# Excurse: Exponential Families

**Definition:** A probability distribution $p$ over $\mathbf{x}$ is a member of the **exponential family** if it can be expressed as

$$p(\mathbf{x} \mid \boldsymbol{\eta}) = h(\mathbf{x})g(\boldsymbol{\eta})\exp(\boldsymbol{\eta}^T \mathbf{u}(\mathbf{x}))$$

where $\boldsymbol{\eta}$ are the **natural parameters** and

$$g(\boldsymbol{\eta}) = \left( \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^T \mathbf{u}(\mathbf{x})) d\mathbf{x} \right)^{-1}$$

is the normalizer.

$h$ and $\mathbf{u}$ are functions of $\mathbf{x}$.

# Exponential Families

Example: Bernoulli-Distribution with parameter $\mu$

$$
\begin{aligned}
p(x \mid \mu) &= \mu^x (1-\mu)^{1-x} \\
&= \exp(x \ln \mu + (1-x) \ln(1-\mu)) \\
&= \exp(x \ln \mu + \ln(1-\mu) - x \ln(1-\mu)) \\
&= (1-\mu) \exp(x \ln \mu - x \ln(1-\mu)) \\
&= (1-\mu) \exp\left(x \ln\left(\frac{\mu}{1-\mu}\right)\right)
\end{aligned}
$$

Thus, we can say

$$
\eta = \ln\left(\frac{\mu}{1-\mu}\right) \Rightarrow \quad \mu = \frac{1}{1+\exp(-\eta)} \Rightarrow 1-\mu = \frac{1}{1+\exp(\eta)} = g(\eta)
$$

# MLE for Exponential Families

From: $$g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^T \mathbf{u}(\mathbf{x})) d\mathbf{x} = 1$$

we get:

$$\nabla g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^T \mathbf{u}(\mathbf{x})) d\mathbf{x} + g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^T \mathbf{u}(\mathbf{x})) \mathbf{u}(\mathbf{x}) d\mathbf{x} = 0$$

$$\Rightarrow \; -\frac{\nabla g(\boldsymbol{\eta})}{g(\boldsymbol{\eta})} = g(\boldsymbol{\eta}) \int h(\mathbf{x}) \exp(\boldsymbol{\eta}^T \mathbf{u}(\mathbf{x})) \mathbf{u}(\mathbf{x}) d\mathbf{x} = \mathbb{E}[\mathbf{u}(\mathbf{x})]$$

which means that $-\nabla \ln g(\boldsymbol{\eta}) = \mathbb{E}[\mathbf{u}(\mathbf{x})]$

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Σu(x) is called the **sufficient statistics** of p.

# 11. Variational Inference: Expectation Propagation

# Expectation Propagation

In mean-field we minimized $\mathrm{KL}(q\|p)$. But: we can also minimize $\mathrm{KL}(p\|q)$. Assume $q$ is from the **exponential family**:

natural parameters

$$q(\mathbf{z}) = h(\mathbf{z})g(\boldsymbol{\eta})\exp(\boldsymbol{\eta}^T\mathbf{u}(\mathbf{z}))$$

normalizer

$$g(\boldsymbol{\eta})\int h(\mathbf{x})\exp(\boldsymbol{\eta}^T\mathbf{u}(\mathbf{z}))d\mathbf{x} = 1$$

Then we have:

$$\mathrm{KL}(p\|q) = -\int p(\mathbf{z})\log\frac{h(\mathbf{z})g(\boldsymbol{\eta})\exp(\boldsymbol{\eta}^T\mathbf{u}(\mathbf{z}))}{p(\mathbf{z})}$$

# Expectation Propagation

This results in $\mathrm{KL}(p\|q) = -\log g(\boldsymbol{\eta}) - \boldsymbol{\eta}^T \mathbb{E}_p[\mathbf{u}(\mathbf{x})] + \mathrm{const}$

We can minimize this with respect to $\boldsymbol{\eta}$

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which is equivalent to

$$\mathbb{E}_q[\mathbf{u}(\mathbf{x})] = \mathbb{E}_p[\mathbf{u}(\mathbf{x})]$$

Thus: the KL-divergence is minimal if the exp. sufficient statistics are the same between $p$ and $q$!

