid \mathbf{x}_{1}, \mathbf{x}_{2}\right)}
$$

... just a brief survey of a subset of current ideas.

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- A theory of many approximations that helps ensure you understand their use and limitations (and may help derive new approaches).

