LECTURE 9: DISTRIBUTIONAL APPROXIMATIONS

- MCMC is expensive, specially for hierarchical models, so a number of approximations have been developed
- Expectation-Maximization
- Variational Inference

Expectation-Maximization (EM) Algorithm

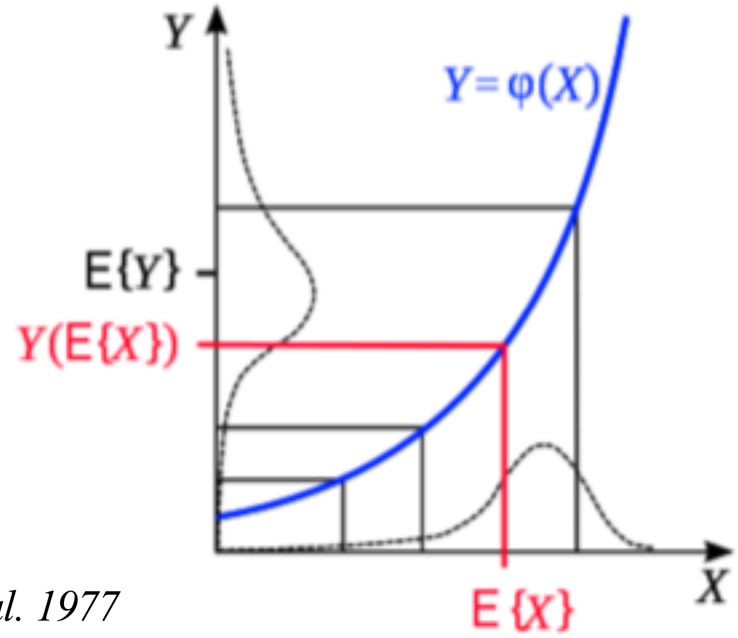
- We have data X, parameters θ and latent variables Z (which often are of the same size as X).
- In hierarchical models we know how to write conditionals $p(X|Z,\theta)$ and $p(Z|\theta)$ but it is hard to integrate out Z to write directly $p(X|\theta)$, and thus posterior $p(\theta|X)$ (we will assume flat prior), i,e. it is hard to compute

$$p(X|\theta) = \int p(X,Z|\theta)dZ = \int p(X|Z,\theta)p(Z|\theta)dZ$$

- Jensen inequality for convex Y:

$$\varphi(\mathbf{E}[X]) \leq \mathbf{E}[\varphi(X)] = \mathbf{E}[Y]$$

- Opposite for concave (log)

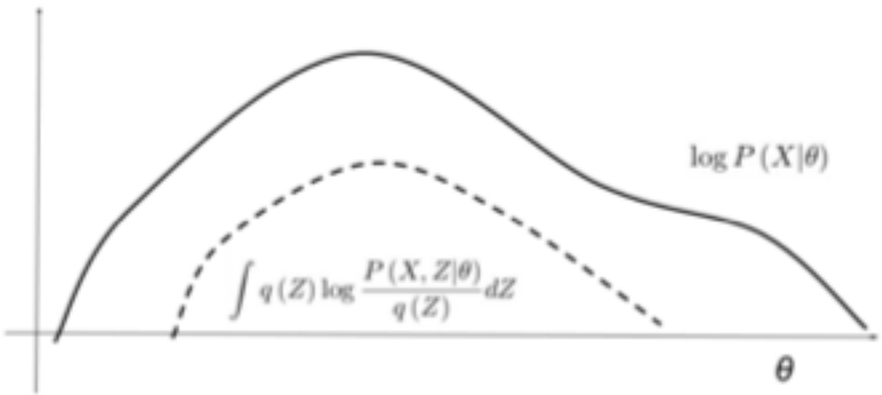


Credit: Dempster et al. 1977

Jensen Inequality applied to log$P$

- For any $q(Z)$ we have

$$\log \int P(X,Z|\theta)\, dZ = \log \int P(X,Z|\theta)\, \frac{q(Z)}{q(Z)} dZ \geq \int q(Z) \log \frac{P(X,Z|\theta)}{q(Z)} dZ$$

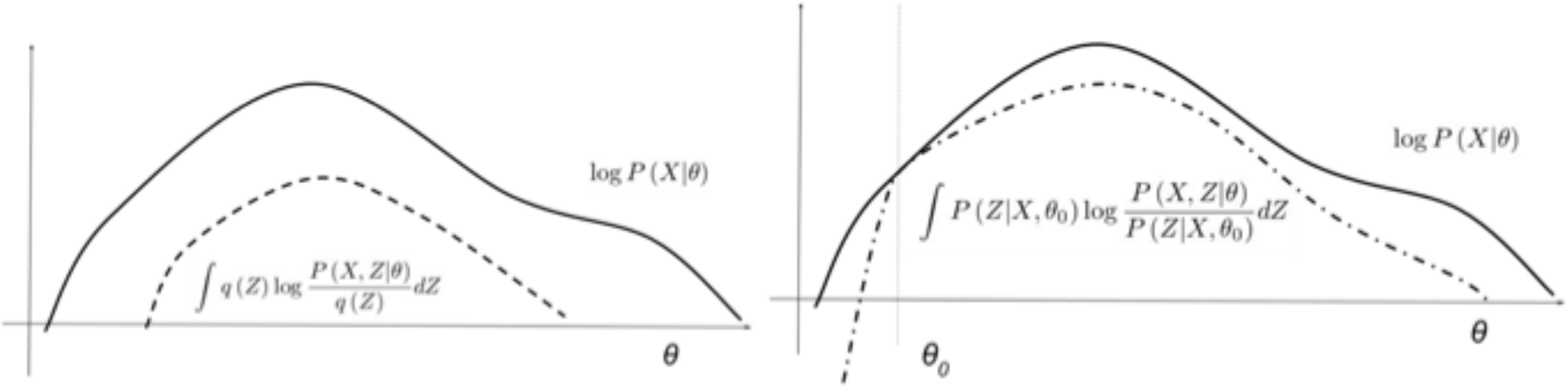


Credit: Slide from R. Giordano

Jensen Equality

- This can be equality if $q(Z) = p(Z|X,\theta_0)$, but only at $\theta = \theta_0$

