Overview

- Some statistics stuff
- Latent variable models, EM, VAE
- Rate vs Distortion
- Improving VAEs
  - Reparameterization
  - A better prior
  - A better encoder through auxiliary variables
  - A better encoder through normalizing flows
  - A better objective (?): Wasserstein VAE
- Variational Bayes
- Local Reparameterization
- Conclusions

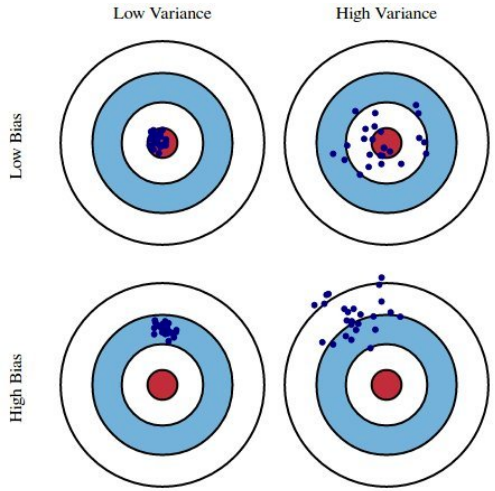
ML as Statistics

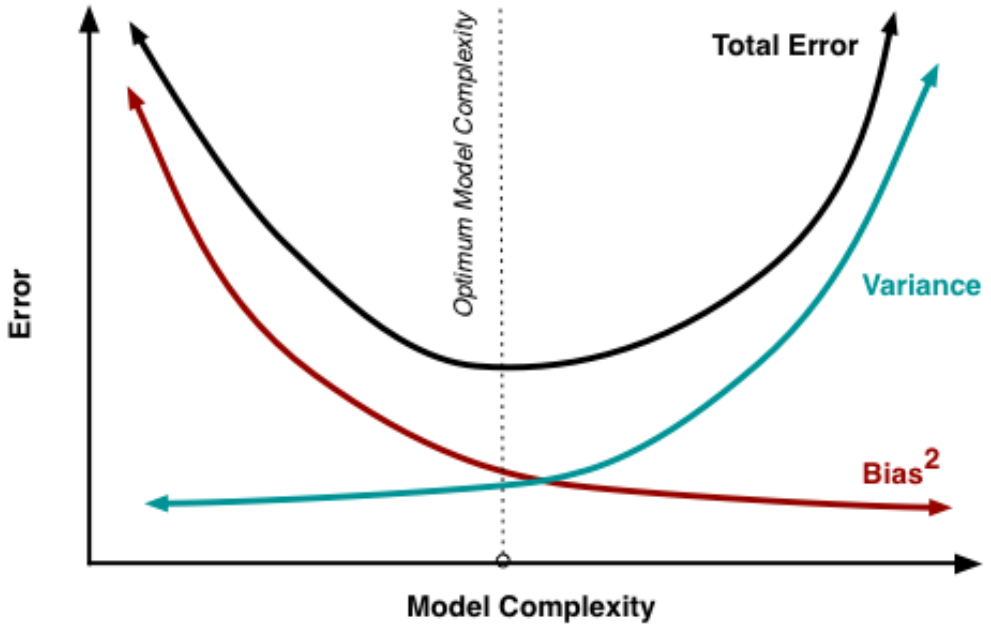
- Data: $\{X_1, ..X_n, Y_1, .., Y_n\} \sim P(X_1, ..X_n, Y_1, .., Y_n)$ (X input, Y label)
- Optimize objective:
  - maximize log likelihood: $\max_{\Theta} \log P(X_1, ...X_n|\Theta)$ (unsupervised)

    $\max_{\Theta} \log P(Y_1, ..Y_n|X_1, ...X_n, \Theta)$ (supervised)
  - minimize loss: $\min_{\Theta} \sum_i Loss(Y_i, \hat{Y}(X_i, \Theta))$ (supervised)

- *ML is more than an optimization problem: it's a statistical inference problem*.
  - E.g.: you should not optimize parameters more precisely than the scale at which the MLE fluctuates under resampling the data: $\Theta_{mle}(X, Y) \approx \Theta'_{mle}(X', Y')$, or risk overfitting.

Bias Variance Tradeoff





$$Y = f(X) + \epsilon \qquad \epsilon \sim \mathcal{N}(0, \sigma_\epsilon).$$

$$Err(x) = E\left[(Y - \hat{f}(x))^2\right]$$

$$Err(x) = \left(E[\hat{f}(x)] - f(x)\right)^2 + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] + \sigma_e^2$$

$$Err(x) = \text{Bias}^2 + \text{Variance} + \text{Irreducible Error}$$

http://scott.fortmann-roe.com/docs/BiasVariance.html

Bayesian Inference

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(model evidence)

$$P(\Theta|X,M) = \frac{P(X|\Theta,M)P(\Theta|M)}{P(X|M)}$$

(posterior)

$$P(x|X,M) = \int d\Theta\ P(x|\Theta,M)P(\Theta|X,M)$$

(prediction)

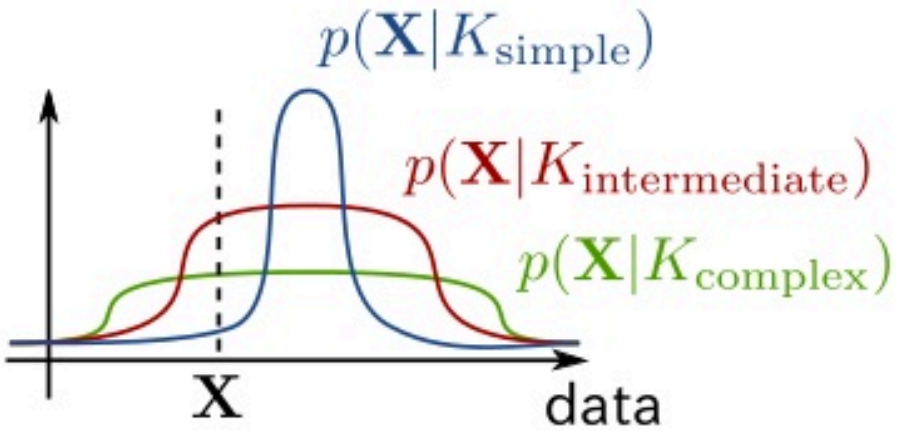
$$P(X) = \sum_M P(X|M)P(M)$$

(evidence)

$$P(M|X) = \frac{P(X|M)P(M)}{P(X)}$$

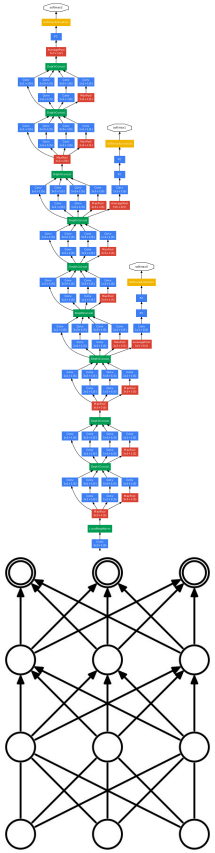
(model selection)

