Lecture 25

Generative Models and Variational Inference

Tutorial paper due

Tues May 1st, 11.59pm

Exam, 2-3 questions, 1-2 simple, 1 a bit hard (bit more work)

Exam released same night. You will have 10 days.

- This course has mostly been about Unsupervised Learning
- That is, estimating a $p(x)$ from data
- Supervised learning can be cast into this density estimation paradigm: $p(x, y)$
- these are "predictive" distributions
- We use some latent variables z, which mat be clusters, or estimation parameters θ

Latent Variables

- key concept: full data likelihood vs partial data likelihood
- probabilistic model is a *joint distribution* $p(\mathbf{x}, \mathbf{z})$, the full data likelihood
- with observed variables $\mathbf{x}$ corresponding to data, and latent variables $\mathbf{z}$

Concrete Formulation of unsupervised learning

Estimate Parameters by $\mathbf{x}$-MLE:

$$
\begin{aligned}
l(x|\lambda, \mu, \Sigma) &= \sum_{i=1}^{m} \log p(x_i|\lambda, \mu, \Sigma) \\
&= \sum_{i=1}^{m} \log \sum_{z} p(x_i|z_i, \mu, \Sigma)\, p(z_i|\lambda)
\end{aligned}
$$

Not Solvable analytically! EM and Variational. Or do MCMC.

EM

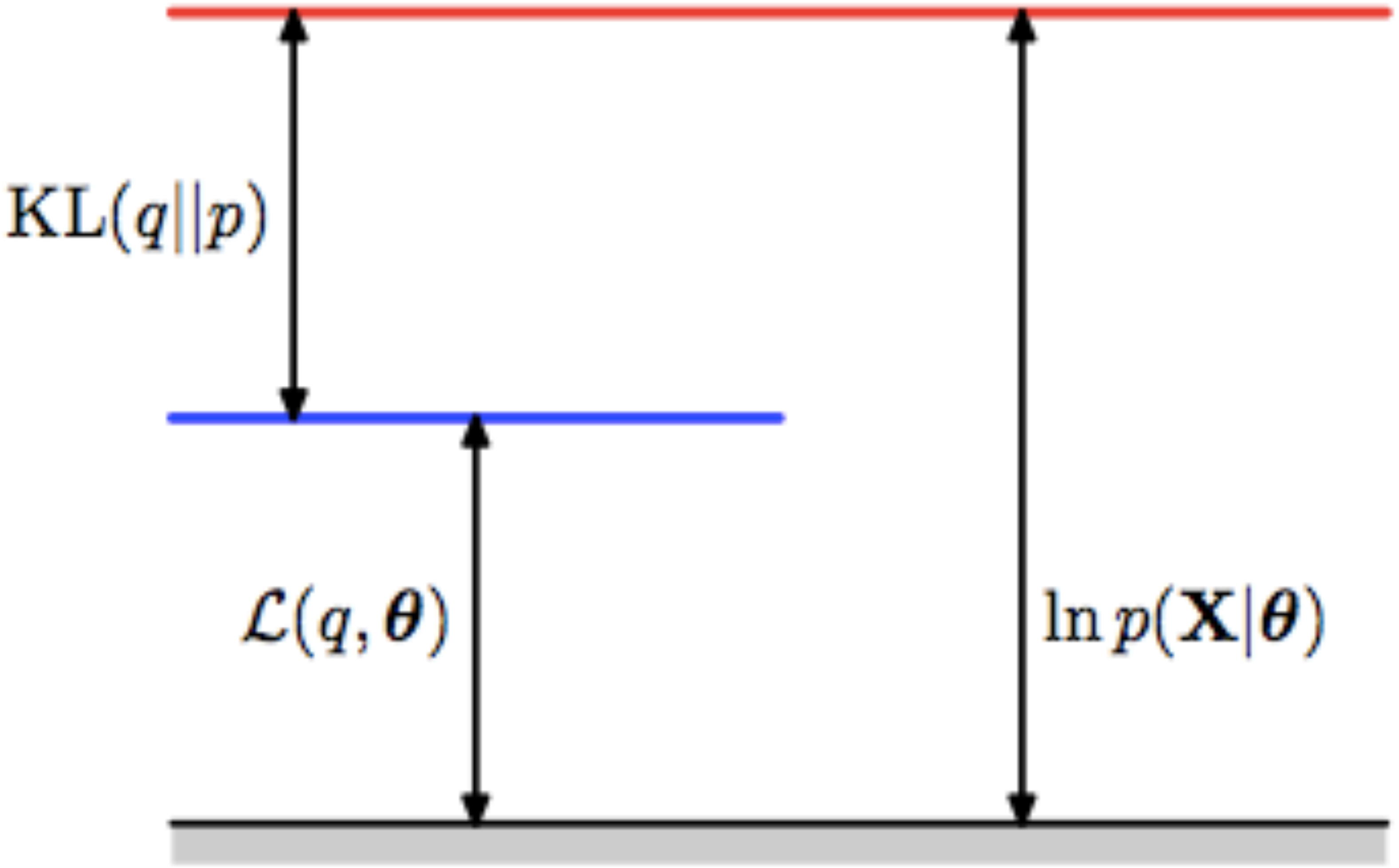
x-data likelihood: carry along θ

$$log\, p(x|\theta) = E_q[log \frac{p(x,z|\theta)}{q}] + D_{KL}(q,p)$$

If we define the ELBO or Evidence Lower bound as:

$$\mathcal{L}(q,\theta) = E_q[log \frac{p(x,z|\theta)}{q}]$$

then $log\, p(x|\theta)$ = ELBO + KL-divergence

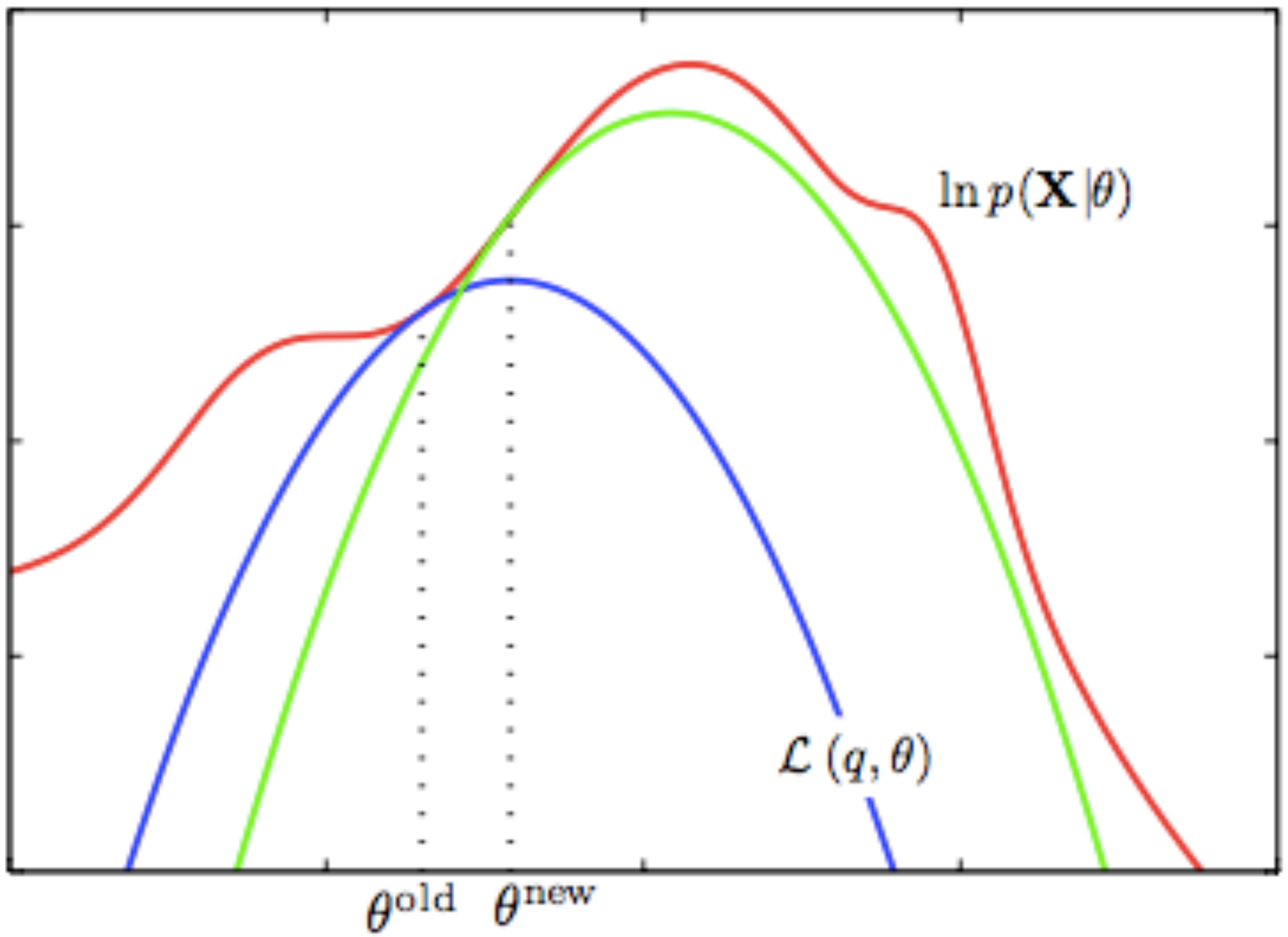


- KL divergence only 0 when $p = q$ exactly everywhere
- minimizing KL means maximizing ELBO
- ELBO $\mathcal{L}(q, \theta)$ is a lower bound on the log-likelihood.
- ELBO is average full-data likelihood minus entropy of q:

$$\mathcal{L}(q, \theta) = E_q[log\frac{p(x, z|\theta)}{q}] = E_q[logp(x, z|\theta)] - E_q[log\, q]$$

Process

1. Start with $p(x|\theta)$(red curve), θ_{old}.
2. Until convergence:
    1. E-step: Evaluate $q(z, \theta_{old}) = p(z|x, \theta_{old})$ which gives rise to $Q(\theta, \theta_{old})$ or $ELBO(\theta, \theta_{old})$ (blue curve) whose value equals the value of $p(x|\theta)$ at θ_{old}.
    2. M-step: maximize Q or $ELBO$ wrt θ to get θ_{new}.
    3. Set $\theta_{old} = \theta_{new}$



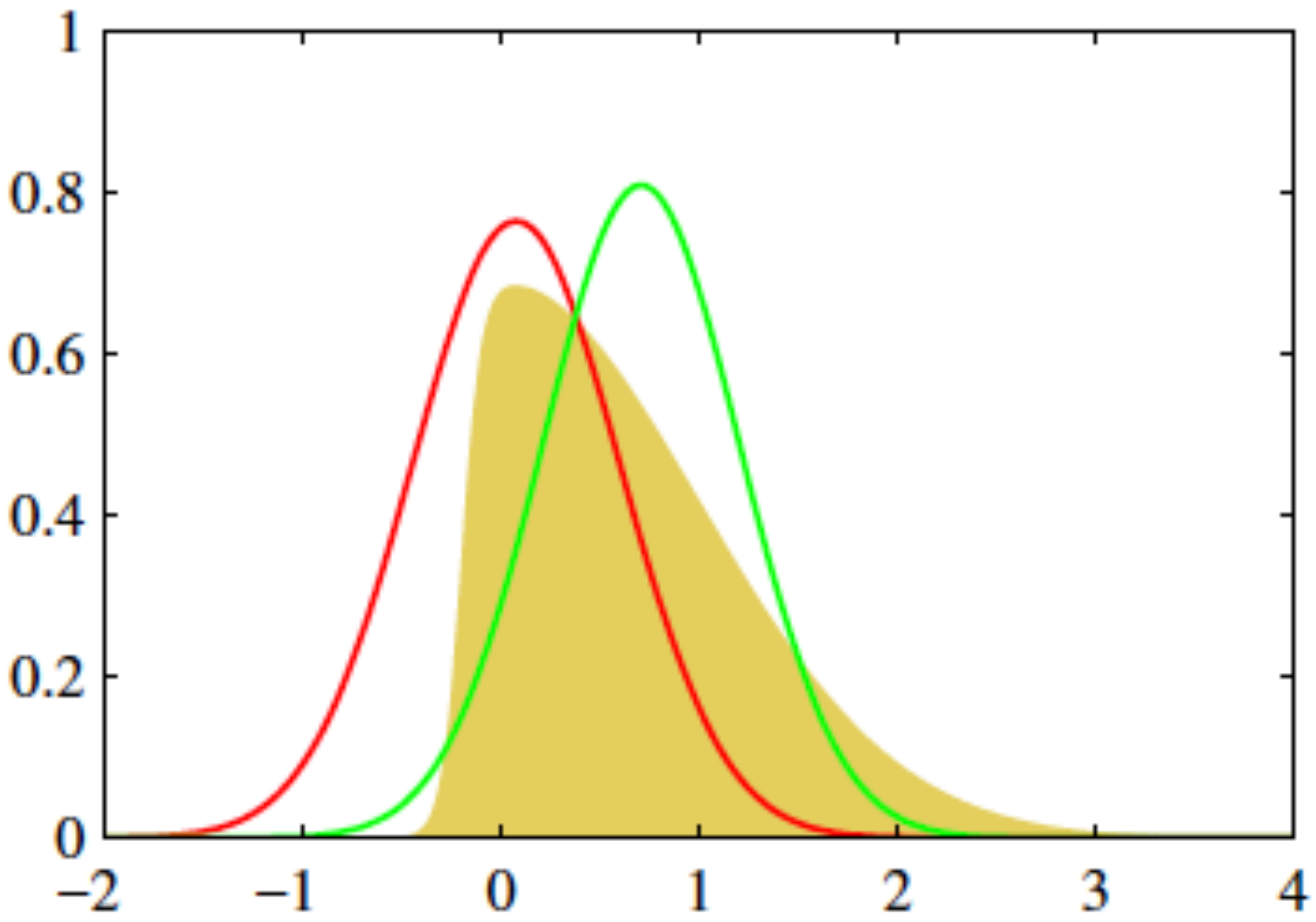
VARIATIONAL INFERENCE

Core Idea

z is now all parameters. Dont distinguish from θ.

Restricting to a family of approximate distributions D over z, find a member of that family that minimizes the KL divergence to the exact posterior. An optimization problem:

$$q^*(z) = \underset{q(z)\in D}{\arg\min} \quad KL(q(z)||p(z|x))$$



VI vs MCMC

MCMC	**VI**
More computationally intensive	Less intensive
Guarantees producing asymptotically exact samples from target distribution	No such guarantees
Slower	Faster, especially for large data sets and complex distributions
Best for precise inference	Useful to explore many scenarios quickly or large data sets

Basic Setup in EM

Recall that $KL + ELBO = log(p(x))$,
$ELBO(q) = E_q[(log(p(z, x))] - E_q[log(q(z))]$

EM alternates between computing the expected complete log likelihood according to $p(z|x)$ (the E step) and optimizing it with respect to the model parameters (the M step).

EM assumes the expectation under $p(z|x)$ is computable and uses it in otherwise difficult parameter estimation problems.