For example, if $q$ is Gaussian: $\mathbf{u}(x) = \begin{pmatrix} x \\ x^2 \end{pmatrix}$

Then, mean and covariance of $q$ must be the same as for $p$ (**moment matching**)

# Expectation Propagation

Assume we have a factorization $p(\mathcal{D}, \boldsymbol{\theta}) = \prod_{i=1}^{M} f_i(\boldsymbol{\theta})$

and we are interested in the posterior:

$$p(\boldsymbol{\theta} \mid \mathcal{D}) = \frac{1}{p(\mathcal{D})} \prod_{i=1}^{M} f_i(\boldsymbol{\theta})$$

we use an approximation $q(\boldsymbol{\theta}) = \frac{1}{Z} \prod_{i=1}^{M} \tilde{f}_i(\boldsymbol{\theta})$

Aim: minimize $\mathrm{KL}\left( \frac{1}{p(\mathcal{D})} \prod_{i=1}^{M} f_i(\boldsymbol{\theta}) \middle\| \frac{1}{Z} \prod_{i=1}^{M} \tilde{f}_i(\boldsymbol{\theta}) \right)$

**Idea:** optimize each of the approximating factors in turn, assume exponential family

# The EP Algorithm

- Given: a joint distribution over data and variables

$$p(\mathcal{D}, \boldsymbol{\theta}) = \prod_{i=1}^{M} f_i(\boldsymbol{\theta})$$

- Goal: approximate the posterior $p(\boldsymbol{\theta} \mid \mathcal{D})$ with $q$
- Initialize all approximating factors $\tilde{f}_i(\boldsymbol{\theta})$
- Initialize the posterior approximation $q(\boldsymbol{\theta}) \propto \prod_i \tilde{f}_i(\boldsymbol{\theta})$
- Do until convergence:
  - choose a factor $\tilde{f}_j(\boldsymbol{\theta})$
  - remove the factor from $q$ by division: $q^{\setminus j}(\boldsymbol{\theta}) = \dfrac{q(\boldsymbol{\theta})}{\tilde{f}_j(\boldsymbol{\theta})}$

# The EP Algorithm

- find $q^{\text{new}}$ that minimizes

$$\mathrm{KL}\left(\frac{f_j(\theta)q^{\setminus j}(\boldsymbol{\theta})}{Z_j}\middle|q^{\text{new}}(\boldsymbol{\theta})\right)$$

  using moment matching, including the zeroth order moment:

$$Z_j = \int q^{\setminus j}(\boldsymbol{\theta}) f_j(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

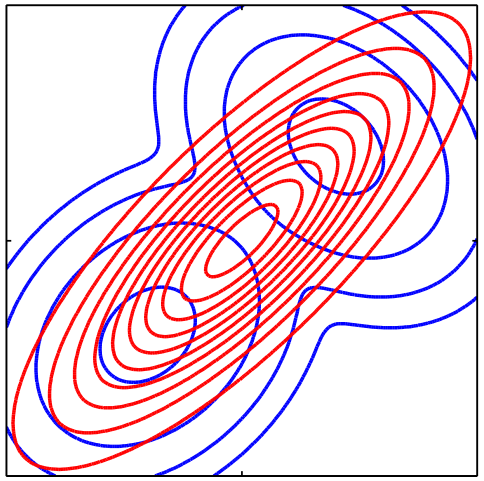
- evaluate the new factor

$$\tilde{f}_j(\boldsymbol{\theta}) = Z_j \frac{q^{\text{new}}(\boldsymbol{\theta})}{q^{\setminus j}(\boldsymbol{\theta})}$$

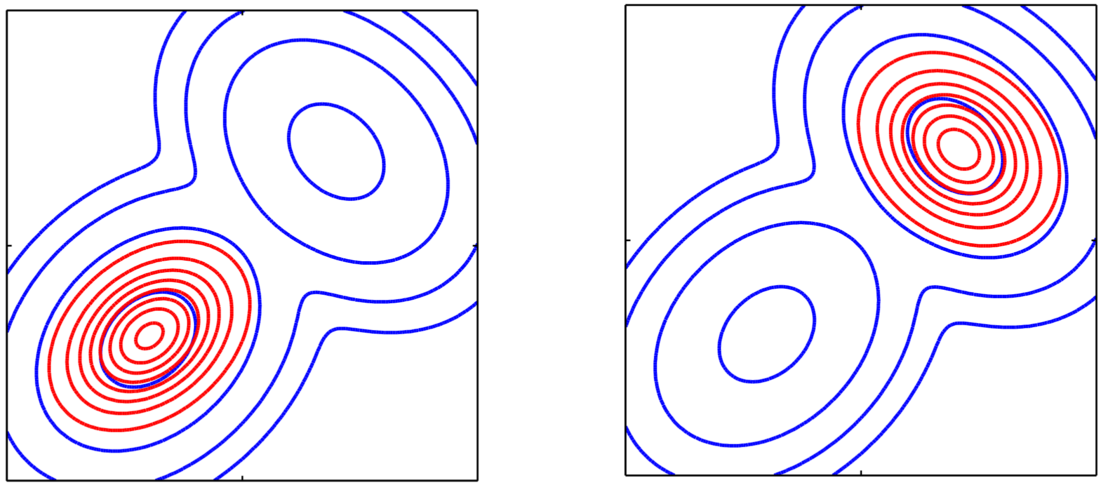
- After convergence, we have $p(\mathcal{D}) \approx \int \prod_i \tilde{f}_j(\boldsymbol{\theta}) d\boldsymbol{\theta}$

