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 – most 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.
- Parametric variational methods might extend our reach.
  Define a parametric family of posterior approximations $q(\mathcal{Z}; \rho)$.
  The constrained (approximate) variational E-step becomes:

$$q(\mathcal{Z}) := \operatorname*{argmax}_{q \in \{q(\mathcal{Z};\rho)\}} \mathcal{F}\big(q(\mathcal{Z}), \theta^{(k-1)}\big) \quad \Rightarrow \quad \rho^{(k)} := \operatorname*{argmax}_{\rho} \mathcal{F}\big(q(\mathcal{Z};\rho), \theta^{(k-1)}\big)$$

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

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

  It might still be valuable to use coordinate ascent in ρ and θ, 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).

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  - Recognition network trained simultaneously with generative model using "frozen" samples (Kingma and Welling 2014; Rezende et al. 2014).

Score-based gradient estimate

We have:

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

Now,

$$
\nabla_\rho \log P(\mathcal{X}, \mathcal{Z}|\theta) = 0 \qquad \text{(no direct dependence)}
$$

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\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 \qquad \text{(always normalised)}
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\nabla_\rho q(\mathcal{Z}; \rho) = q(\mathcal{Z}; \rho)\nabla_\rho \log q(\mathcal{Z}; \rho)
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So,

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\nabla_\rho \mathcal{F}(\rho, \theta) = \Big\langle [\nabla_\rho \log q(\mathcal{Z}; \rho)](\log P(\mathcal{X}, \mathcal{Z}|\theta) - \log q(\mathcal{Z}; \rho)) \Big\rangle_{q(\mathcal{Z};\rho)}
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Score-based gradient estimate

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$$= \int d\mathcal{Z}\, [\nabla_\rho q(\mathcal{Z}; \rho)](\log P(\mathcal{X}, \mathcal{Z}|\theta) - \log q(\mathcal{Z}; \rho))$$

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$$\nabla_\rho q(\mathcal{Z}; \rho) = q(\mathcal{Z}; \rho)\nabla_\rho \log q(\mathcal{Z}; \rho)$$

So,

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

Reduced gradient of expectation to expectation of gradient – easier to compute.

Factorisation

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

- 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 $q(\mathcal{Z}) = \prod_i q(\mathcal{Z}_i|\rho_i)$ factor over disjoint cliques; let $\bar{\mathcal{Z}}_i$ be the minimal Markov blanket of $\mathcal{Z}_i$ in the joint; $P_{\bar{\mathcal{Z}}_i}$ be the product of joint factors that include any element of $\mathcal{Z}_i$ (so the union of their arguments is $\bar{\mathcal{Z}}_i$); and $P_{\neg\bar{\mathcal{Z}}_i}$ the remaining factors. Then,

$$\begin{aligned}
\nabla_{\rho_i} \mathcal{F}(\{\rho_j\}, \theta) &= \left\langle [\nabla_{\rho_i} \textstyle\sum_j \log q(\mathcal{Z}_j; \rho_j)](\log P(\mathcal{X}, \mathcal{Z}|\theta) - \textstyle\sum_j \log q(\mathcal{Z}_j; \rho_j)) \right\rangle_{q(\mathcal{Z})} \\
&= \left\langle [\nabla_{\rho_i} \log q(\mathcal{Z}_i; \rho_i)](\log P_{\bar{\mathcal{Z}}_i}(\mathcal{X}, \bar{\mathcal{Z}}_i) - \log q(\mathcal{Z}_i; \rho_i)) \right\rangle_{q(\bar{\mathcal{Z}}_i)} \\
&\quad + \left\langle [\nabla_{\rho_i} \log q(\mathcal{Z}_i; \rho_i)] \underbrace{\left(\log P_{\neg\bar{\mathcal{Z}}_i}(\mathcal{X}, \mathcal{Z}_{\neg i}) - \sum_{j \neq i} \log q(\mathcal{Z}_j; \rho_j)\right)}_{\text{constant wrt } \mathcal{Z}_i} \right\rangle_{q(\mathcal{Z})}
\end{aligned}$$

So the second term is proportional to $\langle \nabla_{\rho_i} \log q(\mathcal{Z}_i; \rho_i) \rangle_{q(\mathcal{Z}_i)}$, which $= 0$ as before. So expectations are only needed wrt $q(\bar{\mathcal{Z}}_i)$ $\rightarrow$ Message passing!