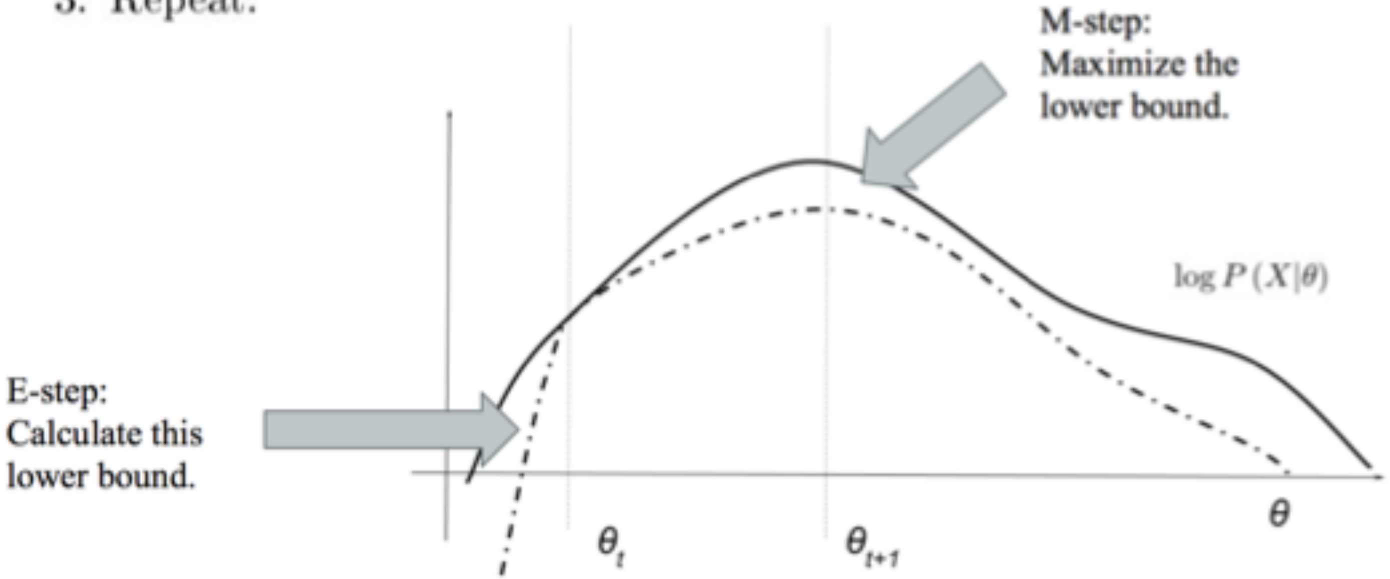
$$\int P(Z|X,\theta_0)\log\frac{P(X,Z|\theta_0)}{P(Z|X,\theta_0)}dZ = \int P(Z|X,\theta_0)\log\frac{P(X,Z|\theta_0)\,P(X|\theta_0)}{P(X,Z|\theta_0)}dZ$$
$$= \log P(X|\theta_0)\int P(Z|X,\theta_0)\,dZ = \log P(X|\theta_0)$$



- Suppose we want to determine MLE/MAP of $p(X|\theta)$ or $p(\theta|X)$ over q: this suggests a strategy is to maximize over θ given previous solution

EM Algorithm

1. E-step: Starting at θ_t, calculate the expectation $E(\theta) = \int P(Z|X, \theta_t) \log P(X, Z|\theta)\, dZ$
2. M-step: Optimize $\theta_{t+1} = \text{argsup} E(\theta)$
3. Repeat.

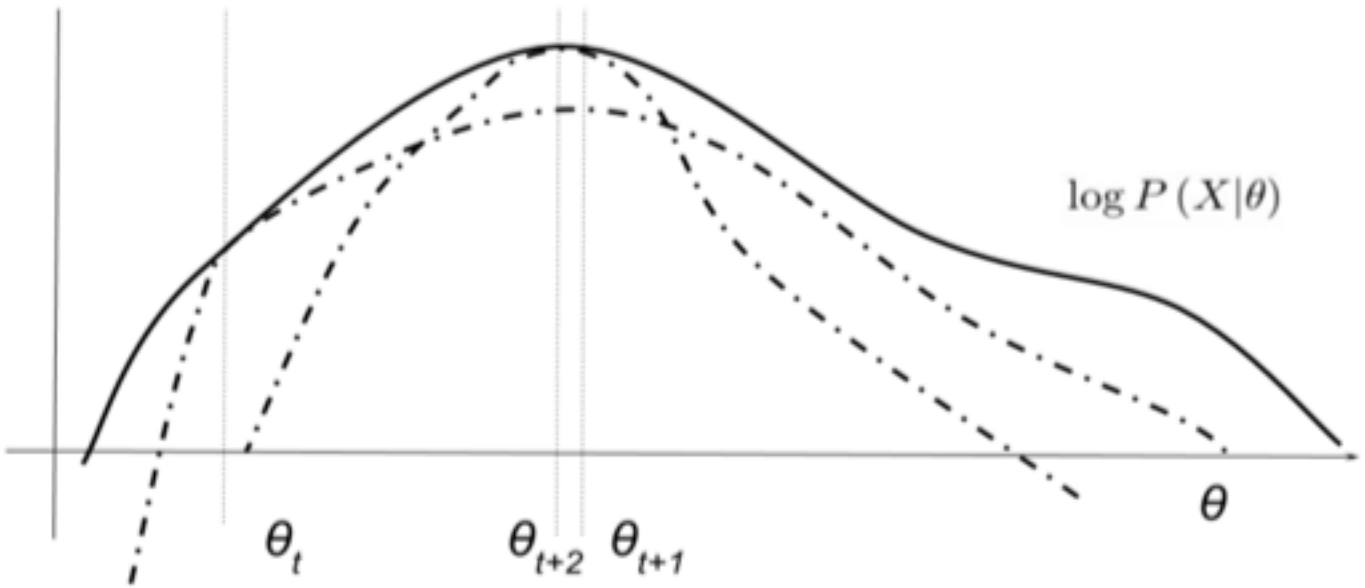


Generalized EM: if M is unsolvable then instead of maximization over θ make any move in the direction of increasing the value (similar to NL optimizations)

Guaranteed to work

This is guaranteed to increase the marginal likelihood $\log P(\theta|X)$ since

$$\sup_\theta \int P(Z|X,\theta_t) \log P(X,Z|\theta)\, dZ = \sup_\theta \int P(Z|X,\theta_t) \log \frac{P(X,Z|\theta)}{P(Z|X,\theta_t)} dZ$$
$$\geq \int P(Z|X,\theta_t) \log \frac{P(X,Z|\theta_t)}{P(Z|X,\theta_t)} dZ = \log P(\theta_t|X)$$



Often rapid convergence if good starting point
Note however that it solves an optimization problem: finds the nearest local maximum

Why is it useful?

- Two reasons: performs marginalization over latent parameters and avoids evaluating the normalizations

$$\sup_\theta \int P\left(Z|X,\theta_t\right) \log P\left(X,Z|\theta\right) dZ$$

Conditionals are simpler than marginals

Log probabilities are simpler than probabilities (no Z in the normalizing constant!)