Basic Setup in VI

$KL + ELBO = log(p(x))$: ELBO bounds log(evidence)

$$ELBO(q) = E_q[log\,\frac{p(z,x)}{q(z)}] = E_q[log\,\frac{p(x|z)p(z)}{q(z)}] = E_q[log\,p(x|z)] + E_q[log\,\frac{p(z)}{q(z)}]$$

$$\implies ELBO(q) = E_{q(z|x)}[(log(p(x|z))] - KL(q(z|x)||p(z))$$

(likelihood-prior balance)

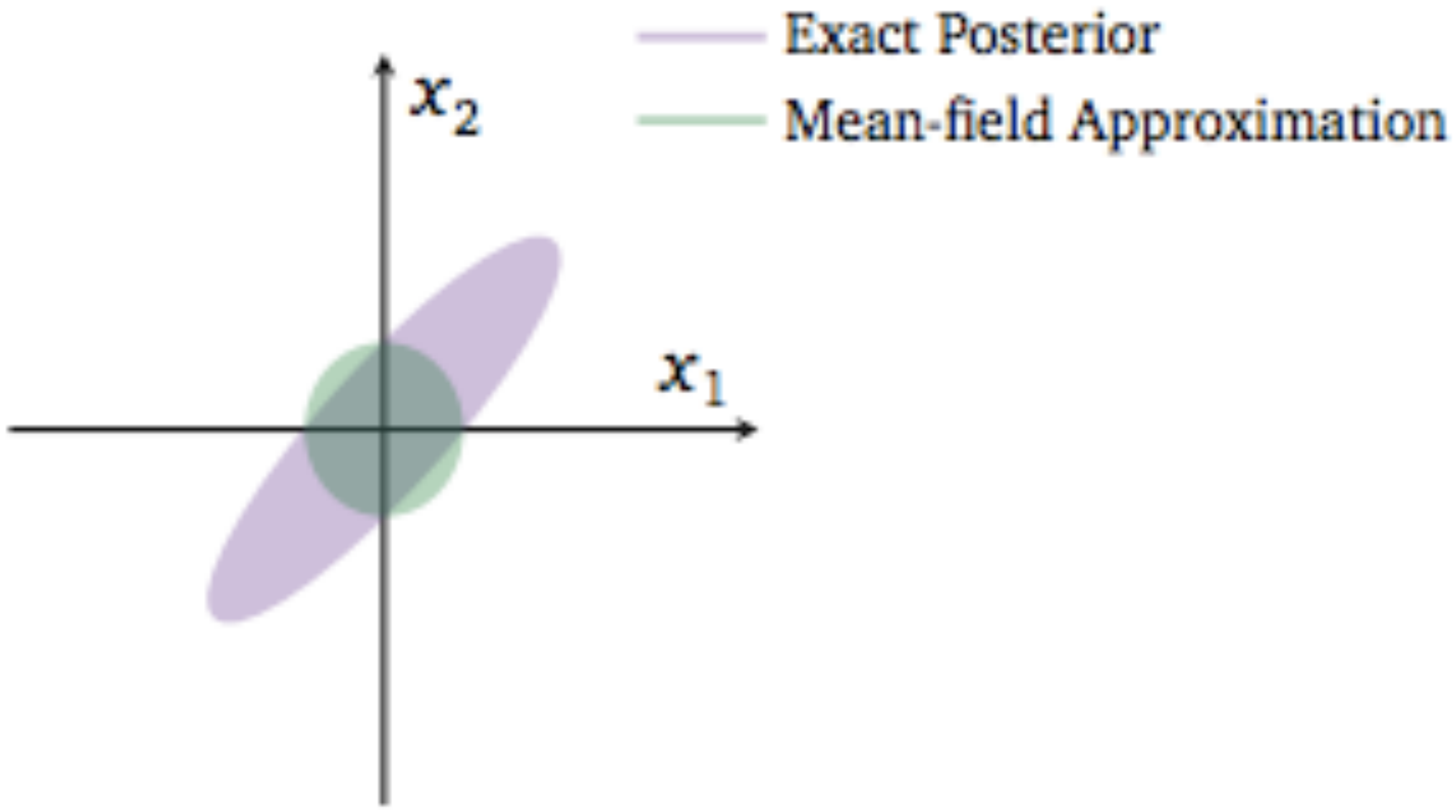
Mean Field: Find a q such that:

$KL + ELBO = log(p(x))$: KL minimized means ELBO maximized.

Choose a "mean-field" q such that:

$$q(z) = \prod_{j=1}^{m} q_j(z_j)$$

Each individual latent factor can take on any paramteric form corresponding to the latent variable.



Example

$$q(z) = \prod_{j=1}^{m} q_j(z_j)$$

a 2D Gaussian Posterior is approximated by a mean-field variational structure with independent gaussians in the 2 dimensions

The variational posterior in green cannot capture the strong correlation in the original posterior because of the mean field approximation.

Optimization: CAVI

Coordinate ascent mean-field variational inference

maximizes ELBO by iteratively optimizing each variational factor of the mean-field variational distribution, while holding the others fixed.

Define Complete Conditional of $z_j = p(z_j | \boldsymbol{z_{-j}}, \boldsymbol{x})$

Algorithm

Input: $p(x, z)$ with data set x, **Output**: $q(z) = \prod_j q_j(z_j)$

Initialize: $q_j(z_j)$

```
while ELBO has not converged (or z have not converged):`
    for each j:
```

$$q_j \propto exp(E_{-j}[logp(z_j | z_{-j}, x])$$

```
    compute ELBO
```

where the expectations above are with respect to the variational distribution over $\boldsymbol{z}_{-\boldsymbol{j}}$:

$$\prod_{\boldsymbol{l} \neq \boldsymbol{j}} q_l(z_l)$$

Assertion: $q_j^*(z_j) \propto \exp\{E_{-j}[log(p(z_j|\boldsymbol{z}_{-\boldsymbol{j}}, \boldsymbol{x}))]\}$
$\implies q_j^*(z_j) \propto \exp\{E_{-j}[log(p(z_j, \boldsymbol{z}_{-\boldsymbol{j}}, \boldsymbol{x}))]\}$

(because the mean-field family assumes that all the latent variables are independent)

Example: "Fake :-) Gaussian"

```
data = np.random.randn(100)
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sd=1)
    sd = pm.HalfNormal('sd', sd=1)
    n = pm.Normal('n', mu=mu, sd=sd, observed=data)
```

Assume Gaussian posteriors for `mu` and `log(sd)`. So, for e.g.,

$$\mu \sim N(\mu_\mu, \sigma_\mu^2), log(\sigma) \sim N(\mu_\sigma, \sigma_\sigma^2)$$

ADVI

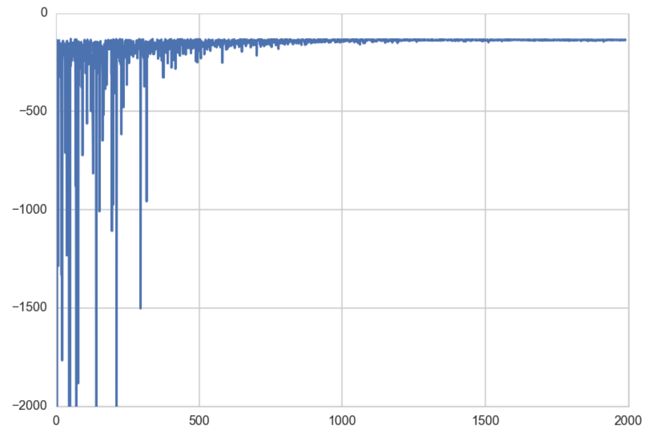
Core Idea:

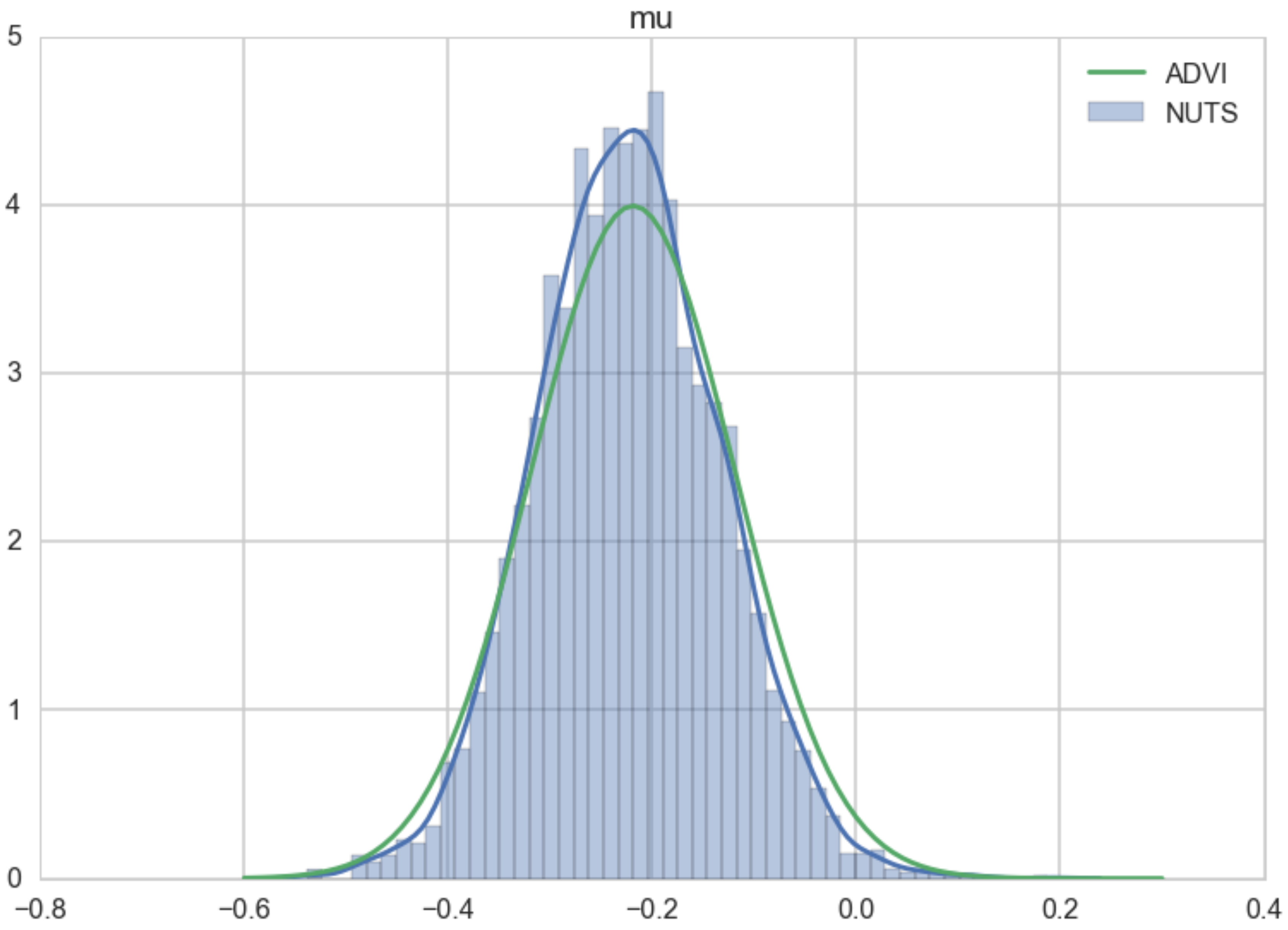
- CAVI does not scale, needs graduate student descent
- Use gradient descent instead
- Use minibatches to do it on less data
- do it automatically using automatic differentiation

ADVI in pymc3

```
data = np.random.randn(100)
with pm.Model() as model:
    mu = pm.Normal('mu', mu=0, sd=1, testval=0)
    sd = pm.HalfNormal('sd', sd=1)
    n = pm.Normal('n', mu=mu, sd=sd, observed=data)
advifit = pm.ADVI( model=model)
advifit.fit(n=50000)
elbo = -advifit.hist
plt.plot(elbo[::10]);
```

elbo:





What does ADVI do?

1. Transformation of latent parameters (**T** transform)
2. Standardization transform for posterior to push gradient inside expectation (**S** transform)
3. Monte-Carlo estimate of expectation
4. Hill-climb using automatic differentiation

Remember:

$$ELBO(q) = E_q[(log(p(z,x))] - E_q[log(q(z))]$$

Need

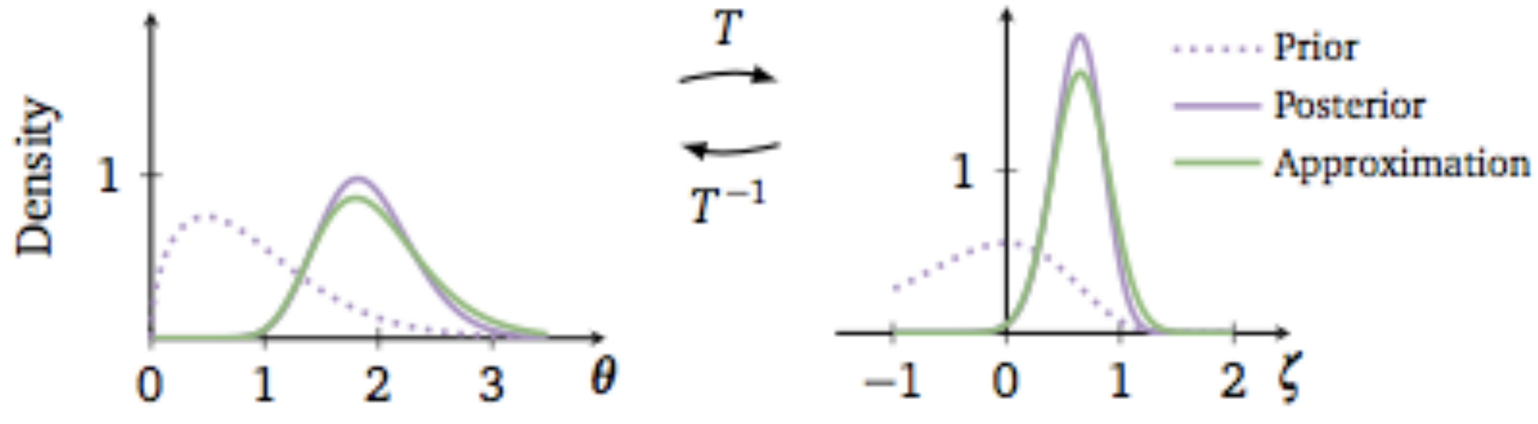
$$\nabla_\eta \mathcal{L} = E[\nabla_\eta[logp(x, T^{-1}(S^{-1}(\eta))) + log(det(J_{T^{-1}}(S^{-1}(\eta))))]$$

where S is the first transform and T is the standardization.

(1) T-Transformation

- Latent parameters are transformed to representations where the 'new" parameters are unconstrained on the real-line. Specifically the joint $p(x, \theta)$ transforms to $p(x, \eta)$ where η is un-constrained.
- Minimize the KL-divergence between the transformed densities.
- This is done for *ALL* latent variables.
- Thus use the same variational family for ALL parameters, and indeed for ALL models,

- Discrete parameters must be marginalized out.
- Optimizing the KL-divergence implicitly assumes that the support of the approximating density lies within the support of the posterior. These transformations make sure that this is the case
- First choose as our family of approximating densities mean-field normal distributions. We'll transform the always positive σ params by simply taking their logs.



(a) Latent variable space (b) Real coordinate space

(2) S-transformation

- we must maximize our suitably transformed ELBO.
- we are optimizing an expectation value with respect to the transformed approximate posterior. This posterior contains our transformed latent parameters so the gradient of this expectation is not simply defined.
- we want to push the gradient inside the expectation. For this, the distribution we use to calculate the expectation must be free of parameters

(3) Compute the expectation

As a result of this, we can now compute the integral as a monte-carlo estimate over a standard Gaussian--superfast, and we can move the gradient inside the expectation (integral) to boot. This means that our job now becomes the calculation of the gradient of the full-data joint-distribution.

(4) Calculate the gradients

We can replace full x data by just one point (SGD) or mini-batch (some-x) and thus use noisy gradients to optimize the variational distribution.

An adaptively tuned step-size is used to provide good convergence.