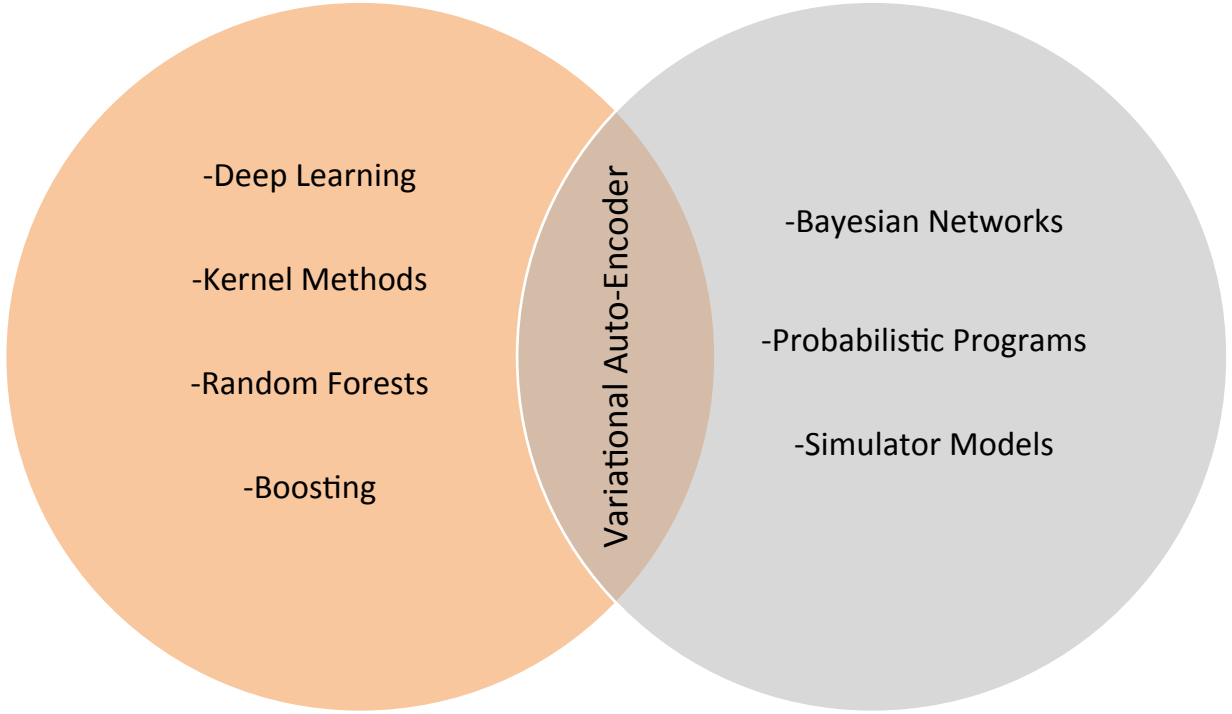
Complex models can have lower marginal likelihood:

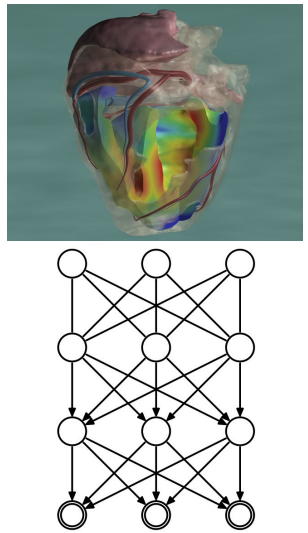


Picture credit: Kohei Hayashi[1,2] Shin-ichi Maeda[3] Ryohei Fujimaki[4]

Discriminative or Generative?





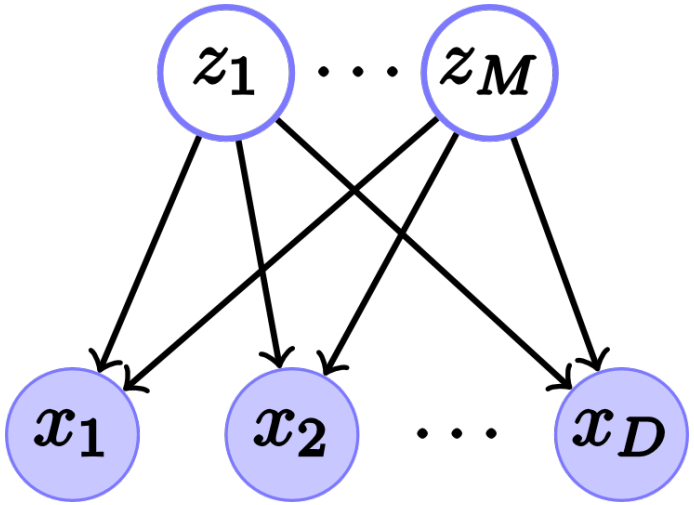


- Advantages discriminative models:
  - Flexible map from input to target (low bias)
  - Efficient training algorithms available
  - Solve the problem you are evaluating on.
  - Very successful and accurate!

- Advantages generative models:
  - Inject expert knowledge
  - Model causal relations, model physics
  - Interpretable
  - Data efficient
  - More robust to domain shift
  - Facilitate un/semi-supervised learning

Latent Variable Models

- Introducing latent (unobserved) variables will dramatically increase the capacity of a model.



$$P(X) = \sum_Z P(X|Z)P(Z)$$

- Problem: P(Z|X) is intractable for most nontrivial models

Learning: Variational Expectation Maximization

$$KL[Q(Z|X)||P(Z||X)]$$

$$\log P(X|\Theta) =$$

$$\log \sum_Z P(X|Z,\Theta)P(Z) \geq$$

$$\sum_Z Q(Z|X,\Phi)\left(\log P(X|Z,\Theta)P(Z) - \log Q(Z|X,\Phi)\right)$$

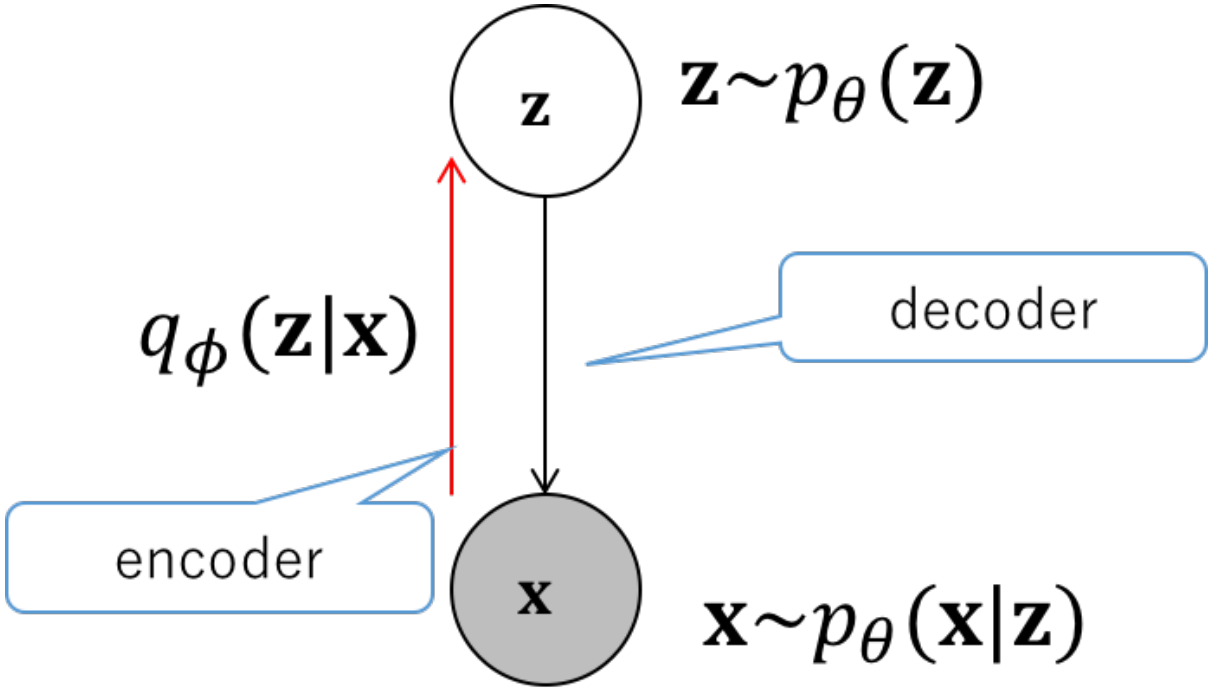
Gap:

Bound $B(\Theta,\Phi)$

E-step: $\arg\max_{\Phi} B(\Theta,\Phi)$ (variational inference)