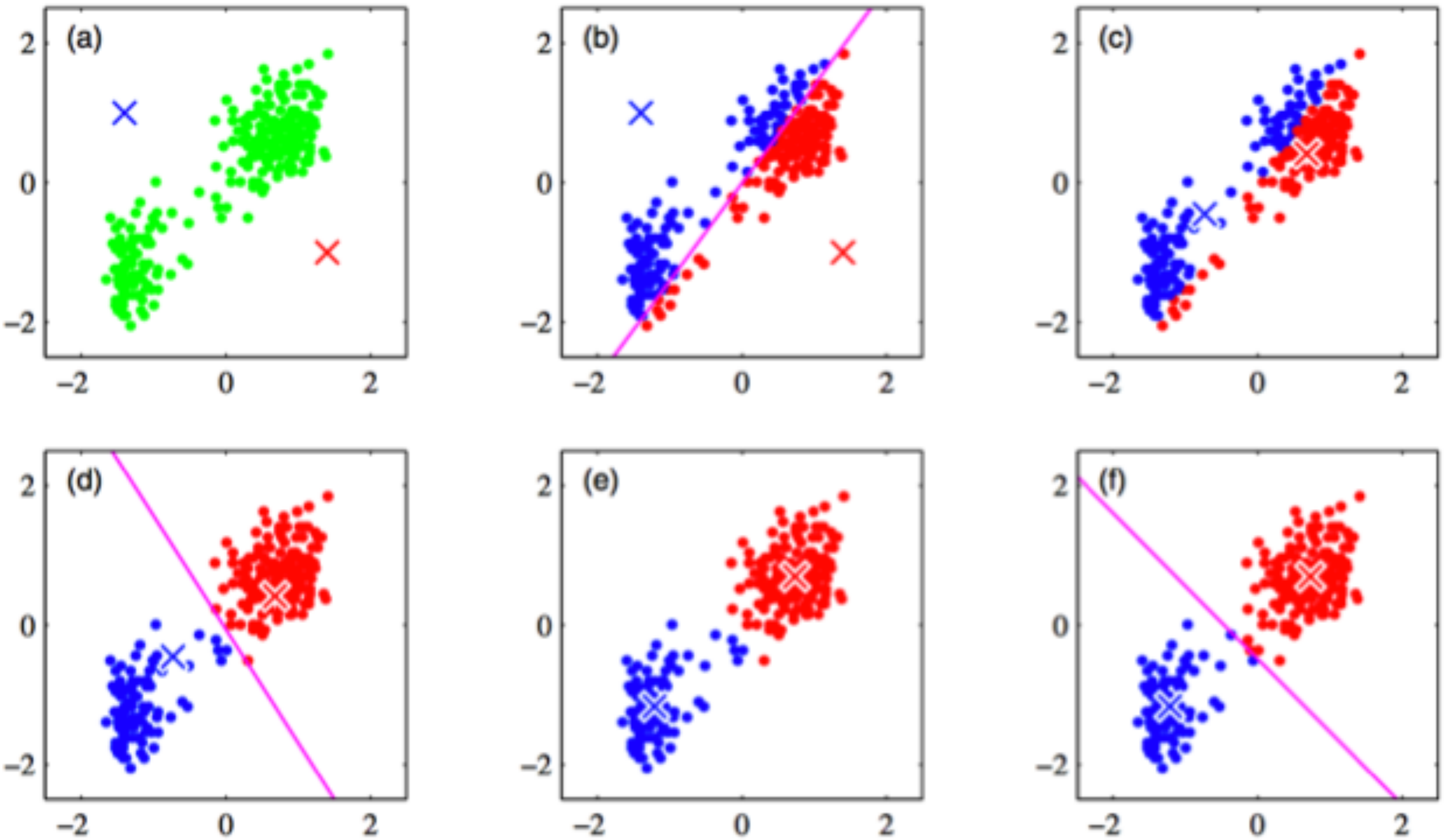
- However, it only gives MLE/MAP
- Extension called supplemented EM evaluates curvature matrix at MLE/MAP (see Gelman etal)

Cluster Classification: K-means

- Before looking at EM let's look at a non-probabilistic approach called K-means clustering
- We have N observations x_n and each x_n is in D-dimensions
- We want to partition it into K clusters
- Let's assume they are given simply by K means μ_k representing cluster centers
- We can define loss or objective function $J = \Sigma_n \Sigma_k r_{nk}(x_n - \mu_n)^2$ where $r_{nk} = 1$ for one k and $r_{nj} = 0$ for $j \neq k$, so that each data point is assigned to a single cluster k.
- Optimizing J for r_{nk} gives us $r_{nk} = 1$ for whichever k minimizes the distance $(x_n - \mu_k)^2$, set $r_{nj} = 0$ for $j \neq k$. This is the expectation part in EM language.
- Optimizing J for μ_k at fixed r_{nk} we take a derivative of J wrt μ_k which gives $\mu_k = \Sigma_n r_{nk} x_n / (\Sigma_n r_{nk})$. This is M part. Repeat.

Example (Bishop Chap. 9)

- Random starting μ_k (crosses). Magenta line is the cluster divider



Gaussian Mixture with Latent Variables

- We have seen GM before: $p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$

- Now we also introduce a latent variable z_{nk} playing the role of r_{nk}, i.e. for each n one is 1 and the other K-1 are 0. The marginal distribution is $p(z_k=1) = \pi_k$, where $\Sigma_k \pi_k = 1$ and $0 \leq \pi_k \leq 1$. Conditional of x given $z_k=1$ is a gaussian

$$p(\mathbf{x}|z_k = 1) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

$$p(\mathbf{z}) = \prod_{k=1}^{K} \pi_k^{z_k} \qquad p(\mathbf{x}|\mathbf{z}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_k}$$

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{z}) p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

More variables make it easier

- We have defined latent variables z we want to marginalize over. Advantage is that we can work with *p(x,z)* rather than *p(x)*. Lesson: adding many parameters sometimes makes the problem easier.
- We also need responsibility $\gamma(z_k) = p(z_k=1|x)$, using Bayes
- Here π_k is prior for $p(z_k=1)$, $\gamma(z_k)$ is posterior given x

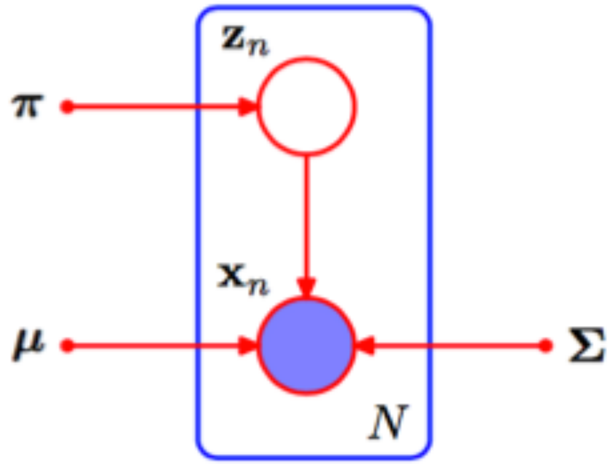
$$
\begin{aligned}
\gamma(z_k) \equiv p(z_k = 1|\mathbf{x}) &= \frac{p(z_k = 1)p(\mathbf{x}|z_k = 1)}{\sum_{j=1}^{K} p(z_j = 1)p(\mathbf{x}|z_j = 1)} \\
&= \frac{\pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}.
\end{aligned}
$$

Mixture Models

- We want to solve

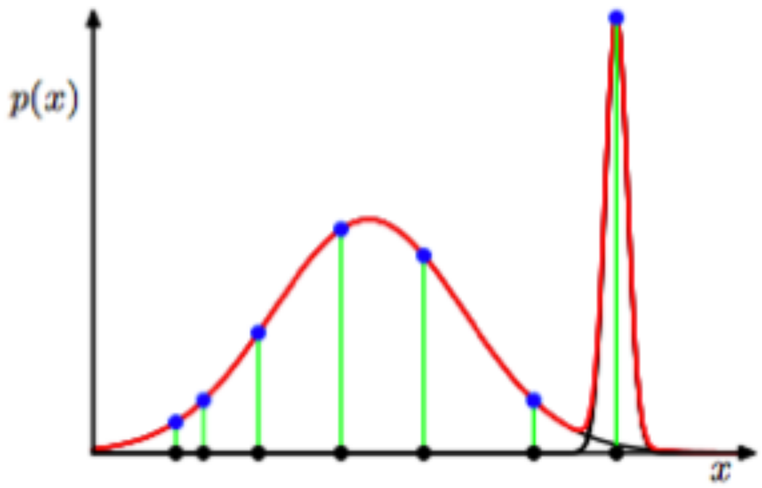
$$\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

- This could have been solved with optimization.
- Instead we solve it with latent variables *z*
- Graphical model



Beware of pitfalls of GM models

- Collapse onto a point: 2^{nd} Gaussian can simply decide to fit a single point with infinitely small error



- Identifiability: there are K! equivalent solutions since we can swap their identities. No big deal, EM will give us one of them.