Relaxing the mean-field approximation

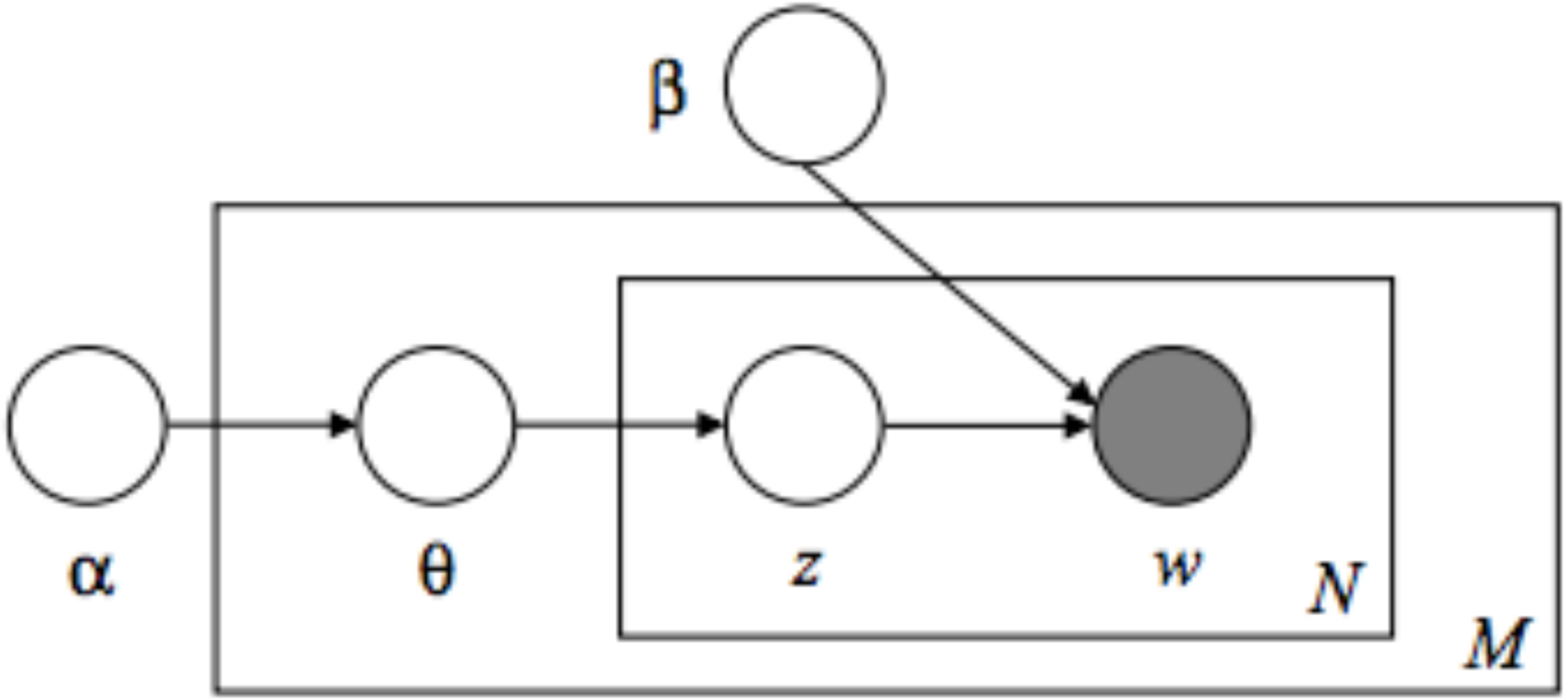
- Full-Rank ADVI: model covariance
- Normalizing Flows
- Operator Variational Inference: allows generalization of many algorithms under one umbrella

(all implemented in pymc3)

How good is variational Bayes?

- its used heavily for models like LDA (latent-dirichlet allocation)
- but surprisingly the "goodness-of-fit" of the posterior approximation has been handled on a case by case basis
- until now: see Yao et. al

LDA: a generative model



See Blei et. al.

LDA assumes the following generative process for *each* document w in a corpus D:

1. Choose $N \sim Poisson(\xi)$.
2. Choose $\theta \sim Dir(\alpha)$.
3. For each of the N words w_n (from vocab size V):
    1. Choose a topic $z_n \sim Multinomial(\theta)$ (size k).
    2. Choose a word w_n from $p(w_n | z_n, \beta)$, β size V x k, a multinomial probability conditioned on the topic z_n.

Two ideas from Yao et. al.

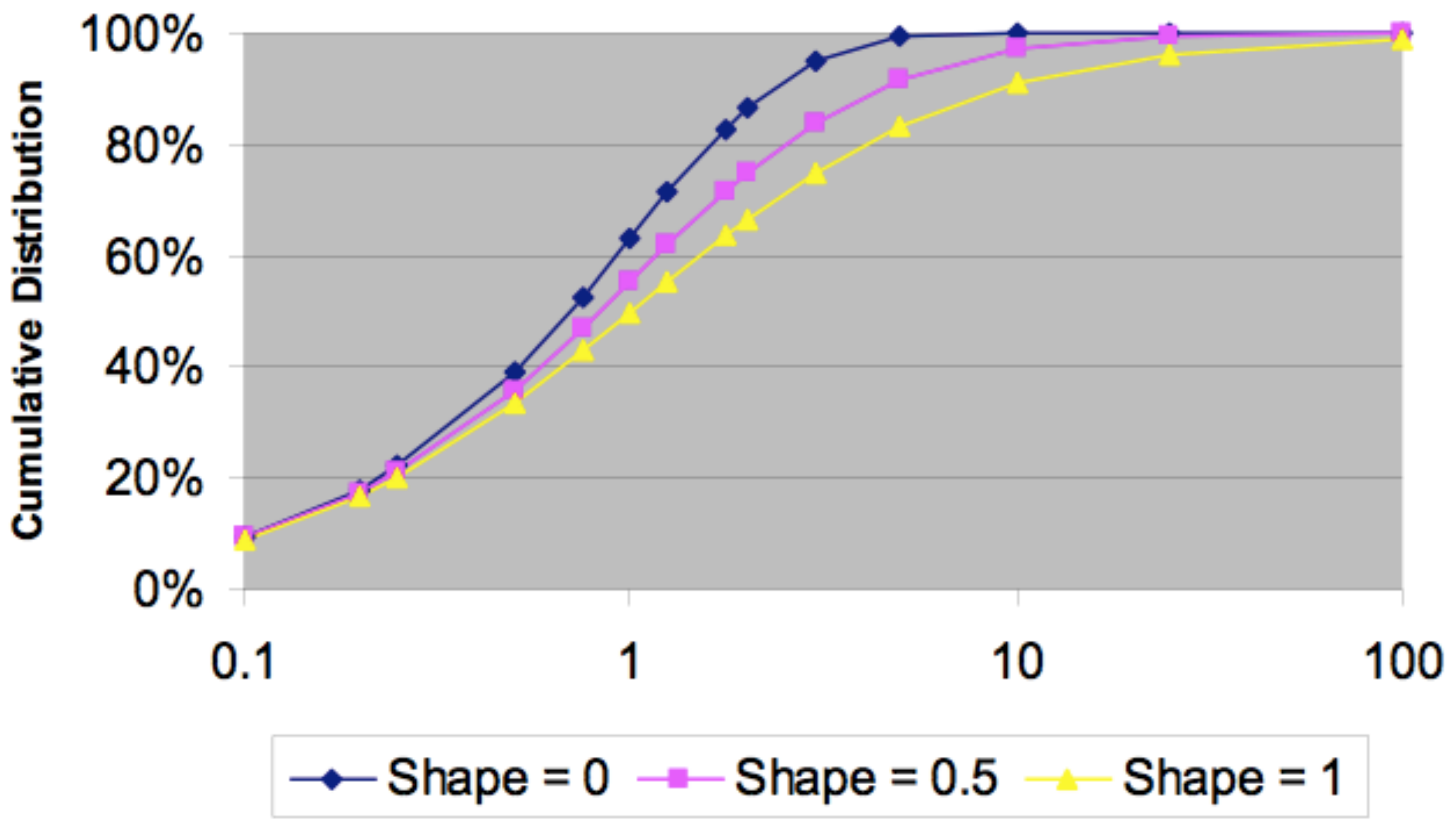
- pareto shape parameter k from PSIS tells you goodness of fit (see here for @junpenglao pymc3 implementation, WIP). The idea comes from the process of smoothing in LOOCV estimation
- VSBC (variational simulation based callibration) : Extends calibration from Bayesian Workflow to variational case. pymc3 experimentation by @junpenglao here, WIP

Pareto Smoothed Importance Sampling

Want $E_p[h(\theta)]$. But we calculate $E_q[h(\theta)] = (1/S) \sum_s h(\theta_s)$ which is biased.