# Properties of EP

- There is no guarantee that the iterations will converge
- This is in contrast to variational Bayes, where iterations do not decrease the lower bound
- EP minimizes $KL(p\|q)$ where variational Bayes minimizes $KL(q\|p)$

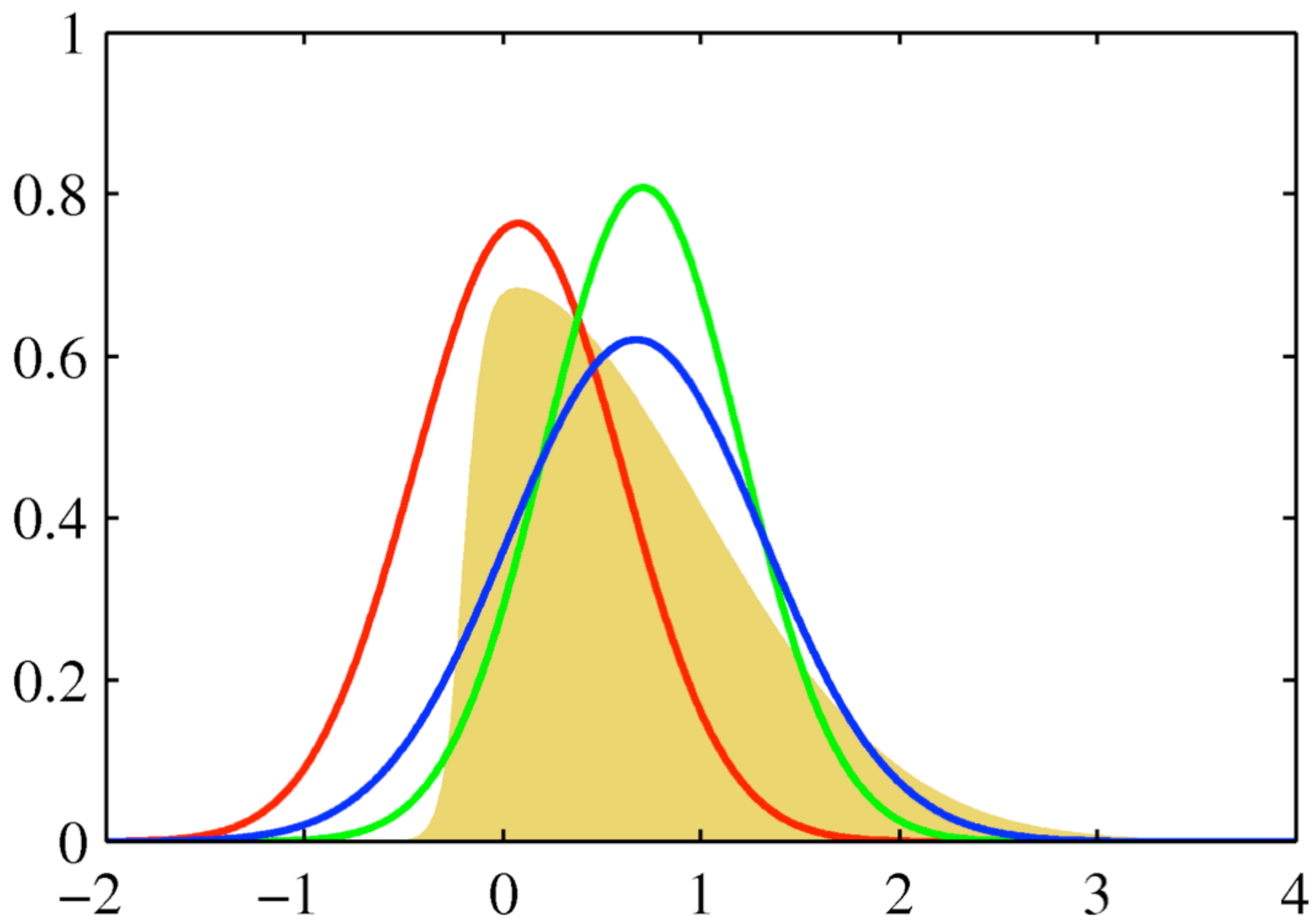


$KL(p\|q)$



$KL(q\|p)$

# Example



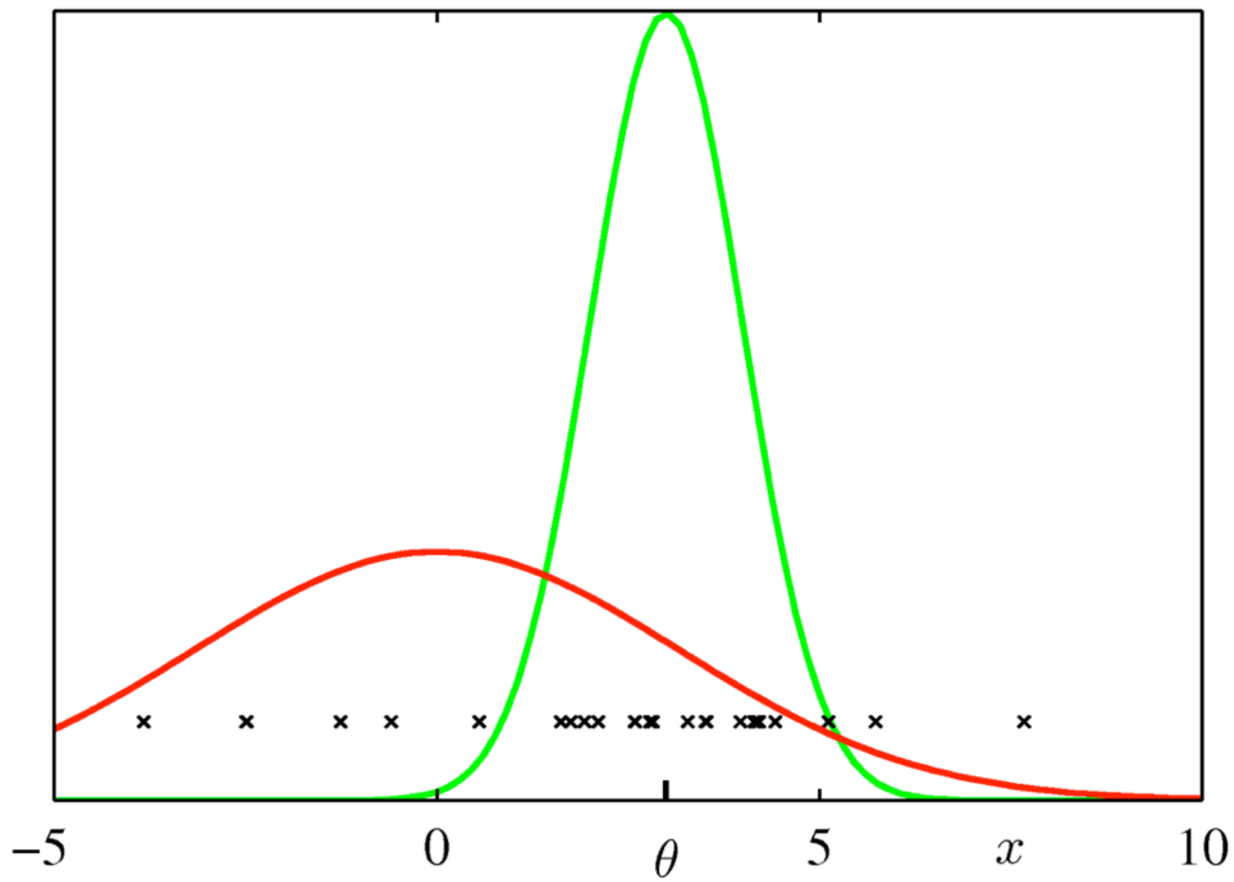

yellow: original distribution

red: Laplace approximation

green: global variation

blue: expectation-propagation

# The Clutter Problem




- Aim: fit a multivariate Gaussian into data in the presence of background clutter (also Gaussian)

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = (1-w)\mathcal{N}(\mathbf{x} \mid \boldsymbol{\theta}, I) + w\mathcal{N}(\mathbf{x} \mid \mathbf{0}, aI)$$

- The prior is Gaussian: $p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta} \mid \mathbf{0}, bI)$