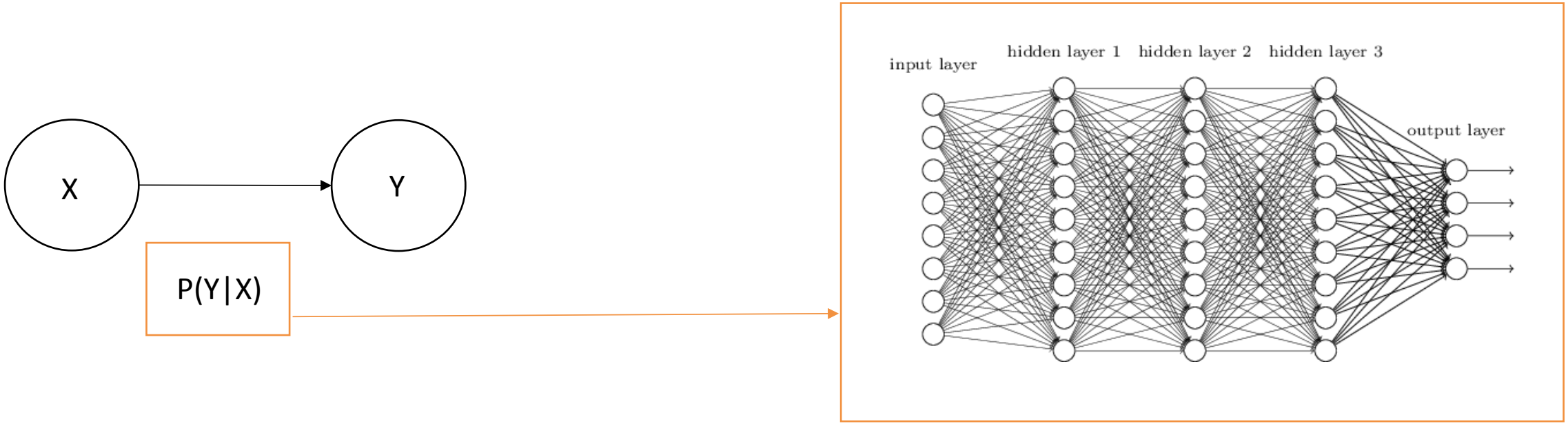
M-step: $\arg\max_{\Theta} B(\Theta,\Phi)$ (approximate learning)

Amortized Inference

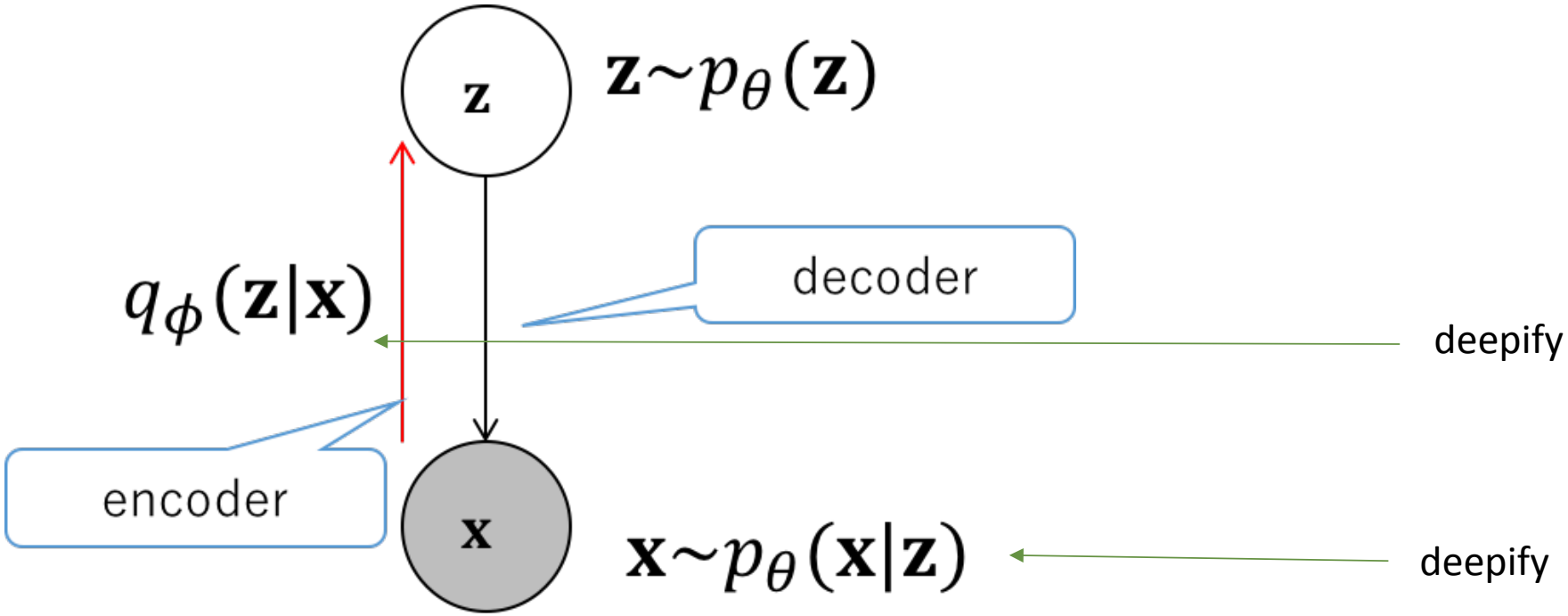


- Bij making q(z|x) a function of x and sharing parameters ϕ , we can do very fast inference at test time (i.e. avoid iterative optimization of $q_{test}(z)$)

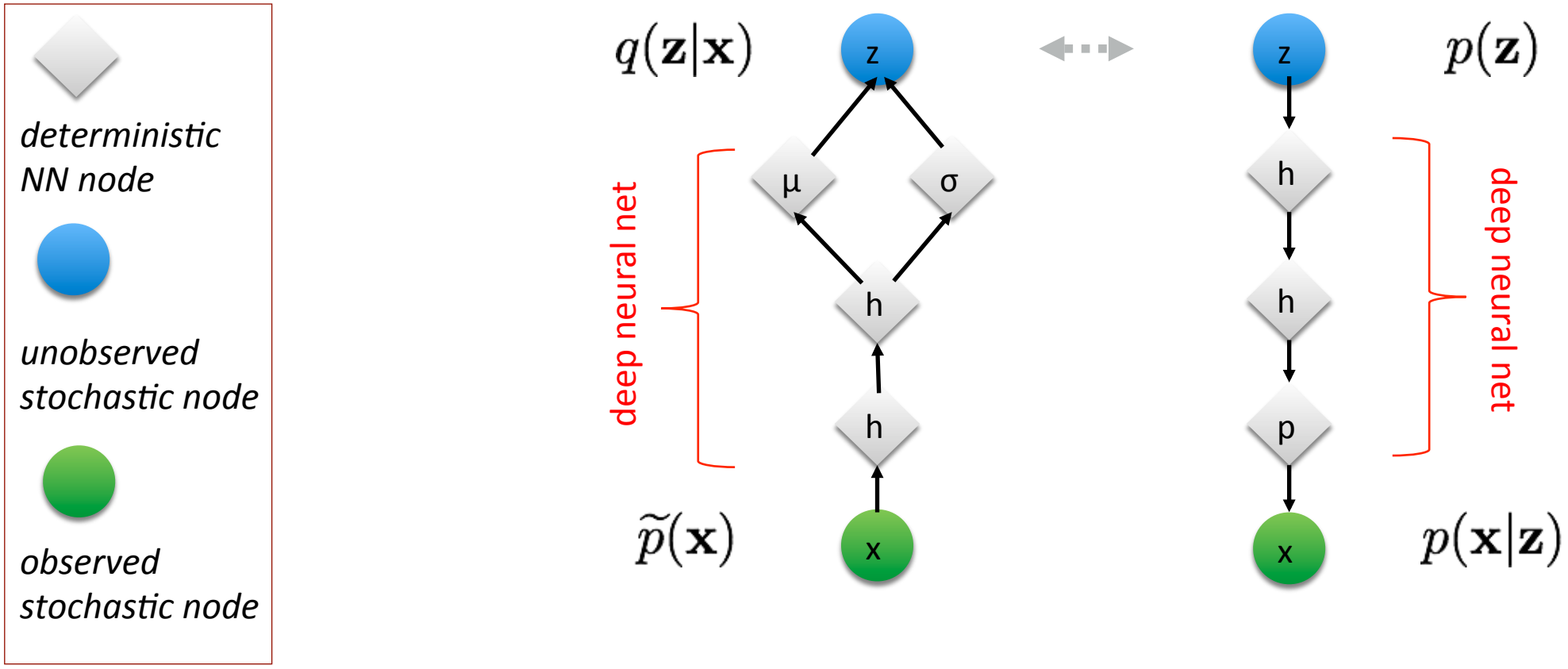
Deep NN as a glorified conditional distribution