Use importance sampling: $E_p[h(\theta)] = \frac{\sum_s w_s h(\theta_s)}{\sum_s w_s}$ where $w_s = p(\theta_s, y)/q$. w_s may have large or infinite variance.

Use PSIS: fit shape k Pareto to M largest w_s and replace them by expected values of corresponding order statistics under the pareto. Also truncate all weights at raw maximum w_s. Use joint as pareto cares not about multiplying factors.



M empirically set as $min(S/5, 3\sqrt{S})$.

Result from extreme value theory (Pickands–Balkema–de Haan theorem): conditional excess distribution function is a generalized pareto

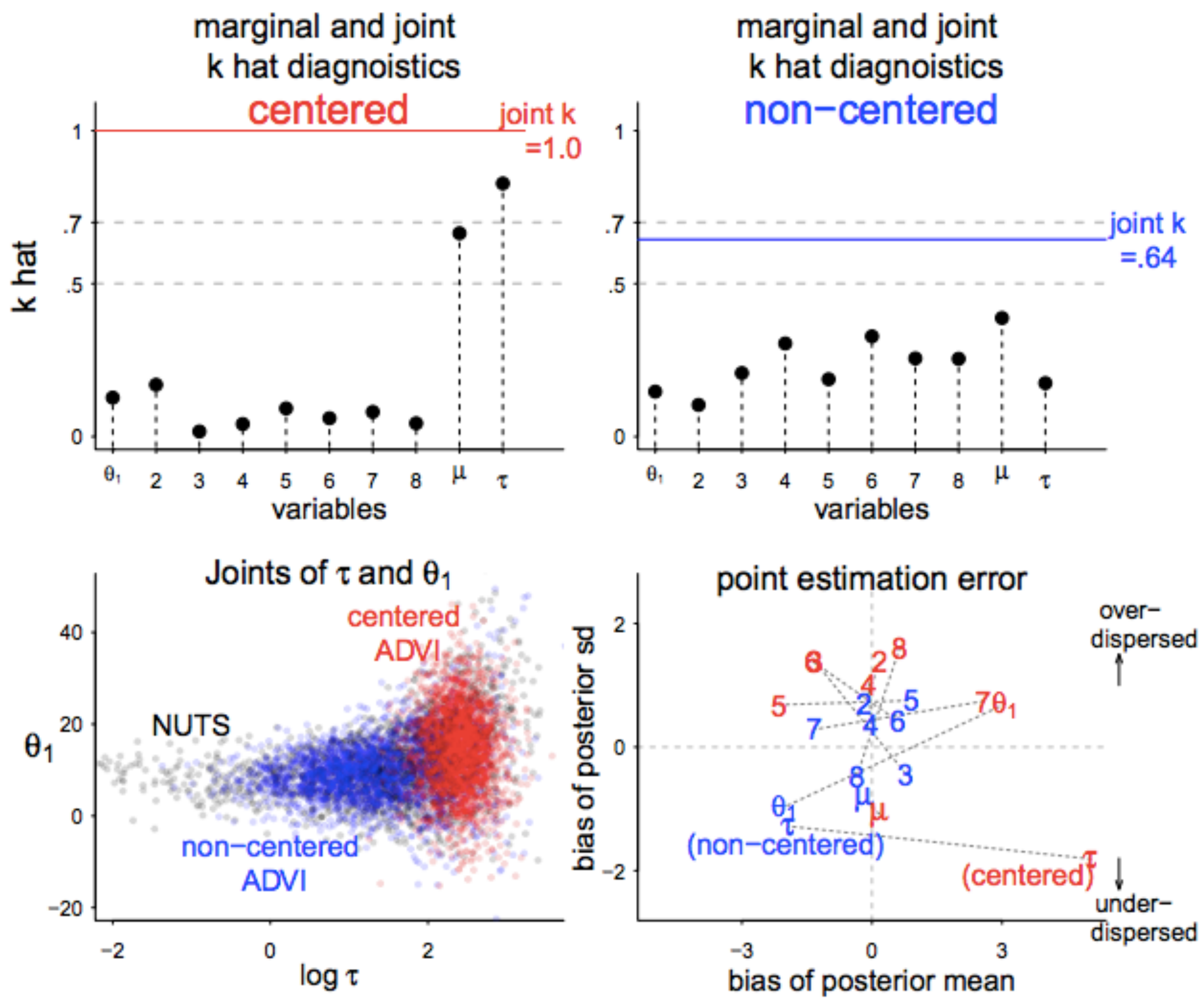
$$p(y|\mu,\sigma,k) = \begin{cases} \frac{1}{\sigma}\left(1+k\left(\frac{y-\mu}{\sigma}\right)\right)^{-\frac{1}{k}-1}, & k \neq 0. \\ \frac{1}{\sigma}\exp\left(\frac{y-\mu}{\sigma}\right), & k = 0. \end{cases}$$

$k < 0.5$ great, ok between 0.5 and 0.7, not so good after 0.7, weights too large.

source

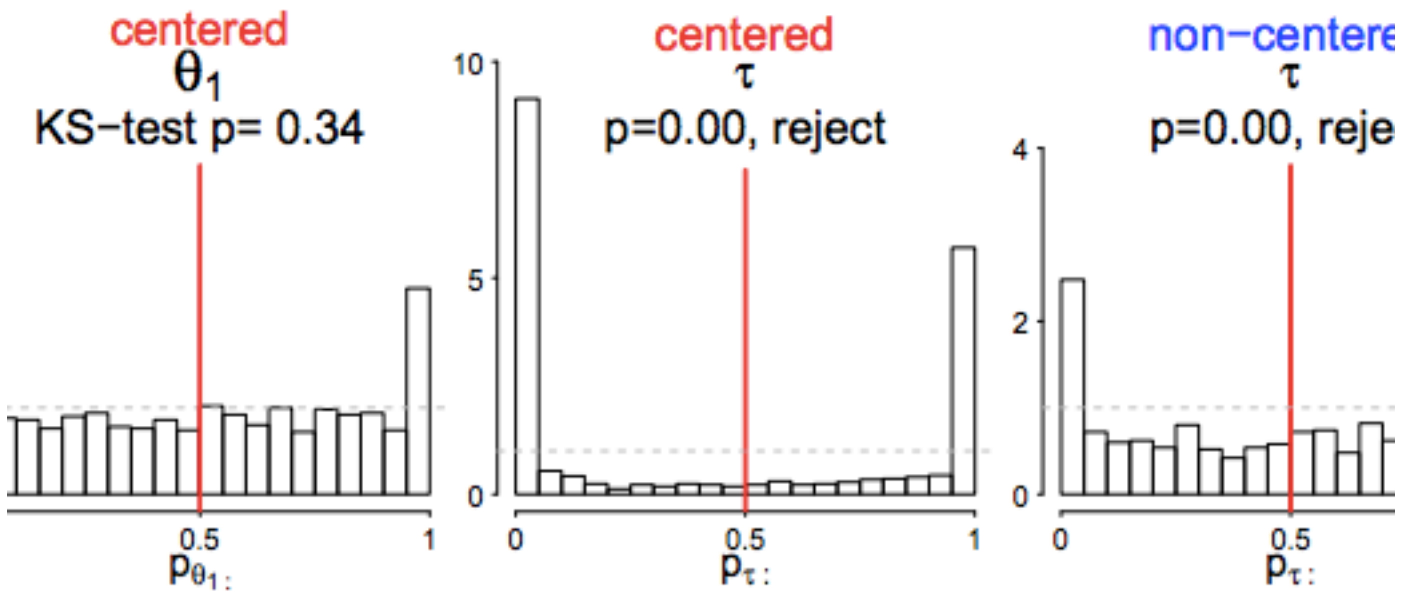
VSBC

- basic idea from bayesian workflow, posterior from data simulated from prior ($\theta_0 \sim p(\theta)$) should look like the prior. That is, ideally order statistics uniform
- in VSBC fit the posterior variationally. Will have some mismatch
- quantify mismatch by asymmetry in histogram of ith marginal callibration probabilities $p_{ij} = P_q(\theta_i < [\theta_j^0]_i)$



