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:

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

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

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

It might still be valuable to use coordinate ascent in ρ and θ , although this is no longer necessary.

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

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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:

$$egin{aligned}
abla_
ho \mathcal{F}(
ho, heta) &=
abla_
ho \int d\mathcal{Z} \, q(\mathcal{Z};
ho)(\log P(\mathcal{X},\mathcal{Z}| heta) - \log q(\mathcal{Z};
ho)) \ &= \int d\mathcal{Z} \, [
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Score-based gradient estimate

We have:

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

Now,

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

$$\int d\mathcal{Z} q(\mathcal{Z}; \rho) \nabla_{\rho} \log q(\mathcal{Z}; \rho) = \nabla_{\rho} \int d\mathcal{Z} q(\mathcal{Z}; \rho) = 0 \qquad (\text{always normalised})$$

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

So,

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

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So,

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

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

Factorisation

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

- 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 $\overline{\mathcal{Z}}_i$ 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,

$$\nabla_{\rho_{i}} \mathcal{F}(\{\rho_{j}\}, \theta) = \left\langle [\nabla_{\rho_{i}} \sum_{j} \log q(\mathcal{Z}_{j}; \rho_{j})] (\log P(\mathcal{X}, \mathcal{Z}|\theta) - \sum_{j} \log q(\mathcal{Z}_{j}; \rho_{j})) \right\rangle_{q(\mathcal{Z})}$$
$$= \left\langle [\nabla_{\rho_{i}} \log q(\mathcal{Z}_{i}; \rho_{i})] (\log P_{\bar{\mathcal{Z}}_{i}}(\mathcal{X}, \bar{\mathcal{Z}}_{i}) - \log q(\mathcal{Z}_{i}; \rho_{i})) \right\rangle_{q(\bar{\mathcal{Z}}_{i})}$$
$$+ \left\langle [\nabla_{\rho_{i}} \log q(\mathcal{Z}_{i}; \rho_{i})] (\log P_{\neg \bar{\mathcal{Z}}_{i}}(\mathcal{X}, \mathcal{Z}_{\neg i}) - \sum_{j \neq i} \log q(\mathcal{Z}_{j}; \rho_{j})) \right\rangle_{q(\mathcal{Z})}$$

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

Sampling

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

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

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

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

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

Sleep phase: sample {z_s, x_s}^S_{s=1} from current generative model. Update recognition parameters φ to direct f(x_s) towards z_s (simple gradient learning).

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

The Helmholtz Machine

- Can sample 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(z) (later).
- Sleep phase learning minimises KL[ρ_θ(z|x)||q(z; f(x, φ))]. 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 **f** gives marginal μ_i and σ_i for latents z_i and $\epsilon_i^s \sim \mathcal{N}(0, 1)$, 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 ε^s fixed.

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

Variational Autoencoders

- Frozen samples ϵ^s can be redrawn to avoid overfitting.
- May be possible to evaluate entropy and log P(z) without sampling, reducing variance.
- Differentiable reparametrisations are available for a number of different distributions.
- Conditional P(x|z, θ) 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
 - Iocal 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:

$$\mathcal{F}(q,\theta) = \left\langle \log \frac{p(\mathbf{x},\mathbf{z})}{q(\mathbf{z})} \right\rangle_{q} = \mathbb{E}_{\mathbf{z} \sim q} \left[\log p(\mathbf{x}) \frac{p(\mathbf{z}|\mathbf{x})}{q(\mathbf{z})} \right]$$

$$\uparrow$$
importance weight

Jensen bound on importance sampled estimate:

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

Suggests more accurate importance sampling:

$$\ell(\theta) = \log \mathbb{E}_{\mathbf{z}_1 \dots \mathbf{z}_K \stackrel{\text{iid}}{\sim} q} \left[\frac{1}{K} \sum_k \frac{p(\mathbf{x}, \mathbf{z}_k)}{q(\mathbf{z}_k)} \right] \geq \mathbb{E}_{\mathbf{z}_1 \dots \mathbf{z}_K \stackrel{\text{iid}}{\sim} q} \left[\log \frac{1}{K} \sum_k \frac{p(\mathbf{x}, \mathbf{z}_k)}{q(\mathbf{z}_k)} \right]$$

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

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

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:

 $\begin{aligned} \mathbf{z}_0 &\sim q_0(\cdot; \mathbf{x}) & \leftarrow \text{ fixed, tractable, e.g. } \mathcal{N}(\mathbf{x}, I) \\ \mathbf{z} &= f_K(f_{K-1}(\dots f_1(\mathbf{z}_0))) & \leftarrow f_k \text{ smooth, invertible, parametrised by } \phi \end{aligned}$

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Then

$$\langle F(\mathbf{z}) \rangle_q = \langle F(f_{\mathcal{K}}(f_{\mathcal{K}-1}(\dots f_1(\mathbf{z}_0)))) \rangle_{q_0} \log q(\mathbf{z}) = \log q_0(f_1^{-1}(f_2^{-1}(\dots f_k^{-1}(\mathbf{z})))) - \sum_k \log |\nabla f_k|$$

where the second result applies from repeated transformations of variables

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

So, given a sample $\mathbf{z}_0^s \overset{\text{iid}}{\sim} q_0(\cdot; \mathbf{x})$:

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

and we can compute gradients of this expression wrt θ and ϕ .

Useful fs (from Rezende & Mohammed 2015):

$$f(\mathbf{z}) = \mathbf{z} + \mathbf{u}h(\mathbf{w}^{\mathsf{T}}\mathbf{z} + b) \qquad \Rightarrow |\nabla f| = \left|1 + \mathbf{u}^{\mathsf{T}}\psi(\mathbf{z})\right| \qquad \psi(\mathbf{z}) = h'(\mathbf{w}^{\mathsf{T}}\mathbf{z} + b)\mathbf{w}$$
$$f(\mathbf{z}) = \mathbf{z} + \frac{\beta}{\alpha + |\mathbf{z} - \mathbf{z}_0|} \qquad \Rightarrow |\nabla f| = [1 + \beta h]^{d-1}[1 + \beta h + \beta h' r]$$
$$r = |\mathbf{z} - \mathbf{z}_0|, h = \frac{1}{\alpha + r}$$

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 $\mu=\langle \phi({\sf z})
angle$: Distributed distributional code (DDC).

Train recognition model using sleep samples:

$$\mu = \langle \boldsymbol{\psi}(\mathbf{z}) \rangle_q = f(\mathbf{x}; \phi)$$
$$\Delta \phi \propto \sum_s (\boldsymbol{\psi}(\mathbf{z}_s) - f(\mathbf{x}_s; \phi)) \nabla_{\phi} f(\mathbf{x}_s; \phi)$$

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

$$\boldsymbol{A} = \Big(\sum_{s} \nabla \log p(\mathbf{x}_{s}, \mathbf{z}_{s} | \theta) \psi(\mathbf{z}_{s})\Big)^{\mathsf{T}} \Big(\sum_{s} \psi(\mathbf{z}_{s}) \psi(\mathbf{z}_{s})^{\mathsf{T}}\Big)^{-1}$$

Then

$$\left\langle
abla \log
ho(\mathbf{x}, \mathbf{z})
ight
angle_q pprox A \left\langle \psi(\mathbf{z})
ight
angle_q pprox A f(\mathbf{x}, \phi)$$

Approach can be generalised to an infinite dimensional ψ using the kernel trick.

Generative models

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

 $egin{aligned} \mathbf{z} &\sim \mathcal{N}\left(\mathbf{0}, \textit{l}
ight) \ \mathbf{x} &\sim \mathcal{N}\left(\mathbf{g}(\mathbf{z}; oldsymbol{ heta}), \psi \textit{l}
ight) \end{aligned}$

where g is a neural network.