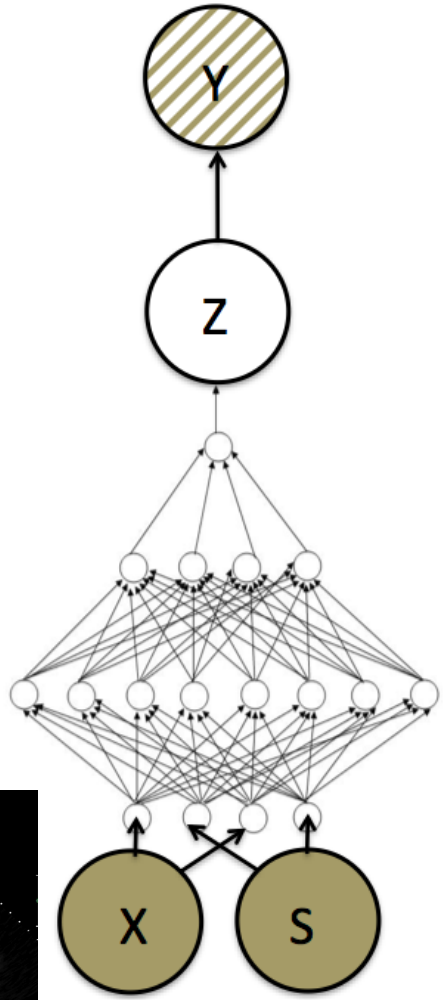
Variational Autoencoder



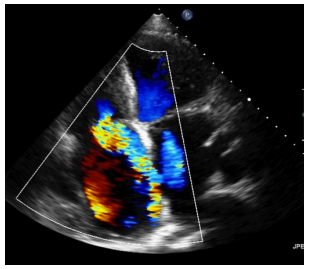
Deep Generative Model: The Variational Auto-Encoder



Combining Generative and Discriminative Models

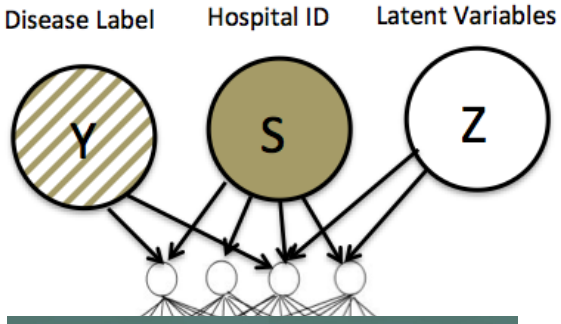


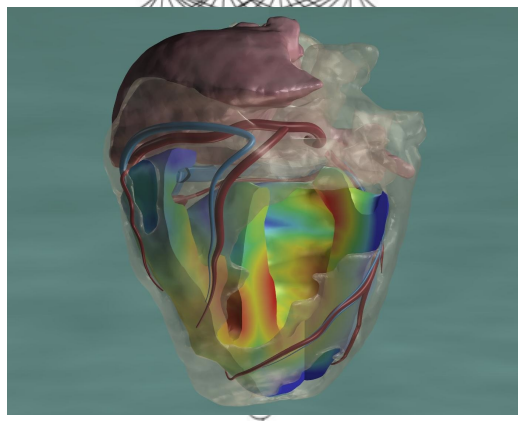
Black box DNN/CNN

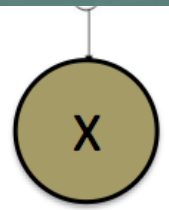


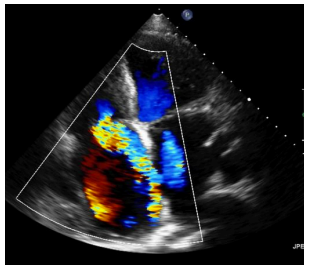
recognition model

generative model









Use physics

Use causality

Use expert knowledge

Stochastic Variational Bayesian Inference

$$B(Q) = \sum_Z Q(Z|X,\Phi)(\log P(X|Z,\Theta) + \log P(Z) - \log Q(Z|X,\Phi))$$

$$\nabla_\Phi B(Q) = \sum_Z Q(Z|X,\Phi)\nabla_\Phi \log Q(Z|X,\Phi)(\log P(X|Z,\Theta) + \log P(Z) - \log Q(Z|X,\Phi))$$

Sample Z

subsample mini-batch X

$$\nabla_\Phi B(Q) = \frac{1}{N}\frac{1}{S}\sum_{i=1}^{N}\sum_{s=1}^{S} \nabla_\Phi \log Q(Z_{is}|X_i,\Phi)(\log P(X_i|Z_{is},\Theta) + \log P(Z_{is}) - \log Q(Z_{is}|X_i,\Phi))$$

very high variance

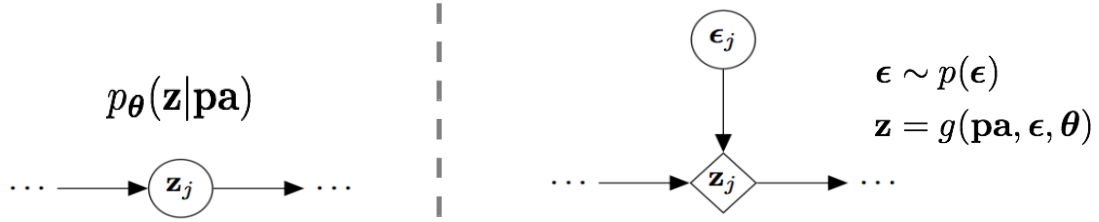
Improving VAEs

- Reducing Variance during learning: e.g. reparameterization, REBAR/RELAX…
- Rate / Distortion tradeoff: e.g. free bits, annealing KL
- More complex models
  - Prior P(z): e.g. VampPrior
  - Decoder P(x|z), e.g. PixelCNN
  - Encoder: e.g. normalizing flows, auxiliary variables

Reducing the Variance: The Reparametrization Trick

Kingma 2013, Bengio 2013, Kingma & Welling 2014

- Reparameterization:



- Applied to VAE:

$$\nabla_\Phi B(\Theta, \Phi) = \nabla_\Phi \int dz\ Q_\Phi(z|x)[\log P_\Theta(x, z) - \log Q_\Phi(z|x)]$$

$$\approx \nabla_\Phi [\log P_\Theta(x, z_s) - \log Q_\Phi(z_s|x)]_{z_s = g(\epsilon_s, \Phi)}, \qquad \epsilon_s \sim P(\epsilon)$$

- Example:

$$\nabla_\mu \int dz \mathcal{N}_z(\mu, \sigma) z$$

$$= \frac{1}{S} \sum_s z_s (z_s - \mu)/\sigma^2, \quad z_s \sim \mathcal{N}_z(\mu, \sigma)$$

$$\text{or } \frac{1}{S} \sum_s 1, \quad \epsilon_s \sim \mathcal{N}_\epsilon(0, 1), \quad z = \mu + \sigma\epsilon$$

Rate vs Distortion

Fixing a Broken ELBO

Alexander A. Alemi [1] Ben Poole [2*] Ian Fischer [1] Joshua V. Dillon [1] Rif A. Saurous [1] Kevin Murphy [1]

- The ELBO objective does not care explicitly about learning good representations Z
- Proposal: look at both distortion and rate.