EM Solution

$$\boldsymbol{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n$$

$$\ln p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}) = \sum_{n=1}^{N}\ln\left\{\sum_{k=1}^{K}\pi_k\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\}$$

$$N_k = \sum_{n=1}^{N}\gamma(z_{nk}).$$

- Take derivative wrt μ_k : $0 = -\sum_{n=1}^{N}\underbrace{\frac{\pi_k\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_j \pi_j\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)}}_{\gamma(z_{nk})}\boldsymbol{\Sigma}_k(\mathbf{x}_n-\boldsymbol{\mu}_k)$
- Derivative wrt Σ_k : $\boldsymbol{\Sigma}_k = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})(\mathbf{x}_n-\boldsymbol{\mu}_k)(\mathbf{x}_n-\boldsymbol{\mu}_k)^{\mathrm{T}}$
- Derivative wrt π_k subject to Lagrange multiplier due to $\Sigma_k \pi_k = 1$ constraint

$$\ln p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}) + \lambda\left(\sum_{k=1}^{K}\pi_k - 1\right)$$

- Gives $0 = \sum_{n=1}^{N}\frac{\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_j \pi_j\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)} + \lambda$. So $\lambda = -N$ and $\pi_k = \frac{N_k}{N}$

Summarizing EM for Gaussian Mixtures

- Iterative, needs more iterations than K-means
- Note that K-means is EM in the limit of variance Σ constant and going to 0

1. Initialize the means $\boldsymbol{\mu}_k$, covariances $\boldsymbol{\Sigma}_k$ and mixing coefficients π_k, and evaluate the initial value of the log likelihood.
2. **E step**. Evaluate the responsibilities using the current parameter values

$$\gamma(z_{nk}) = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_{j=1}^{K} \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}. \tag{9.23}$$

Summarizing EM for Gaussian Mixtures

3. **M step**. Re-estimate the parameters using the current responsibilities

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\mathbf{x}_n \tag{9.24}$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k}\sum_{n=1}^{N}\gamma(z_{nk})\left(\mathbf{x}_n-\boldsymbol{\mu}_k^{\text{new}}\right)\left(\mathbf{x}_n-\boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}} \tag{9.25}$$

$$\pi_k^{\text{new}} = \frac{N_k}{N} \tag{9.26}$$

where

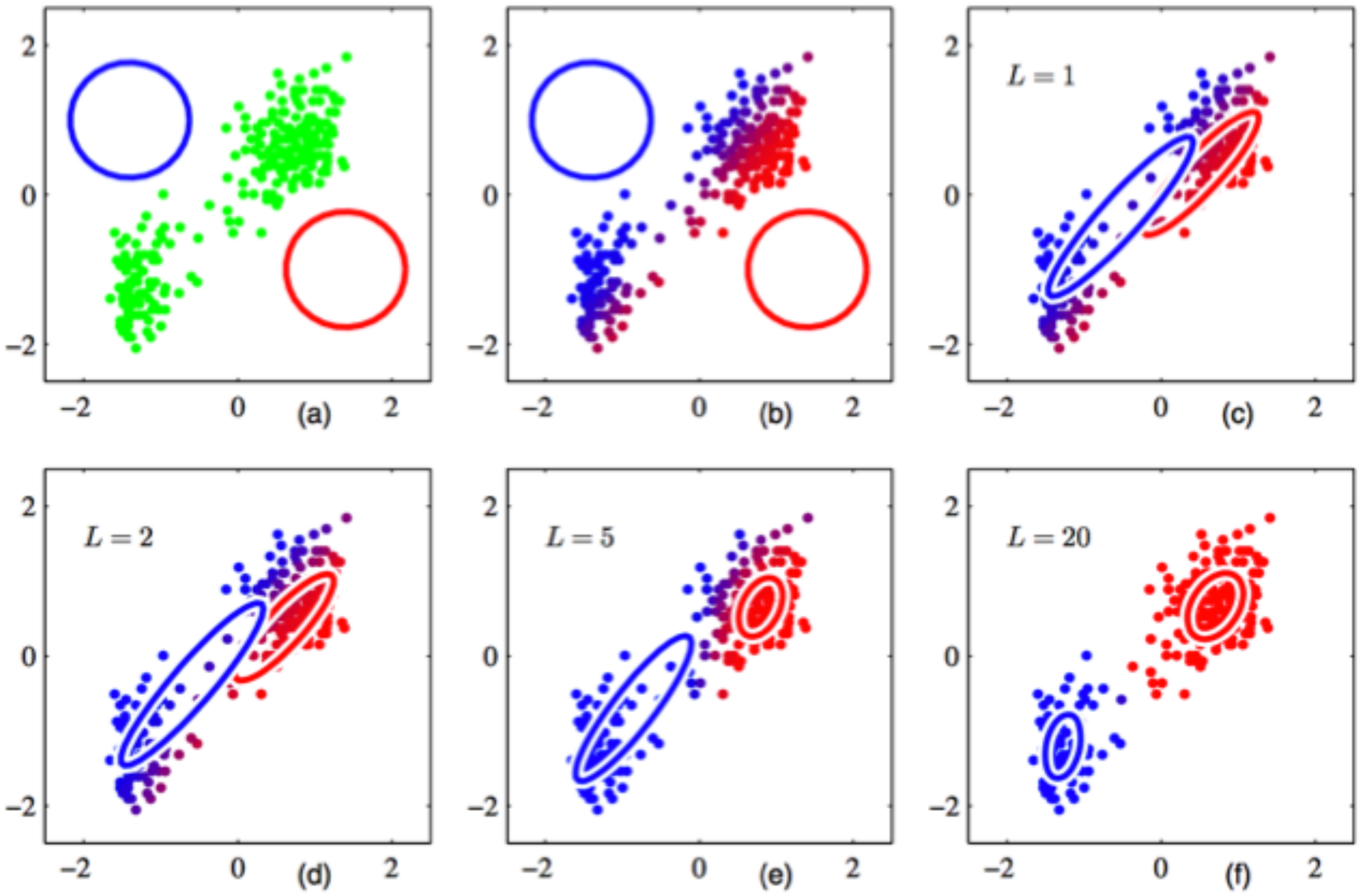
$$N_k = \sum_{n=1}^{N}\gamma(z_{nk}). \tag{9.27}$$

4. Evaluate the log likelihood

$$\ln p(\mathbf{X}|\boldsymbol{\mu},\boldsymbol{\Sigma},\boldsymbol{\pi}) = \sum_{n=1}^{N}\ln\left\{\sum_{k=1}^{K}\pi_k\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\} \tag{9.28}$$

and check for convergence of either the parameters or the log likelihood. If the convergence criterion is not satisfied return to step 2.

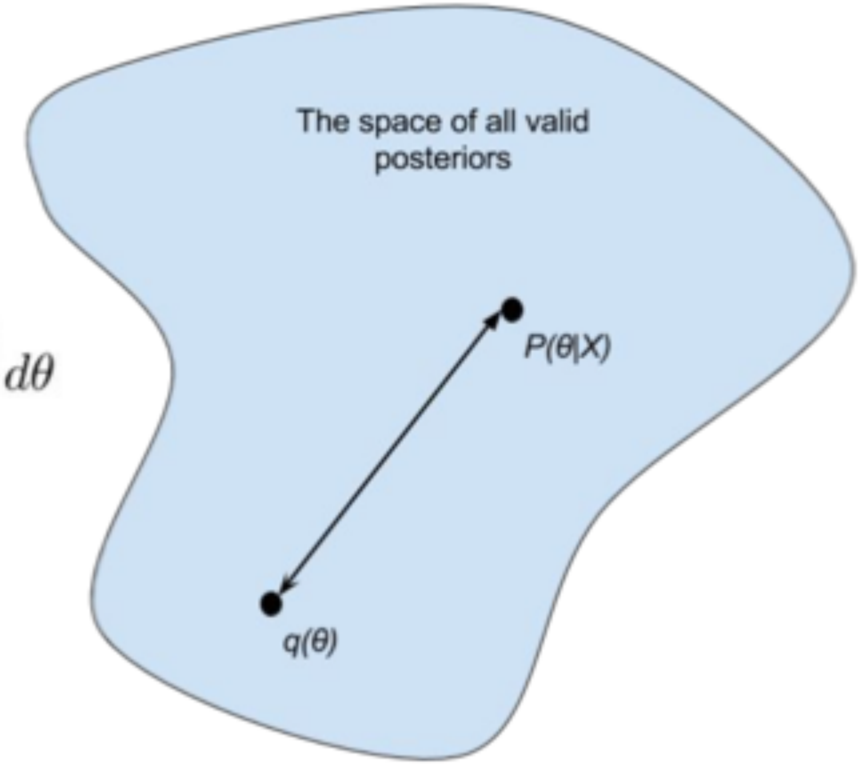
Example (same as before)