Sampling

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

- Choose a parametric (factored) variational family $q(\mathcal{Z}) = \prod_i q(\mathcal{Z}_i; \rho_i)$.
- Initialise factors.
- Repeat to convergence:
  - **Stochastic VE-step**. For each i:
    - Sample from $q(\bar{\mathcal{Z}}_i)$ and estimate expected gradient $\nabla_{\rho_i}\mathcal{F}$.
    - Update ρ_i along gradient.
  - **Stochastic M-step**. For each i:
    - Sample from each $q(\bar{\mathcal{Z}}_i)$.
    - 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.

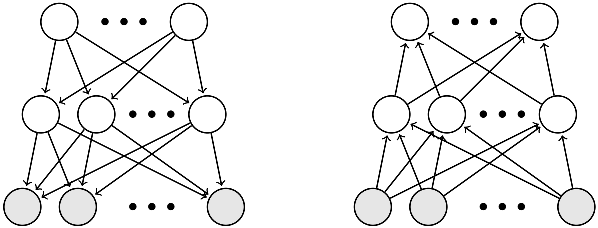
Suppose that we have fixed length vectors $\{(\mathbf{x}_i, \mathbf{z}_i)\}$ ($\mathbf{z}$ is still latent).

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

$$q(\mathbf{z}_i) = \text{Bernoulli}[\hat{\mathbf{z}}_i] \qquad \hat{\mathbf{z}}_i = f(\mathbf{x}_i; \phi)$$

  Update generative parameters θ according to $\nabla_\theta \mathcal{F}(\{\hat{\mathbf{z}}_i\}, \theta)$.

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

$$\Delta\phi \propto \sum_s (\mathbf{z}_s - f(\mathbf{x}_s; \phi)) \nabla_\phi f(\mathbf{x}_s; \phi)$$

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 $q(\mathbf{z})$:

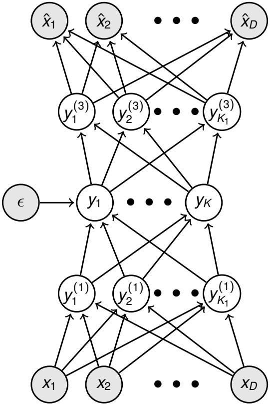
$$q(\mathbf{z}; \boldsymbol{\rho}) \propto e^{\eta(\boldsymbol{\rho})^{\mathsf{T}} \mathbf{s}_q(\mathbf{z})} \qquad \boldsymbol{\rho} = \langle \mathbf{z} \rangle_q = f(\mathbf{x}; \phi)$$

$$\Delta\phi \propto \sum_s (\mathbf{s}_q(\mathbf{z}_s) - f(\mathbf{x}_s; \phi)) \nabla_\phi f(\mathbf{x}_s; \phi)$$

  Current work uses flexible (but non-normalisable) exponential families (the "DDC-Helmholtz machine")

- Sleep phase learning minimises $\mathbf{KL}[p_\theta(\mathbf{z}|\mathbf{x}) \| q(\mathbf{z}; f(\mathbf{x}, \phi))]$. 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 μ_i and σ_i for latents y_i and $\epsilon_i^s \sim \mathcal{N}(0,1)$, then $y_i^s = \mu_i + \sigma_i \epsilon_i^s$.
- Now generative and recognition parameters can be trained together by gradient descent (backprop), holding $\boldsymbol{\epsilon}^s$ fixed.

$$\mathcal{F}_i(\theta,\phi) = \sum_s \log P(\mathbf{x}_i, \mathbf{z}_i^s; \theta) - \log q(\mathbf{z}_i^s; \mathbf{f}(\mathbf{x}_i, \phi))$$

$$\frac{\partial}{\partial \theta}\mathcal{F}_i = \sum_s \nabla_\theta \log P(\mathbf{x}_i, \mathbf{z}_i^s; \theta)$$

$$\frac{\partial}{\partial \phi}\mathcal{F}_i = \sum_s \frac{\partial}{\partial \mathbf{z}_i^s}(\log P(\mathbf{x}_i, \mathbf{z}_i^s; \theta) - \log q(\mathbf{z}_i^s; \mathbf{f}(\mathbf{x}_i))) \frac{d\mathbf{z}_i^s}{d\phi}$$

$$+ \frac{\partial}{\partial \mathbf{f}(\mathbf{x}_i)} \log q(\mathbf{z}_i^s; \mathbf{f}(\mathbf{x}_i)) \frac{d\mathbf{f}(\mathbf{x}_i)}{d\phi}$$

Variational Autoencoders

- Frozen samples ϵ^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 $P(\mathbf{x}|\mathbf{z}, \theta)$ 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

- Dynamical VAE (to train RNNs) – “draw” network.
- Train proposal networks for particle filtering.
- Importance weighted VAE.
- DDC Helmholt machines – arbitrary (non-normalisable) ExpFam posteriors.
- ...