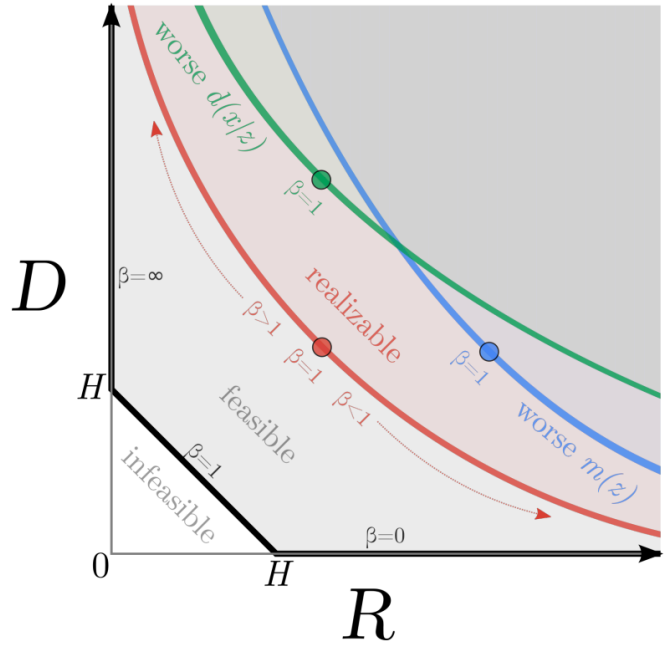
$$\min_{e(z|x),m(z),d(x|z)} D + \beta R.$$

$$\min_{e(z|x),m(z),d(x|z)} \int dx\, p^*(x) \int dz\, e(z|x) \left[-\log d(x|z) + \beta \log \frac{e(z|x)}{m(z)} \right].$$

$$H \equiv -\int dx\, p^*(x) \log p^*(x)$$

$$D \equiv -\int dx\, p^*(x) \int dz\, e(z|x) \log d(x|z)$$

$$R \equiv \int dx\, p^*(x) \int dz\, e(z|x) \log \frac{e(z|x)}{m(z)}$$



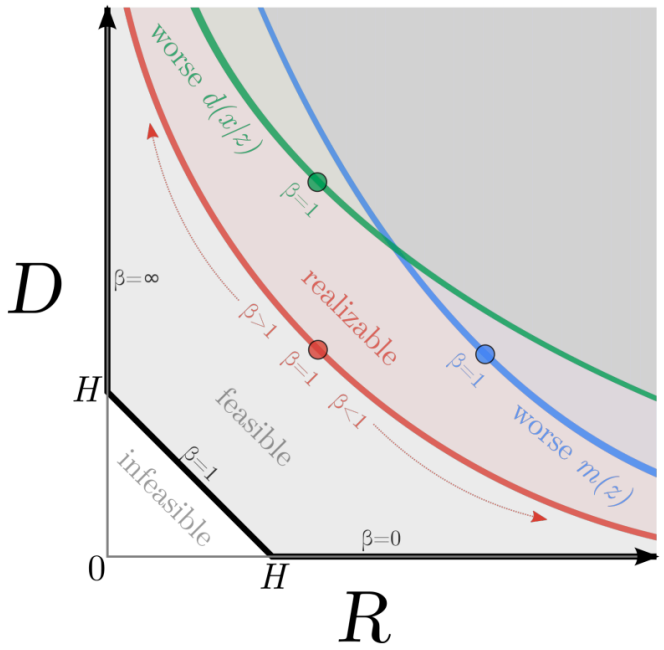
$$H - D \leq \mathrm{I}_e(X;Z) \leq R$$

$$\mathrm{I}_e(X;Z) = \iint dx\, dz\, p_e(x,z) \log \frac{p_e(x,z)}{p^*(x) p_e(z)}.$$

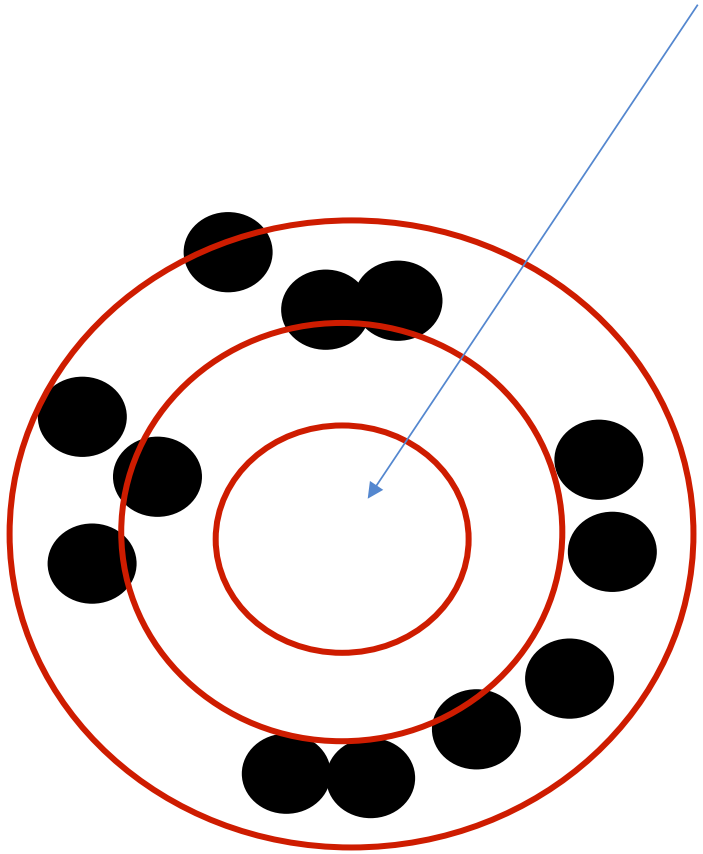
$$p_e(x,z) = e(z|x)p^*(x)\ ;\ \ p_e(z) = \int dx\, p^*(x) e(z|x)$$

Rate vs Distortion Conclusions

- ELBO is too one dimensional, it does not care about representations.
- We can improve R-D by changing encoder, decoder, or prior.



Improving the Prior



“hole”

Model was not trained to generate from the hole.

Improving the Prior (Tomczak & W, 2018)

- We can simply solve for the best prior p(.):

$$p^*(z) = \arg\max_{p(\cdot)} \sum_n \int dz_n q(z_n|x_n) \left[\log p(x_n|z_n) + \log p(z_n) - \log q(z_n|x_n)\right]$$

$$= \frac{1}{N}\sum_{n=1}^{N} q(z|x_n)$$ "Variational Mixture of Posteriors Prior" or VampPrior

- Too expensive because it scales with N. Approximate using K pseudo data points {u_k}:

$$p^*(z) \approx \frac{1}{K}\sum_{k=1}^{K} q(z|u_k) \quad \text{or} \quad p^*(z) \approx \frac{1}{K}\sum_{k=1}^{K} w_k q(z|u_k); \quad \sum_k w_k = 1$$ (Alemi et al 2018)

- Learn the {w_k, u_k} alongside the parameters of the posterior q(z|u)

Improving the Encoder: Auxiliary Variables

(Salimans & Knowles, 2013

- Introduce new latent variables y and distributions:

$$p(x,z) \rightarrow p(x,z)r(y|x,z)$$
$$q(z|x) \rightarrow q(z,y|x)$$

- The variational posterior is now a mixture distribution: Note that q(z|x) can now be very complicated and intractable.

$$q(z|x) = \int dy\ q(z,y|x)$$

- New, but looser bound, on joint space : Note that this bound can still be better than the usual ELBO with a simpler q(z|x).

$$\begin{aligned}
&\mathcal{L}_{\text{aux}} \qquad (3)\\
&= \mathbb{E}_{q(y,z_T|x)}[\log[p(x,z_T)r(y|x,z_T)] - \log q(y,z_T|x)]\\
&= \mathcal{L} - \mathbb{E}_{q(z_T|x)}\{D_{KL}[q(y|z_T,x)||r(y|z_T,x)]\}\\
&\leq \mathcal{L} \ \leq \ \log[p(x)],
\end{aligned}$$

- (Homework: derive (3) by first proving the following general triangle inequality for KL-divergences:

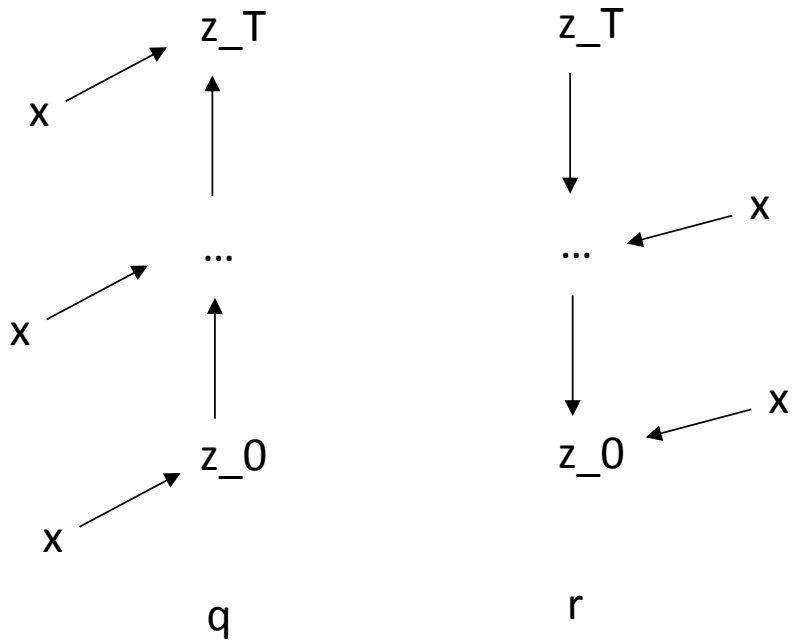
$$KL[q(x,z)||p(x,z)] = KL[q(x)||p(x)] + E_{q(x)}\left[KL[q(z|x)||p(z|x)]\right]\ )$$

Auxiliary Variables

Salimans et al 2015

Choose Markov Chains:

$$r(y|z,x) = r(z_{T-1}|x,z_T)r(z_{T-2}|z_{T-1},x)...r(z_0|z_1,x)$$
$$q(z,y|x) = q(z_0|x)q(z_1|z_0,x)...q(z_T|z_{T-1},x)$$



$$\begin{aligned}\log p(x) &\geq \mathbb{E}_q[\log p(x,z_T) - \log q(z_0,\ldots,z_T|x) \\ &\quad + \log r(z_0,\ldots,z_{t-1}|x,z_T)] \\ &= \mathbb{E}_q\big[\log[p(x,z_T)/q(z_0|x)] \\ &\quad + \sum_{t=1}^{T} \log[r_t(z_{t-1}|x,z_t)/q_t(z_t|x,z_{t-1})]\big].\end{aligned}$$

Algorithm to compute bound:

Draw an initial random variable $z_0 \sim q(z_0|x)$
Initialize the lower bound estimate as
$L = \log p(x,z_0) - \log q(z_0|x)$
for $t = 1:T$ **do**
  Perform random transition $z_t \sim q_t(z_t|x,z_{t-1})$
  Calculate the ratio $\alpha_t = \frac{p(x,z_t)r_t(z_{t-1}|x,z_t)}{p(x,z_{t-1})q_t(z_t|x,z_{t-1})}$
  Update the lower bound $L = L + \log[\alpha_t]$
end for

Improving the Encoder: Normalizing Flows (I)

- The usual VAE predicts mean and log-variance functions $\mu(x), \log \sigma(x)$, and then samples $z_n \sim N(z; \mu(x_n), \sigma(x_n))$ This is unimodal and this quite limited.
- How can we produce more complicated distributions?
- Consider an invertible transformation f(z): $\mathbf{z}' = f(\mathbf{z}),\ \mathbf{z}, \mathbf{z}' \in \mathbb{R}^D \text{ and } f : \mathbb{R}^D \mapsto \mathbb{R}^D$
- The density then transforms as: $p_1(\mathbf{z}') = p_0(\mathbf{z}) \left| \det \left(\frac{\partial f(\mathbf{z})}{\partial \mathbf{z}} \right) \right|^{-1}$
- Let's take a simple distribution q0 for z0 and then transform K times z0→z1→z2→…→zK.
- The final log distribution is now given as:

$$\log q_K(\mathbf{z}_K|\mathbf{x}) = \log q_0(\mathbf{z}_0|\mathbf{x}) - \sum_{k=1}^{K} \log \left| \det \left(\frac{\partial f_k(\mathbf{z}_{k-1}; \lambda_k(\mathbf{x}))}{\partial \mathbf{z}_{k-1}} \right) \right|$$

Improving the Encoder: Normalizing Flows (II)

- Final variational objective is now:

$$\begin{aligned}\mathcal{F}(\theta, \phi) &= \mathbb{E}_{q_\phi}[\log q_\phi(\mathbf{z}|\mathbf{x}) - \log p_\theta(\mathbf{x}, \mathbf{z})] \\ &= \mathbb{E}_{q_0}[\log q_0(\mathbf{z}_0|\mathbf{x}) - \log p_\theta(\mathbf{x}, \mathbf{z})] \\ &- \mathbb{E}_{q_0}\left[\sum_{k=1}^{K} \log \left|\det \left(\frac{\partial f_k(\mathbf{z}_{k-1}; \lambda_k(\mathbf{x}))}{\partial \mathbf{z}_{k-1}}\right)\right|\right]\end{aligned}$$

- Planar flows (Rezende & Mohamed, 2015) are convenient functions: $\mathbf{z}' = \mathbf{z} + \mathbf{u}h(\mathbf{w}^T\mathbf{z} + b)$

  with efficiently computed Jacobian:

$$\begin{aligned}\det \frac{\partial \mathbf{z}'}{\partial \mathbf{z}} &= \det\left(\mathbf{I} + \mathbf{u}h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{w}^T\right) \\ &= 1 + \mathbf{u}^T h'(\mathbf{w}^T\mathbf{z} + b)\mathbf{w},\end{aligned}$$

- Note: h is a scalar function and acts as a one-neuron bottleneck.

Improving the Encoder: Sylvester Flows

Van den Berg et al 2018

- A more general flow without the bottleneck is: $\mathbf{z}' = \mathbf{z} + \mathbf{A}h(\mathbf{B}\mathbf{z} + \mathbf{b})$,
  with $\mathbf{A} \in \mathbb{R}^{D \times M}$, $\mathbf{B} \in \mathbb{R}^{M \times D}$, $\mathbf{b} \in \mathbb{R}^{M}$, and $M \leq D$

- We can now the following theorem:

Theorem 1 (Sylvester's determinant identity)**.** *For all* $\mathbf{A} \in \mathbb{R}^{D \times M}$, $\mathbf{B} \in \mathbb{R}^{M \times D}$,

$$\det\left(\mathbf{I}_D + \mathbf{A}\mathbf{B}\right) = \det\left(\mathbf{I}_M + \mathbf{B}\mathbf{A}\right), \qquad (11)$$

where $\mathbf{I}_M$ *and* $\mathbf{I}_D$ *are* M *and* D*-dimensional identity matrices, respectively.*

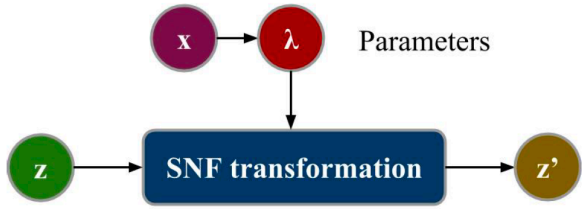
Improving the Encoder: Sylvester Flows

$$\mathbf{z}' = \mathbf{z} + \mathbf{A}h(\mathbf{B}\mathbf{z} + \mathbf{b}),$$

- To achieve invertibility we use: $A = QR$ and $B = \tilde{R}Q^T$ with R & $\tilde{R}$ upper-triangular and

  $\mathbf{Q} = (\mathbf{q}_1 \dots \mathbf{q}_M)$ with q_i an orthonormal set of vectors.

- The parameters of R, Q are all functions of x.