Variational Inference/ Bayes

- We want to approximate the posterior $P(\theta|X)$ using simple distributions $q(\theta)$ that are analytically tractable
- We do this by minimizing KL divergence

$$KL\left(q\left(\theta\right)||P\left(\theta|X\right)\right)=\int q\left(\theta\right)\log\frac{P\left(\theta|X\right)}{q\left(\theta\right)}d\theta$$



Slides credit from here to end of lecture : R. Giordano

Why is this useful?

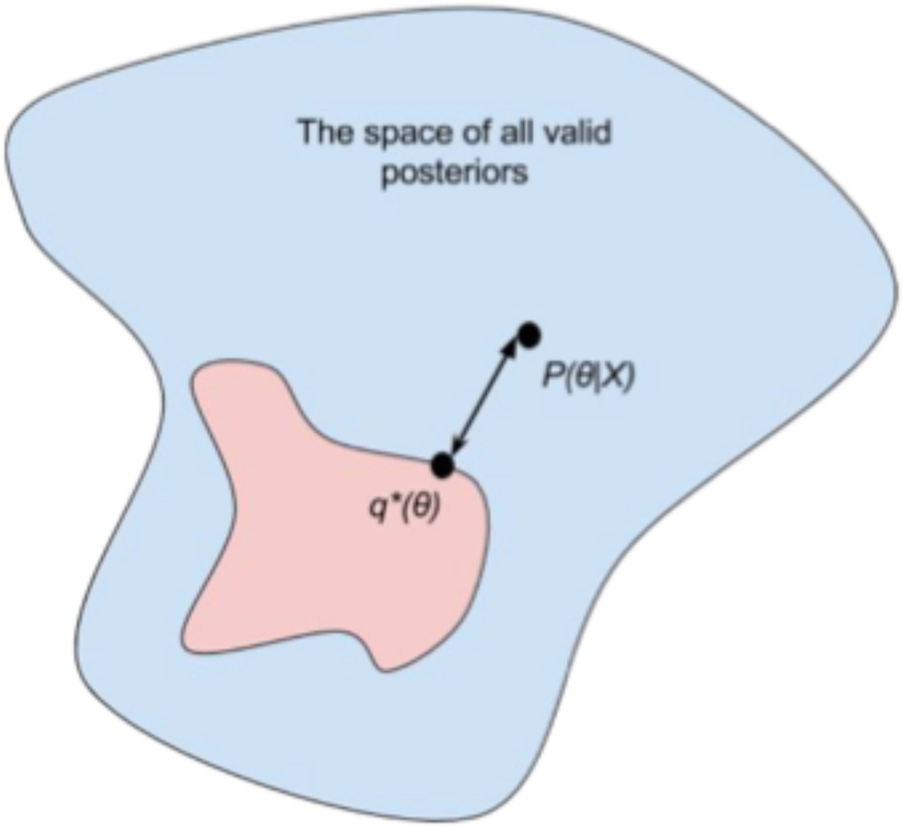
- We do not know the normalizing integral constant of *P(θ|X)* but we know it for *q(θ)*

$$
\begin{aligned}
P\left(\theta|X\right) &= \mathrm{argmin_q} KL\left(q\left(\theta\right)||P\left(\theta|X\right)\right) \\
&= \mathrm{argmin_q} \int q\left(\theta\right) \log \frac{q\left(\theta\right)}{P\left(\theta|X\right)} d\theta \\
&= \mathrm{argmin_q} \left\{ \int q\left(\theta\right) \log q\left(\theta\right) d\theta - \int q\left(\theta\right) \log P\left(\theta, X\right) P\left(\theta\right) d\theta - P\left(X\right) \right\} \\
&= \mathrm{argmax_q} \left\{ \underbrace{- \int q\left(\theta\right) \log q\left(\theta\right) d\theta}_{\text{Entropy of approximation}} + \underbrace{\int q\left(\theta\right) \log P\left(\theta, X\right) P\left(\theta\right) d\theta}_{\text{Data fit (without the normalizing constant!)}} \right\}
\end{aligned}
$$

We limit $q(\theta)$ to tractable distributions

- Entropies are hard to compute except for tractable distributions
- We find $q^*(q)$ that minimizes KL distance in this space
- Mean field approach:

$$\mathcal{Q} = \left\{ q(\theta) = \prod_k q(\theta_k) \right\}$$



Bivariate Gaussian Example

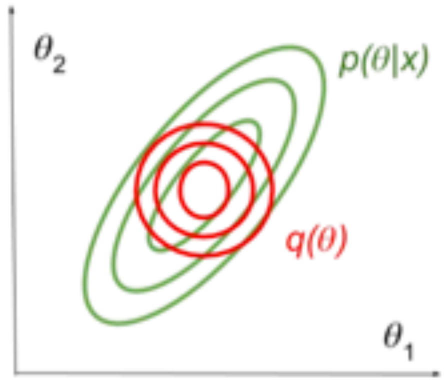
- MFVB does a good job at finding the mean
- MFVB does not describe correlations and tends to underestimate the variance

$$\mathcal{Q} = \left\{ q(\theta) = \mathcal{N}\left(\theta_1; \mu_1, \sigma_1^2\right) \mathcal{N}\left(\theta_2; \mu_2, \sigma_2^2\right) \right\}$$

$$\eta_1 = \left(\mu_1, \sigma_1^2\right)$$

$$\eta_2 = \left(\mu_2, \sigma_2^2\right)$$

$$\eta = \left(\mu_1, \sigma_1^2, \mu_2, \sigma_2^2\right)$$

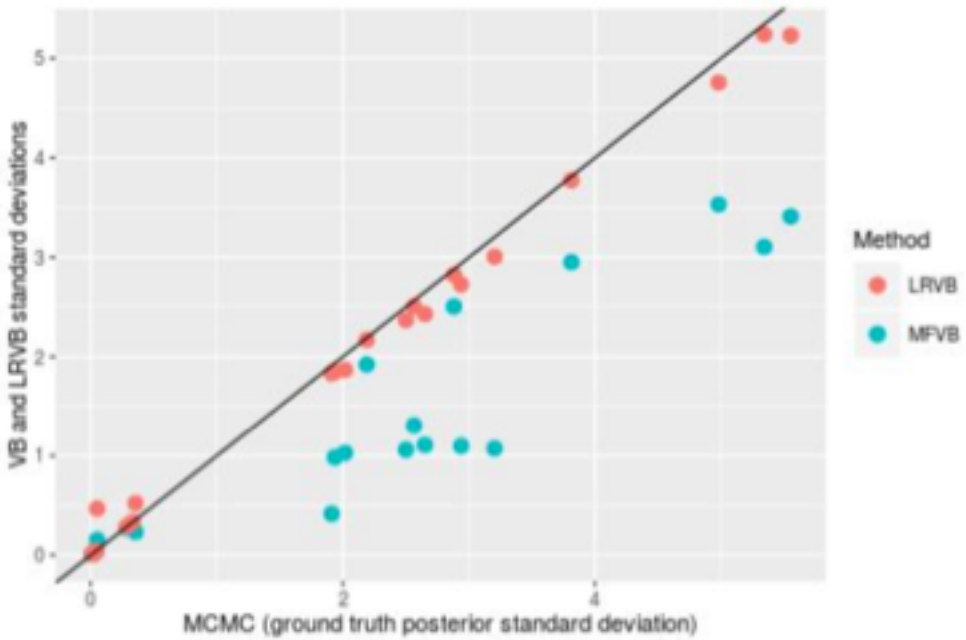


VB and EM

- EM can be viewed as a special case of VB where $q(\theta,Z) = \delta(\theta-\theta_0)q(Z)$
- E step: update $q(Z)$ keeping θ_0 fixed
- M step: update θ_0 at fixed Z

Why use (or not) VB?