Left: ADVI posterior and pareto shape statistics

Below: VSBC histogram

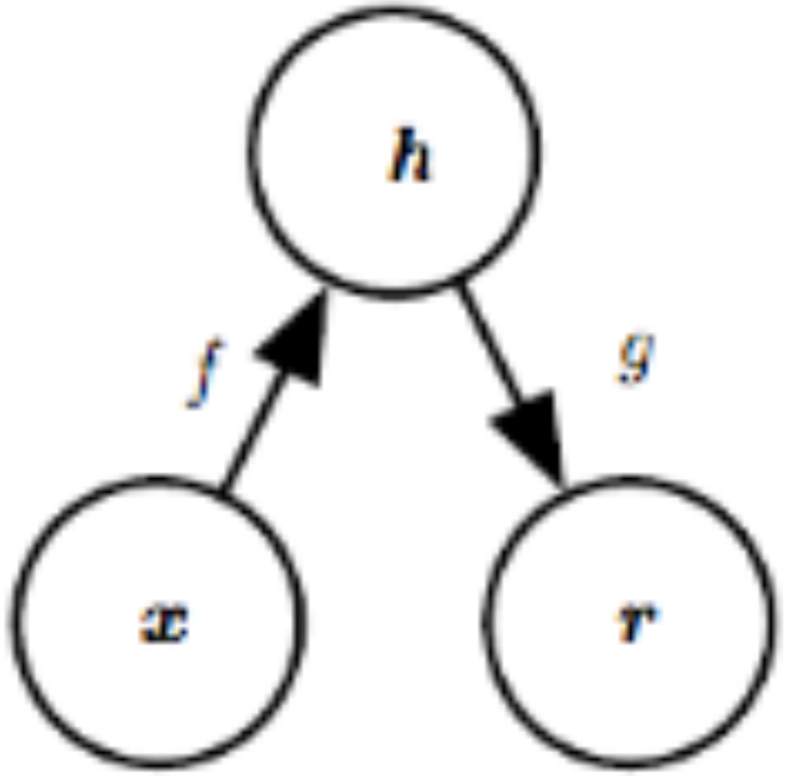


Why use VB

- simply not possible to do inference in large models
- inference in neural networks: understanding robustness, etc
- hierarchical neural networks (perhaps on exam)
- Mixture density networks: mixture parameters are fitted using ANNs
- extension to generative semisupervised learning
- variational autoencoders

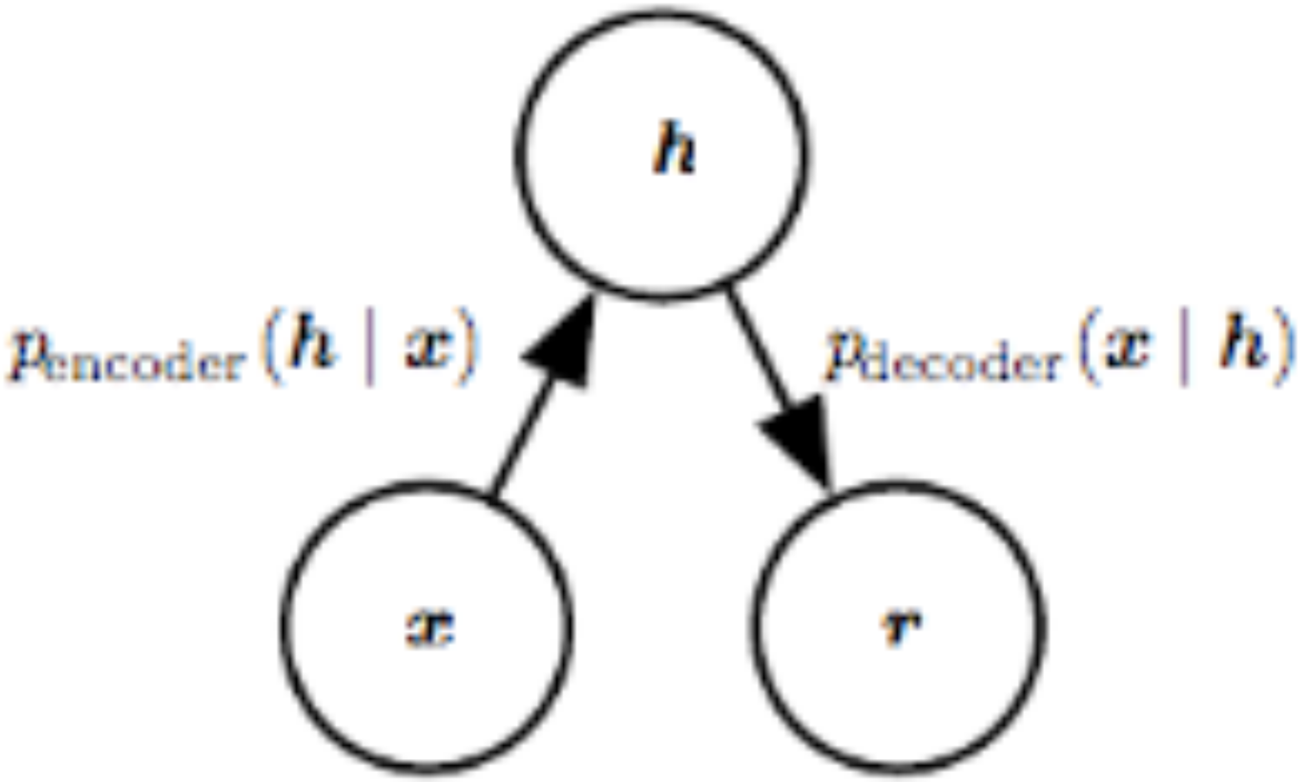
Variational Autoencoders

Autoencoders: basic idea



- **h** is the representation. An *undercomplete* autoencoder makes **h** of smaller dimension than x
- f is the encoder and g the decoder
- simplest idea: minimize $L(x, g(f(x)))$
- can regularize instead of being undercomplete

- can think of an autoencoder as a way of approximately training a generative model.
- the features of the autoencoder describe the latent variables that explain the input
- can go deep!
- generalize to a stochastic autoencoder. The standard autoencoder then is a specific hidden state h or z



Variational Autoencoder

- just as in ADVI, we want to learn an approximate "encoding posterior" $p(z|x)$
- note that we have now again gone back to thinking of z as a (possibly) deep latent variable, or "representation".

We know how to do this:

ELBO maximization

Basic Setup in VI

$KL + ELBO = log(p(x))$: ELBO bounds log(evidence)

$$ELBO(q) = E_q[log\,\frac{p(z,x)}{q(z)}] = E_q[log\,\frac{p(x|z)p(z)}{q(z)}] = E_q[log\,p(x|z)] + E_q[log\,\frac{p(z)}{q(z)}]$$