- We then finally have:

Theorem 2. *Let* $\mathbf{R}$ *and* $\tilde{\mathbf{R}}$ *be upper triangular matrices. Let* $h : \mathbb{R} \longrightarrow \mathbb{R}$ *be a smooth function with bounded, positive derivative. Then, if the diagonal entries of* $\mathbf{R}$ *and* $\tilde{\mathbf{R}}$ *satisfy* $r_{ii}\tilde{r}_{ii} > -1/\|h'\|_\infty$ *and* $\tilde{\mathbf{R}}$ *is invertible, the transformation given by* (13) *is invertible.*

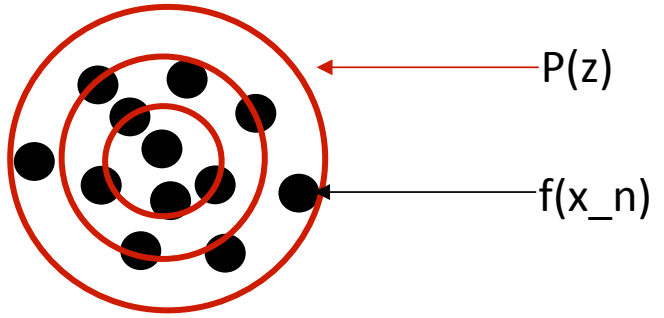
Changing the Objective: Wasserstein AE

- The term $E_{p(x)}\left[KL[q(z|x)||p(z)]\right]$ puts pressure on keeping q(z|x) close to p(z) for every value of x!
- An alternative requirement is to only force the aggregated posterior q(z) close to p(z):

$$E_{p(x)}\left[KL[q(z|x)||p(z)]\right] \longrightarrow KL[E_{p(x)}q(z|x)||p(z)]$$

- This says that the embedded data-points should distribute according to p(z), a much weaker condition!
- Amazingly, with this new KL the objective the ELBO becomes the dual formulation of the Wasserstein GAN! (Tolstikhin et al 2018)

$$\mathrm{POT}_{\|\cdot\|}(\mathbb{P}_{\text{data}}, \mathbb{P}_G) = \inf_{\mathbb{Q}_{Z|X}} \mathop{\mathbb{E}}_{\substack{\mathbf{x}\sim\mathbb{P}_{\text{data}} \\ \mathbf{z}\sim\mathbb{Q}_{Z|X=\mathbf{x}}}} \|\mathbf{x} - G(\mathbf{z})\| + \lambda_Z \cdot \mathfrak{D}(\mathbb{Q}_Z \,\|\, \mathbb{P}_Z)$$



(Wasserstein autoencoder, if D is enforced using a GAN this is a adversarial autoencoder Makhzani et al)

Learning as Bayesian Inference

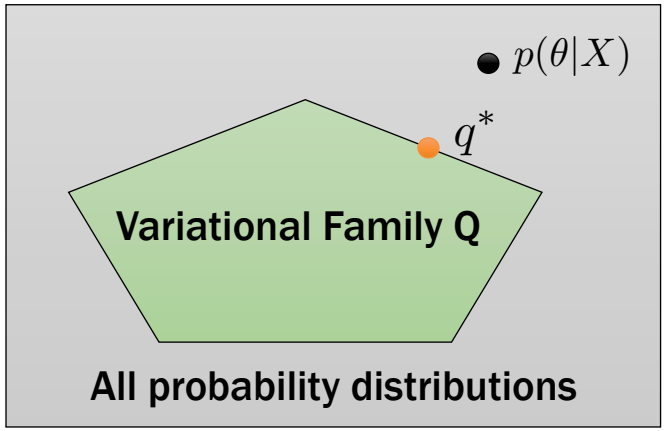
Bayes vs ML

- What's the difference between a prior p(z) over latent variables and a prior over p(w) over parameters?
- Why is Bayesian learning conceptually very different from maximum likelihood learning?
- Is a "Bayesian Network" Bayesian?
- Why Bayes:
  - Less overfitting
  - Uncertainties over predictions due to model
  - Compression

Bayesian Posterior Inference

Variational Inference

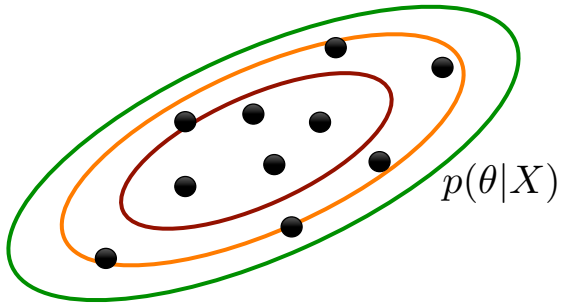
$$q^* = \min_{q \in Q} \mathrm{KL}[q(\theta)||p(\theta|X)]$$



- Deterministic
- Biased
- Local minima
- Easy to assess convergence

Sampling

$$\mathbb{E}_{p(\theta|X)}[f(\theta)] \approx \frac{1}{T}\sum_{t=1}^{T} f(\theta_t) \quad : \quad \theta_t \sim p(\theta|X)$$



- Stochastic (sample error)
- Unbiased
- Hard to mix between modes
- Hard to assess convergence

Hinton

Hinton & Van Camp, 1993,
"Keeping Neural Networks Simple by Minimizing the Description Length of the Weights"

Neal & Hinton, 1998
"A view of the EM algorithm that justifies incremental, sparse, and other variants"

$$\log P(X) = \int \mathrm{d}\Theta\ Q(\Theta) \log P(X|\Theta) - \mathrm{KL}[Q(\Theta)||P(\Theta)] + \mathrm{KL}[Q(\Theta)||P(\Theta|X)]$$

$$\log P(X) \geq \int \mathrm{d}\Theta\ Q(\Theta) \log P(X|\Theta) - \mathrm{KL}[Q(\Theta)||P(\Theta)]$$

$$= \int \mathrm{d}\Theta\ Q(\Theta) \log P(X|\Theta)P(\Theta) - \int \mathrm{d}\Theta\ Q(\Theta) \log Q(\Theta)$$

- Free Energy = - Energy + Entropy

Stochastic Variational Bayes

$$B(Q(\Theta)|X) = \int_{\Theta} d\Theta \;\; Q(\Theta) \left[\log P(X|\Theta) + \log P(\Theta) - \log Q(\Theta)\right]$$

$$\nabla_{\Phi} B = \int_{\Theta} d\Theta \;\; Q_{\Phi}(\Theta) \; \nabla_{\Phi} \log Q_{\Phi}(\Theta) \left[\log P(X|\Theta) + \log P(\Theta) - \log Q_{\Phi}(\Theta)\right]$$

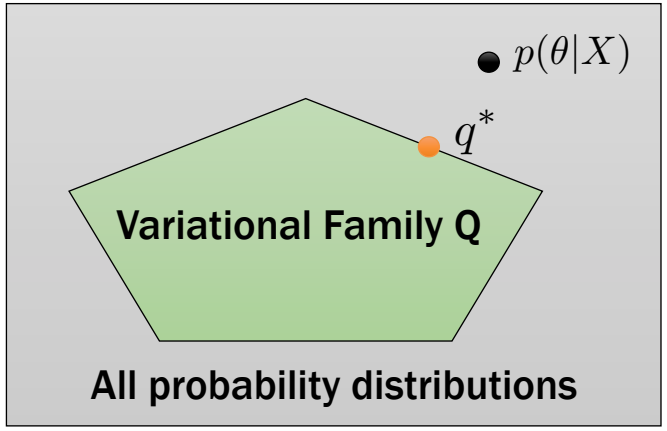
sample

subsample mini-batch X

$$\nabla_{\Phi} B = \frac{1}{S} \sum_{s=1}^{S} \nabla_{\Phi} \log Q_{\Phi}(\Theta_s) \left[\frac{N}{n} \sum_{i=1}^{n} \log P(x_i|\Theta_s) + \log P(\Theta_s) - \log Q_{\Phi}(\Theta_s)\right]$$

very high variance 

Variational Bayesian Learning



$$\Phi^* = \text{argmax}_\Phi \int \mathrm{d}\Theta\ Q_\Phi(\Theta)[\log P(X|\Theta)P(\Theta) - \log Q_\Phi(\Theta)]$$

$$= \text{argmax}_\Phi \int \mathrm{d}\Omega\ P_0(\Omega)[\log P(X|f(\Omega,\Phi))P(f(\Omega,\Phi)) - \log Q_\Phi(f(\Omega,\Phi))]$$

$$\Theta = f(\Omega,\Phi), \quad \text{s.t.} \quad Q_\Phi(\Theta)\mathrm{d}\Theta = P_0(\Omega)\mathrm{d}\Omega$$