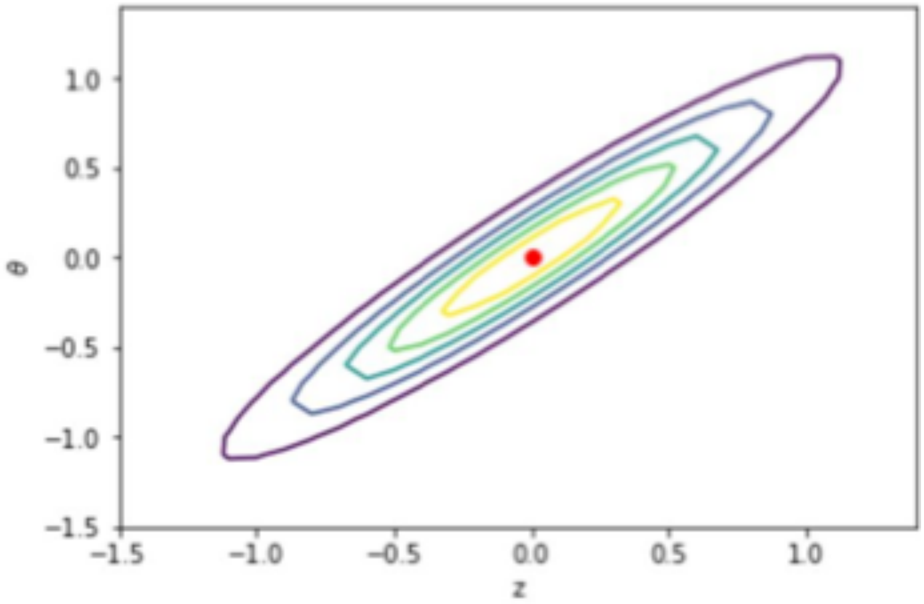
- Very fast compared to MCMC
- Typically gives good means
- Mean field often fails on variance
- Recent developments (ADVI, LRVB) improve on MFVB variance, but still no full posteriors