$$\implies ELBO(q) = E_{q(z|x)}[(log(p(x|z))] - KL(q(z|x)||p(z))$$

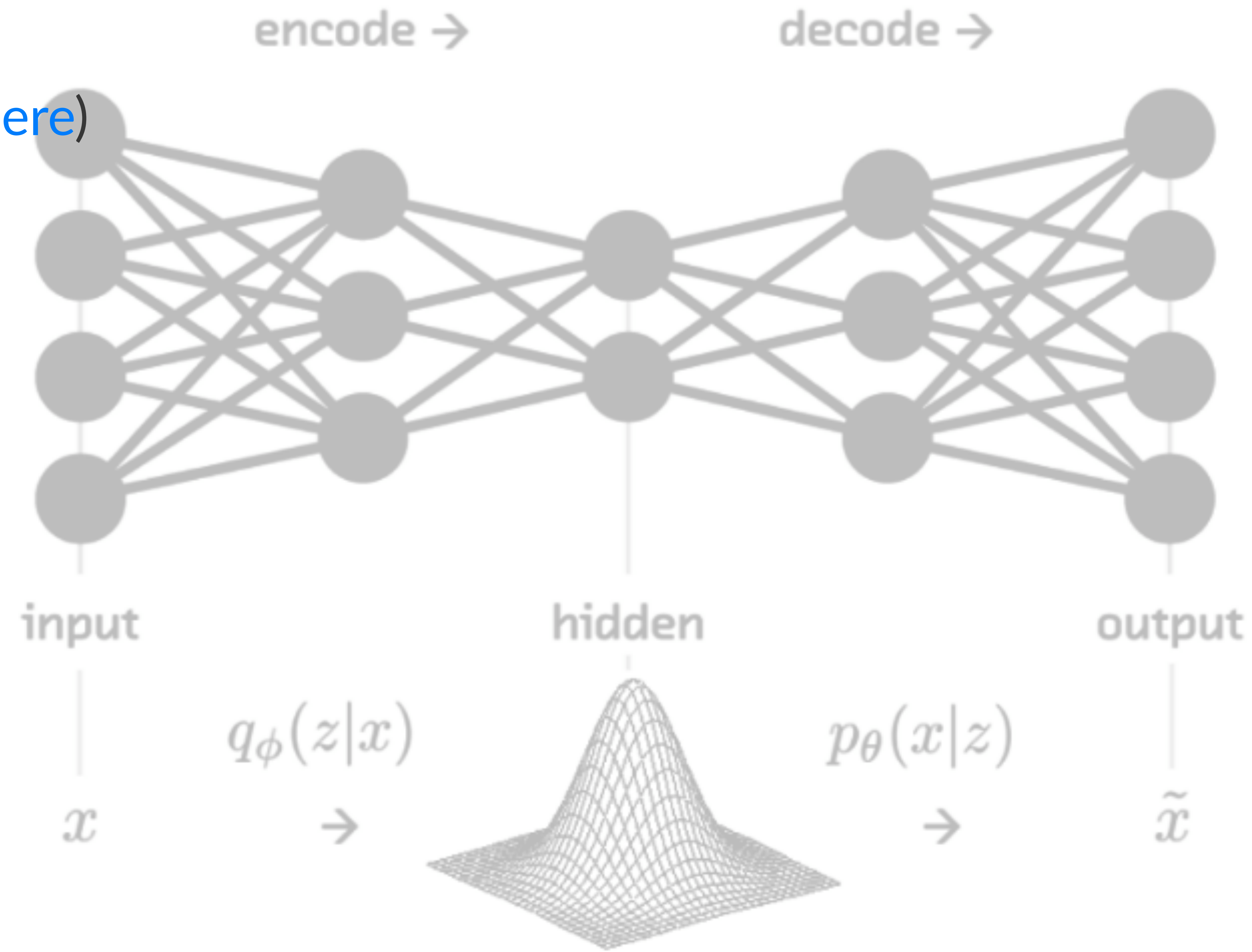
(likelihood-prior balance)

The Game

$$ELBO(q) = E_{q(z|x)}[(log(p(x|z))] - KL(q(z|x)||p(z))$$

- get z samples coming from x, $q(z|x)$- to be close to some prior, $p(z)$, typically chosen as an isotropic gaussian...the regularization term
- first term is called "reconstruction loss", or "capacity of model to generate something like the data".

(from here)



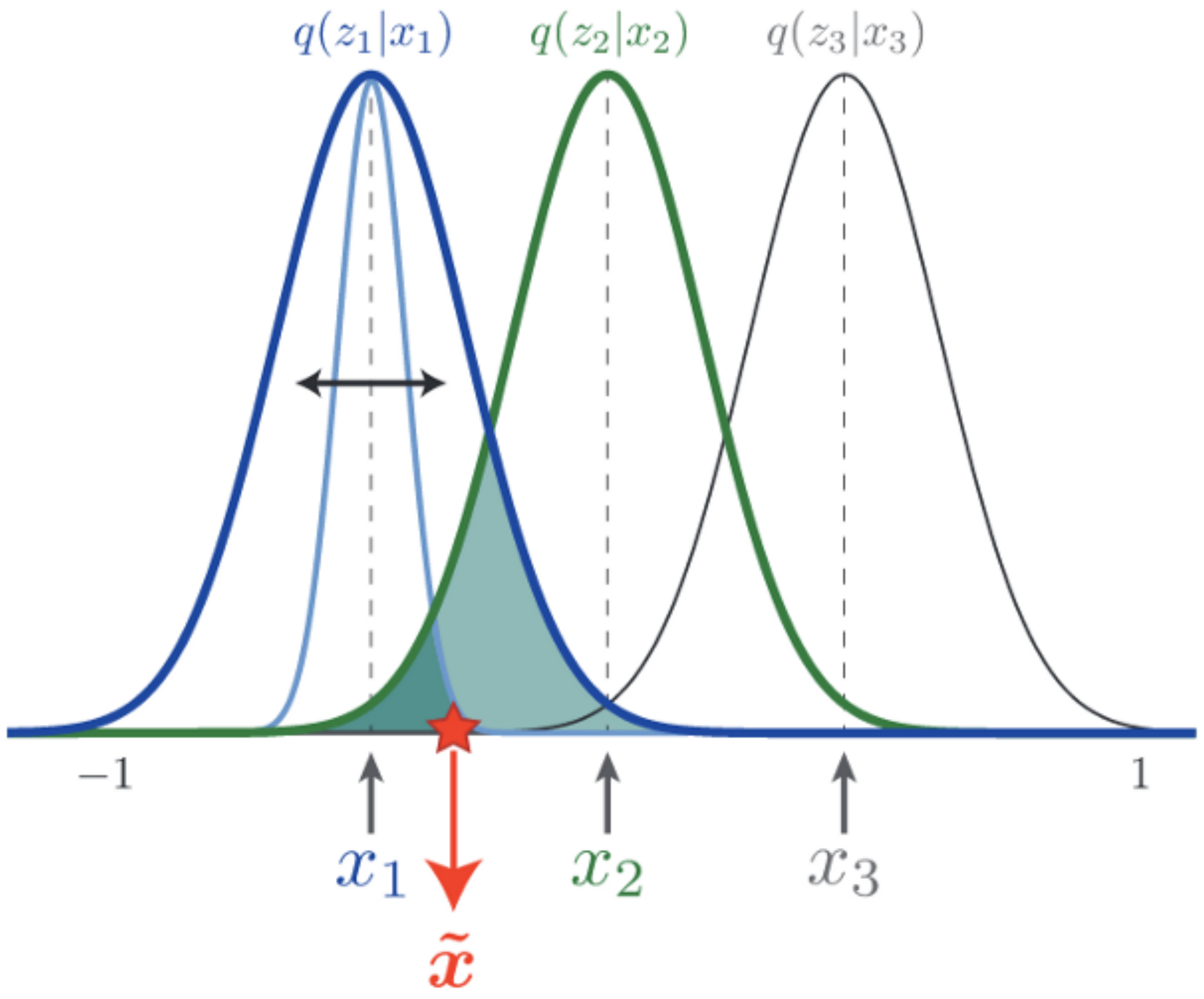
encode →
decode →
input
hidden
output
$q_\phi(z|x)$
$p_\theta(x|z)$
x
→
→
$\tilde{x}$

VAE steps for MNIST

- details in original paper and notebook
- linear encoder for both μ and $log(\sigma^2)$
- then transformation to $N(0,1)$ to be able to take gradient inside expectation as in ADVI
- then decode using a loss: binary cross-entropy $p(x|z)$ (for images) minus KL

Disentanglement Issues

- can be understood from a gaussian mixtures perspective
- we would prefer data locality
- thus crank up the prior (regularization) term
- this is called the βVAE



How to implement?

- possible in pytorch, also in pymc3
- see convolutional VAE for MNIST in pymc3
- notice that MNIST, which we did earlier as supervised is now being done unsupervised.

Why?

See pymc3 for e.g. for auto-encoding LDA

- variational auto-encoders algorithm which allows us to perform inference efficiently for large datasets
- use tunable and flexible encoders such as multilayer perceptrons (MLPs) as our variational distribution to approximate complex variational posterior
  -then its just ADVI with mini-batch on PyMC3 or pytorch. Can use for any posterior, example LDA, or custom for MNIST