("reparameterization trick", Kingma & W. 2013)

High Variance Gradient Estimator

$$L_{\mathcal{D}}(\phi) \simeq L_{\mathcal{D}}^{\mathrm{SGVB}}(\phi) = \frac{N}{M} \sum_{i=1}^{M} \log p(\mathbf{y}^i | \mathbf{x}^i, \mathbf{w} = f(\epsilon, \phi)),$$

- Sample epsilon once, then compute gradients on each data-case and sum.
- This has high variance because the data terms are now correlated because they share single epsilon
- Solution (?): draw different samples epsilon for every datacase
- Problem: very expensive: at every layer we have to multiply M times (M=nr. data in minibatch) a KxK matrix of random weights (K is nr. neurons in layer).

Local Reparameterization for Deep NNs

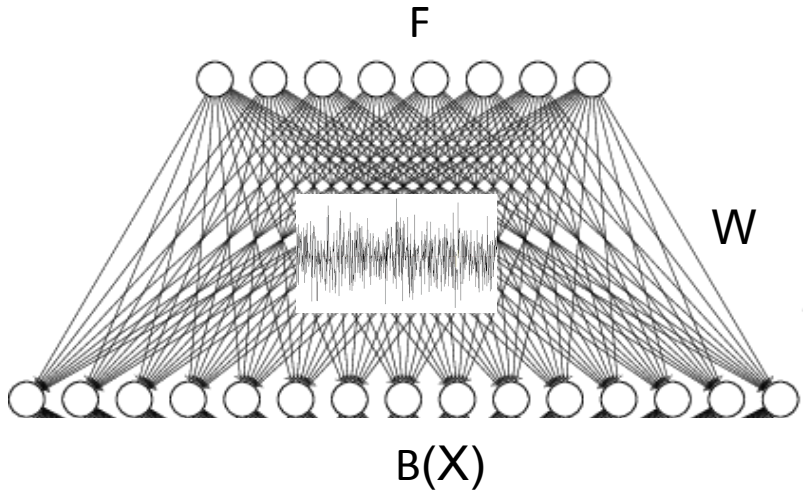
Kingma, Salimans & W. 2015

$$\int dW Q(W) \log P(Y|X,W) - \mathrm{KL}(Q(W)||P(W))$$

Reparameterize: compute exactly

$$\sum_{i=1}^{N} \int dW \; Q(W) \log P(y_i|W\phi(b_i)) \int df_i \; I(f_i - W\phi(b_i))$$

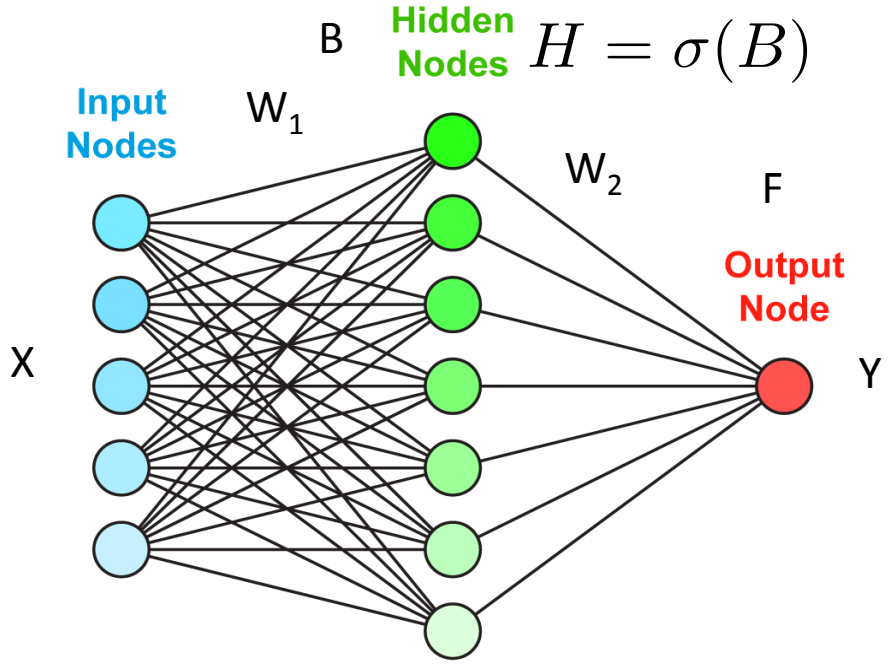
$$\sum_{i=1}^{N} \int df_i \; Q(f_i|b_i) \log P(y_i|f_i)$$



- Sampling f (KxM) for every data case is cheaper than sampling W for every data case (KxKxM)
- This trick reduces also variance

Bayesian Neural Networks

$$\mathbb{E}_{\tilde{p}(\mathbf{x},\mathbf{y})}[\log p(\mathbf{Y}|\mathbf{X})] \leq \mathbb{E}_{\tilde{p}(\mathbf{x},\mathbf{y})}\left[\mathbb{E}_{\tilde{q}_{\phi_1}(\mathbf{B}|\mathbf{X})\tilde{q}_{\phi_2}(\mathbf{F}|\mathbf{B})}\left[\log p(\mathbf{Y}|\mathbf{F})\right] - \sum_{i=1}^{2} KL(q_{\phi_i}(\mathbf{W}_i)||p_{\theta_i}(\mathbf{W}_i))\right]$$



Interesting relations to Deep GPs and Information Bottleneck

Extensions

$$\mathbb{E}_{\tilde{p}(\mathbf{x},\mathbf{y})}[\log p(\mathbf{Y}|\mathbf{X})] \leq \mathbb{E}_{\tilde{p}(\mathbf{x},\mathbf{y})}\left[\mathbb{E}_{\tilde{q}_{\phi_1}(\mathbf{B}|\mathbf{X})\tilde{q}_{\phi_2}(\mathbf{F}|\mathbf{B})}\left[\log p(\mathbf{Y}|\mathbf{F})\right] - \sum_{i=1}^{2} KL(q_{\phi_i}(\mathbf{W}_i)||p_{\theta_i}(\mathbf{W}_i))\right]$$

- Use matrix normal priors and posteriors $p(\mathbf{W}) = \mathcal{MN}(\mathbf{M}, \mathbf{U}, \mathbf{V})$
$$= \frac{\exp\left(-\frac{1}{2}\operatorname{tr}\left[\mathbf{V}^{-1}(\mathbf{W}-\mathbf{M})^T\mathbf{U}^{-1}(\mathbf{W}-\mathbf{M})\right]\right)}{(2\pi)^{np/2}|\mathbf{V}|^{n/2}|\mathbf{U}|^{n/2}}$$
- Use normalizing flows: $q_\phi(\mathbf{W}|\mathbf{z}) = \prod_{i=1}^{D_{in}}\prod_{j=1}^{D_{out}}\mathcal{N}(z_i\mu_{ij}, \sigma_{ij}^2)$, $\mathbf{z} \sim q_\phi(\mathbf{z})$ = normalizing flow

Louizos & W. "Structured and efficient variational deep learning with matrix Gaussian posteriors 2016.

Louizos & W. "Multiplicative Normalizing Flows for Variational Bayesian Neural Networks, 2017

Conclusions

- Think about variance and bias for parameter estimators or gradient estimators.
- There is more to representation learning than just the ELBO
- VAEs can be improved along many dimensions (prior, encoder, decoder, objective)
- A model is not Bayesian when there is a prior over latent variables
- Local reparameterization can help reduce variance and computation in Variational Bayesian Learning