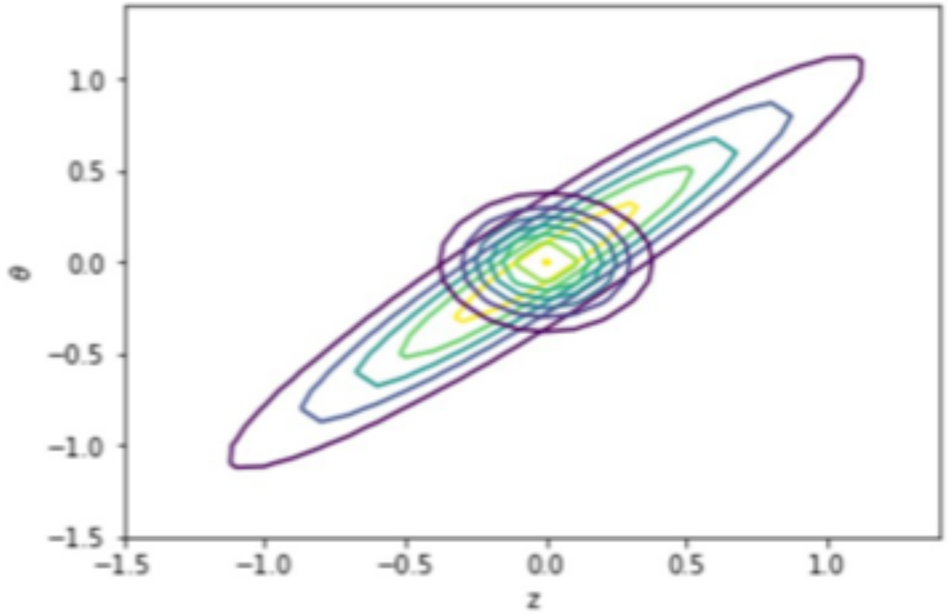


Example: MAP/Laplace vs. MFVB

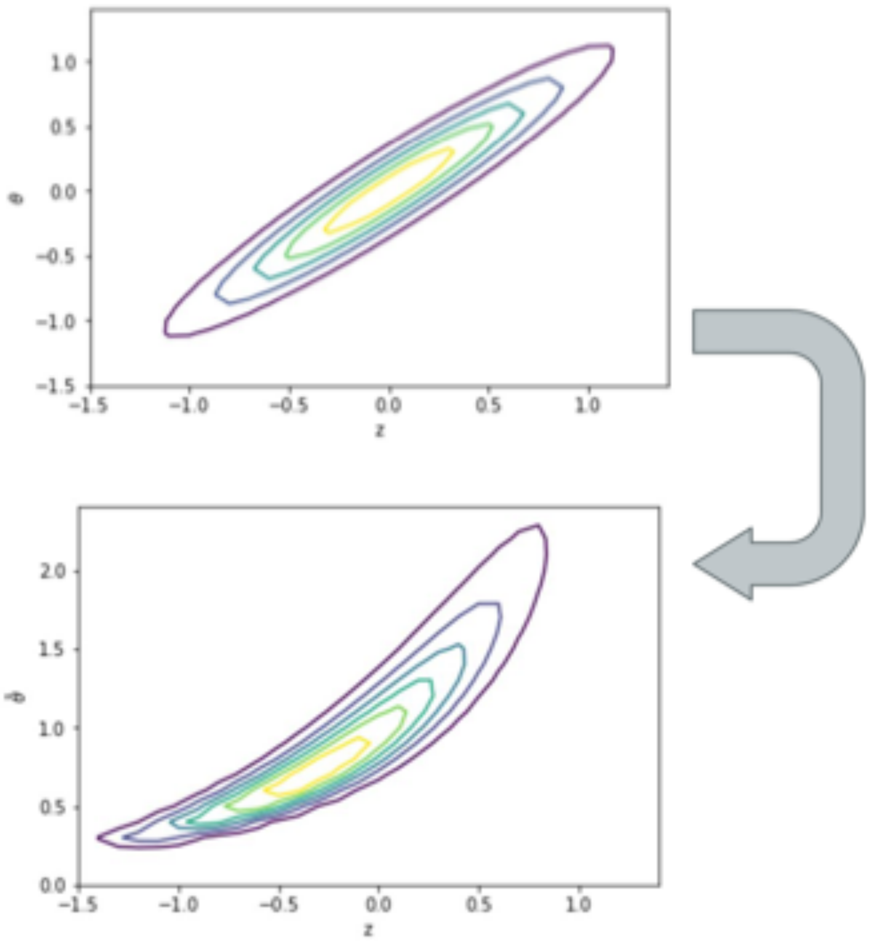
- On a multivariate Gaussian

MAP+Laplace beats MFVB





Example: bad banana



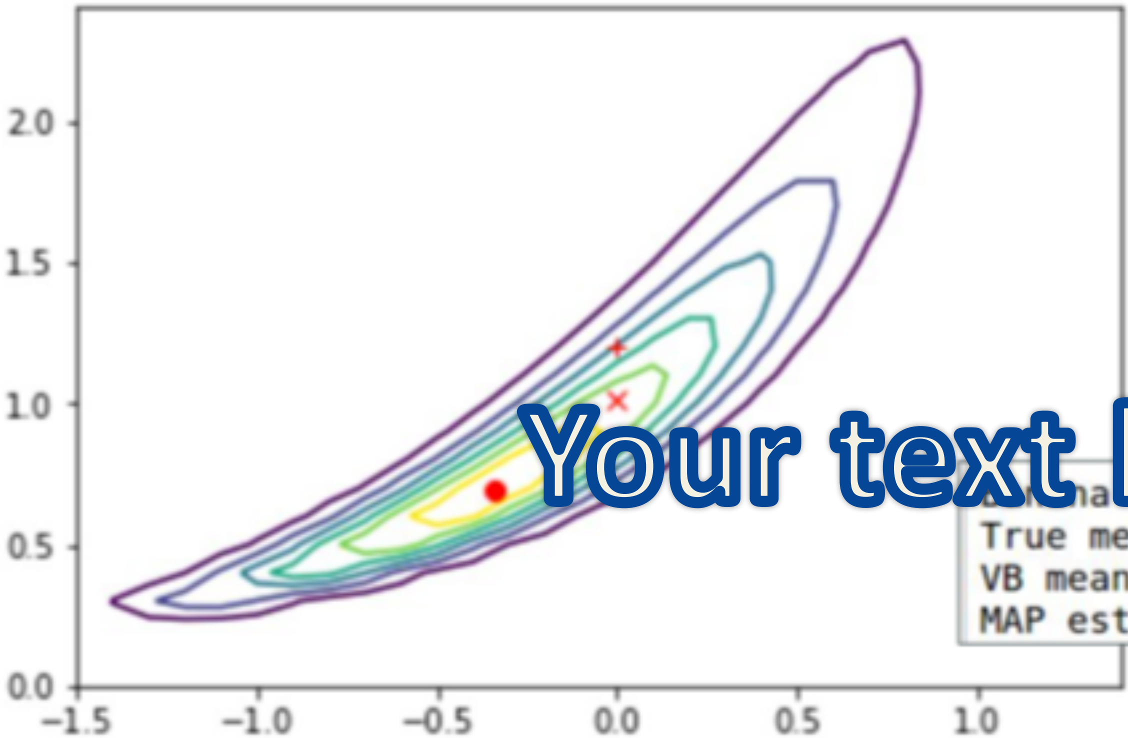
Suppose we instead had modeled

$$\tilde{\theta} = \exp(\theta)$$

$$P_{\tilde{\theta},z}\left(\tilde{\theta}, z\right) = P_{\theta,z}\left(\log\tilde{\theta}, z\right)\frac{d\theta}{d\tilde{\theta}}$$
$$= P_{\theta,z}\left(\log\tilde{\theta}, z\right)\exp(-\theta)$$

In $\left(\tilde{\theta}, Z\right)$ space the problem is not as easy.

Both MAP and MFVB get mean wrong



- o: The MAP
- +: The posterior mean
- x: The MFVB estimate

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... theta tilde:
True mean:              1.19721736312
VB mean:                1.01770490612
MAP estimate:           0.697601425656
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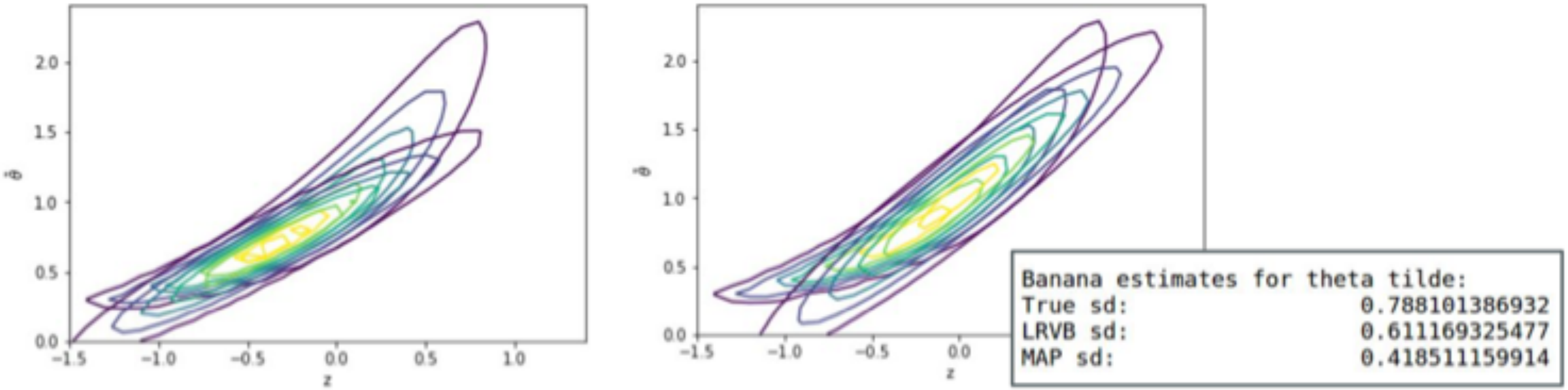
- MFVB is better than MAP on the mean

Covariances for MAP can also be wrong, but so are for MFVB and LRVB



Neyman-Scott "Paradox"

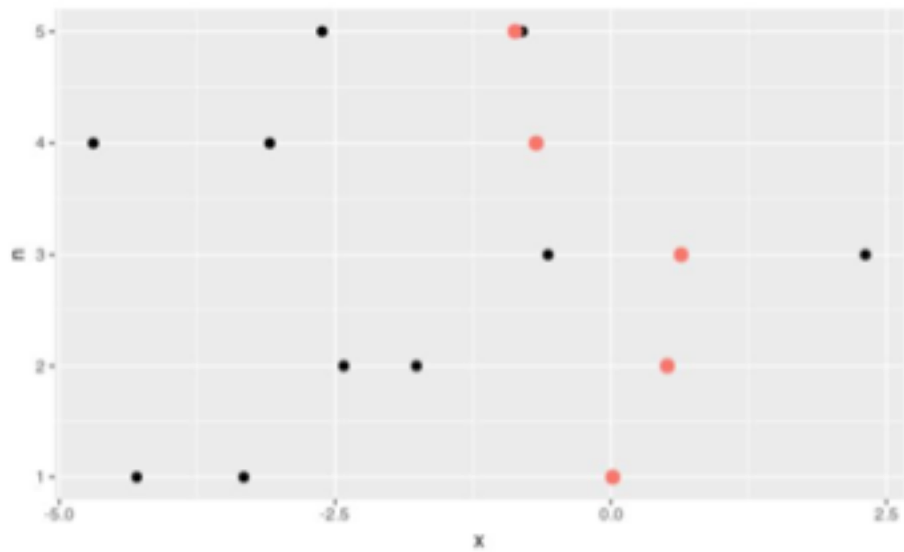
- Setup: we have N experiments, each measures $M = 2$ data X_{1n}, X_{2n}. Experiments are trying to determine the variance θ. However, there is an unknown mean offset for each experiment z_n.

For $n = 1, \ldots, N$

$$X_{1n} \sim \mathcal{N}(z_n, \theta)$$

$$X_{2n} \sim \mathcal{N}(z_n, \theta)$$

We will investigate the "joint maximum likelihood estimator".