- Overcomplicated: if dim(z) is large enough the optimal solution has ψ → 0, q(z; x) → δ(z − f(x, φ)). In effect, the generative model learns a flow to transform a normal density to the target.
- Oversimplified: if dim(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 $p(\mathcal{Z}|\theta)$ has tractable joint exponential-family potentials and

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

are intractable (say neural net + normal) cond ind observations. γ_i might be the same for all *i*.

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$$\begin{split} \log q_i^*(\mathbf{z}_i) &= \langle \log p(\mathcal{Z}, \mathcal{X}) \rangle_{q_{\neg i}} = \langle \log p(\mathbf{z}_i | \mathcal{Z}_{\neg i}) + \log p(\mathbf{x}_i | \mathbf{z}_i) \rangle_{q_{\neg i}} \\ &= \langle \boldsymbol{\eta}_{\neg i} \rangle_{q_{\neg i}}^{\mathsf{T}} \psi_i(\mathbf{z}_i) + \log p(\mathbf{x}_i | \mathbf{z}_i) \end{split}$$

where we have exploited the exponential-family form of $p(\mathcal{Z})$. ψ_i are effective suff stats – including log normalisers of children in a DAG; $\eta_{\neg i}$ is a function of $\mathcal{Z}_{\neg i}$.

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Now, choose the parametric form $q_i(\mathbf{z}_i) = e^{\tilde{\eta}_i^{\mathsf{T}} \psi_i(\mathbf{z}_i) - \Phi_i(\tilde{\eta}_i)}$. Constrained optimum has form

$$\log q_i^*(\mathbf{z}_i) \underset{+C}{=} \langle \boldsymbol{\eta}_{\neg i} \rangle_{q_{\neg i}}^{\mathsf{T}} \psi_i(\mathbf{z}_i) + \rho(\mathbf{x}_i)^{\mathsf{T}} \psi_i(\mathbf{z}_i)$$

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

$$\boldsymbol{\rho}(\mathbf{x}_i) = f_i(\mathbf{x}_i, \phi_i)$$

Recognition function f_i might be same for all *i* if all likelihoods are the same (*e.g.* HMM).

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

$$\mathcal{F}(\theta, \mathsf{\Gamma}, \{\phi_i\}) = \left\langle \sum_i \log p(\mathbf{x}_i | \mathbf{z}_i, \gamma_i) + \log p(\mathcal{Z} | \theta) \right\rangle_{q(\mathcal{Z}; \theta, \{\phi_i\})} + \sum_i \mathsf{H}[q_i]$$

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To update each ϕ_i and γ_i , find $\langle \eta_{\neg i} \rangle_{q_{\neg i}}$ to give the "prior". Generate reparametrised samples $\mathbf{z}_i^s \sim q_i$. Then

$$\begin{split} &\frac{\partial}{\partial \gamma_i} \mathcal{F}_i = \sum_{s} \nabla_{\gamma_i} \log p(\mathbf{x}_i, \mathbf{z}_i^s; \gamma_i) \\ &\frac{\partial}{\partial \phi_i} \mathcal{F}_i = \sum_{s} \frac{\partial}{\partial \mathbf{z}_i^s} (\log p(\mathbf{x}_i, \mathbf{z}_i^s; \gamma_i) - \log q(\mathbf{z}_i^s; \mathbf{f}(\mathbf{x}_i))) \frac{d\mathbf{z}_i^s}{d\phi} + \frac{\partial}{\partial \mathbf{f}(\mathbf{x}_i)} \log q(\mathbf{z}_i^s; \mathbf{f}(\mathbf{x}_i)) \frac{d\mathbf{f}(\mathbf{x}_i)}{d\phi} \end{split}$$

as for the standard VAE.

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Convergent messages



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Then

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... 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).