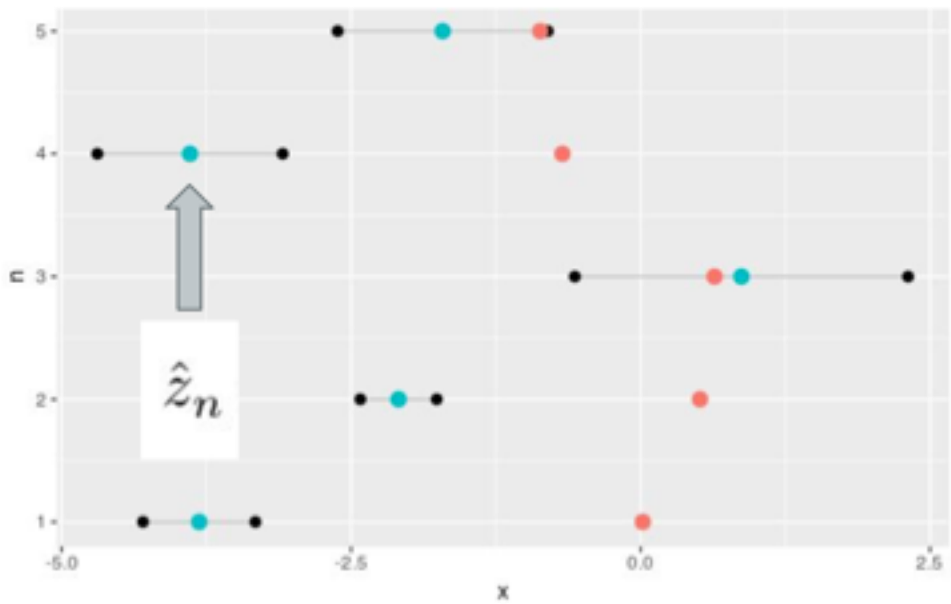
Means are easy enough

For $n = 1, ..., N$

$$X_{1n} \sim \mathcal{N}(z_n, \theta)$$
$$X_{2n} \sim \mathcal{N}(z_n, \theta)$$

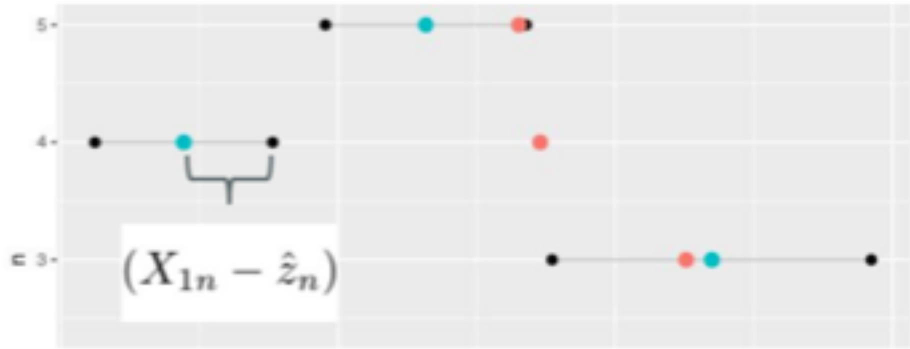
Irrespective of θ,

$$\hat{z}_n = \text{argmax}_{z_n} P(X_{1n}, X_{2n} | z_n, \theta) = \frac{X_{1n} + X_{2n}}{2}$$



How about variance θ?

$$\hat{z}_n = \frac{X_{1n} + X_{2n}}{2}$$



$$\begin{aligned}\hat{\theta} &= \text{argmax}_\theta P\left(X_{1n}, X_{2n} | \hat{z}_n, \theta\right) \\ &= \frac{1}{2}\left(\frac{1}{N}\sum_n \left(X_{1n} - \hat{z}_n\right)^2 + \frac{1}{N}\sum_n \left(X_{2n} - \hat{z}_n\right)^2\right) \\ &= \frac{1}{4N}\sum_n \left(X_{1n} - X_{2n}\right)^2\end{aligned}$$

- In intro labs/statistics courses we learn that the variance is computed from mean square distance of each point from mean divided by number of measurements *M* (here 2) if mean is known and divided by *M-1* (here 1) if unknown. Where did it come from?

Even for large *N*, MLE is biased for low *M* by *M*/(*M*-1) (=2 here)

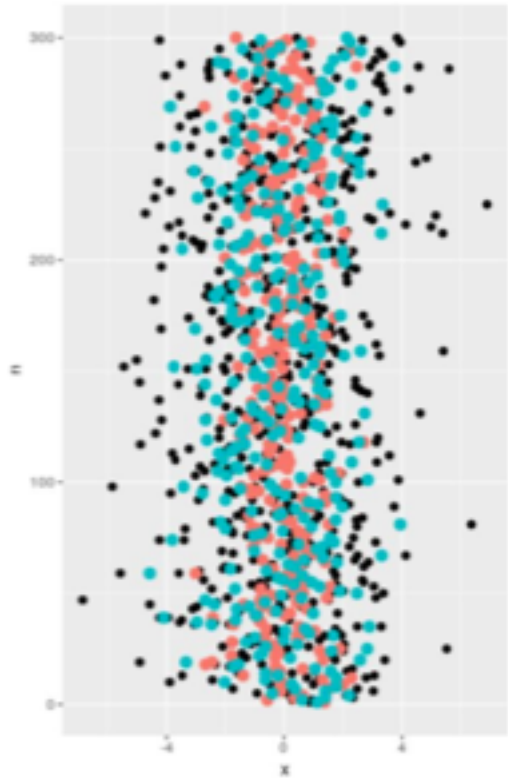
$$\hat{z}_n = \frac{X_{1n} + X_{2n}}{2} \qquad \hat{\theta} = \frac{1}{4N}\sum_n (X_{1n} - X_{2n})^2$$

What does our estimate converge to as we get more data?

$$\mathbb{E}\left[(X_{1n} - X_{2n})^2\right] = \mathbb{E}\left[\mathbb{E}\left[(X_{1n} - X_{2n})^2 \,|z_n\right]\right] = 2\theta$$

So

$$\hat{\theta} \xrightarrow[n\to\infty]{} \frac{1}{4}2\theta = \frac{\theta}{2} \neq \theta$$



- We failed to account for uncertainty in mean z_n: we only measure it from 2 data points
- We need to marginalize over z_n

MAP/MLE vs. Bayes

- We see that MAP/MLE is strongly biased here even in large N limit: one has to be careful with asymptotics theorems
- Full Bayesian analysis (e.g. MCMC) gives posterior of θ marginalized over z_n and automatically takes care of the problem. Bayesian analysis gives correct answer, i.e. it gives $M/(M-1)$ correction without "thinking".
- EM also solves this problem correctly: it gives point estimator of θ averaging over z_n. So frequentist analyses that perform marginals over latent variables can also be correct "without thinking" (or without simulations telling us there is a problem).
- VB solves it too, and converges to the correct answer
- Lesson: sometimes we need to account for uncertainty in latent variables by marginalizing over them, even if we just want point estimators

Summary

- MCMC is great, but slow
- EM is a point estimator (like MAP/MLE) which marginalizes over latent variables
- Its Bayesian generalization is VB
- Both of these are able to perform marginalization and solve Neyman-Scott paradox, while MLE/MAP fails
- VB is not perfect and can provide wrong means or variances, and is never used for full posteriors

Literature

- *Bayesian Data Analysis,* Gelman et al. , Chapter 13
- D. Mackay, *Information Theory, Inference, and Learning Algorithms* (See course website), Chapter 33
- R. Giordano https://docs.google.com/presentation/d/1TZYdzn1jMQY8pCnZxmN6bgzm6jZCPzyg9MNwVldLP8k/edit