# The Clutter Problem

The joint distribution for $\mathcal{D} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$ is

$$p(\mathcal{D}, \boldsymbol{\theta}) = p(\boldsymbol{\theta}) \prod_{n=1}^{N} p(\mathbf{x}_n \mid \boldsymbol{\theta})$$

this is a mixture of $2^N$ Gaussians! This is intractable for large $N$. Instead, we approximate it using a spherical Gaussian:

$$q(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta} \mid \mathbf{m}, vI) = \tilde{f}_0(\boldsymbol{\theta}) \prod_{n=1}^{N} \tilde{f}_n(\boldsymbol{\theta})$$

the factors are (unnormalized) Gaussians:

$$\tilde{f}_0(\boldsymbol{\theta}) = p(\boldsymbol{\theta}) \qquad \tilde{f}_n(\boldsymbol{\theta}) = s_n \mathcal{N}(\boldsymbol{\theta} \mid \mathbf{m}_n, v_n I)$$

# EP for the Clutter Problem

- First, we initialize $\tilde{f}_n(\boldsymbol{\theta}) = 1$, i.e. $q(\boldsymbol{\theta}) = p(\boldsymbol{\theta})$
- Iterate:
  - Remove the current estimate of $\tilde{f}_n(\boldsymbol{\theta})$ from $q$ by division of Gaussians:

$$q_{-n}(\boldsymbol{\theta}) = \frac{q(\boldsymbol{\theta})}{\tilde{f}_n(\boldsymbol{\theta})}$$

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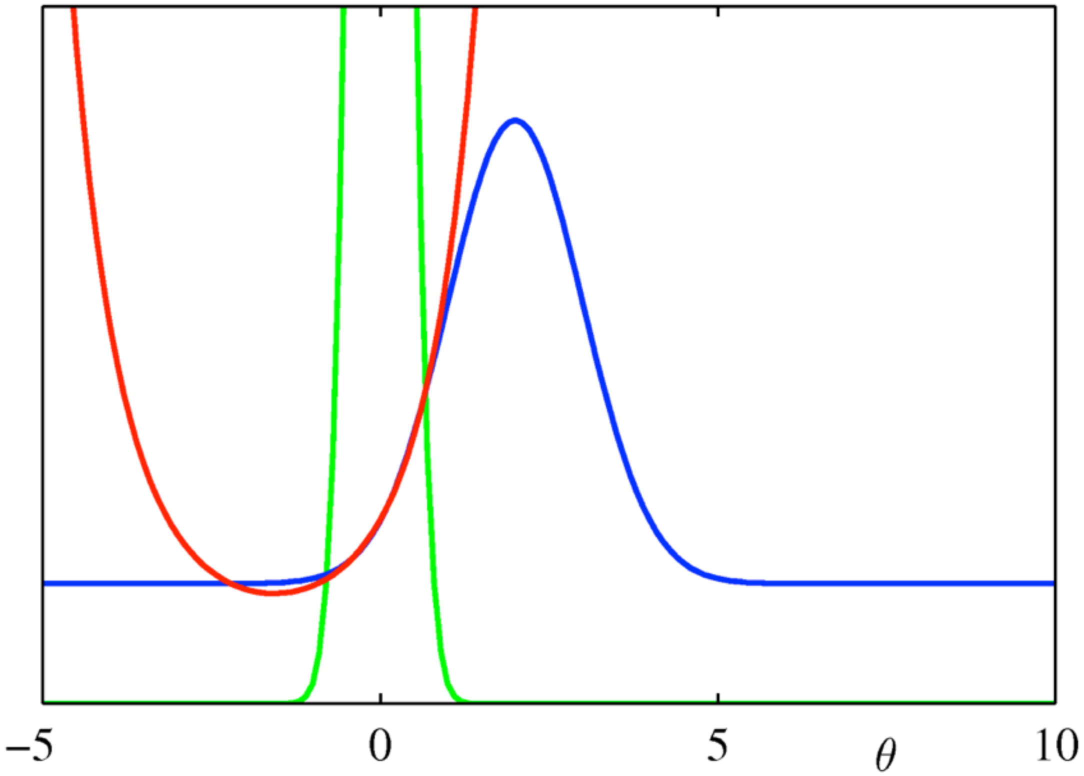
$$q_{-n}(\boldsymbol{\theta}) = \frac{q(\boldsymbol{\theta})}{\tilde{f}_n(\boldsymbol{\theta})} \qquad q_{-n}(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta} \mid \mathbf{m}_{-n}, v_{-n} I)$$

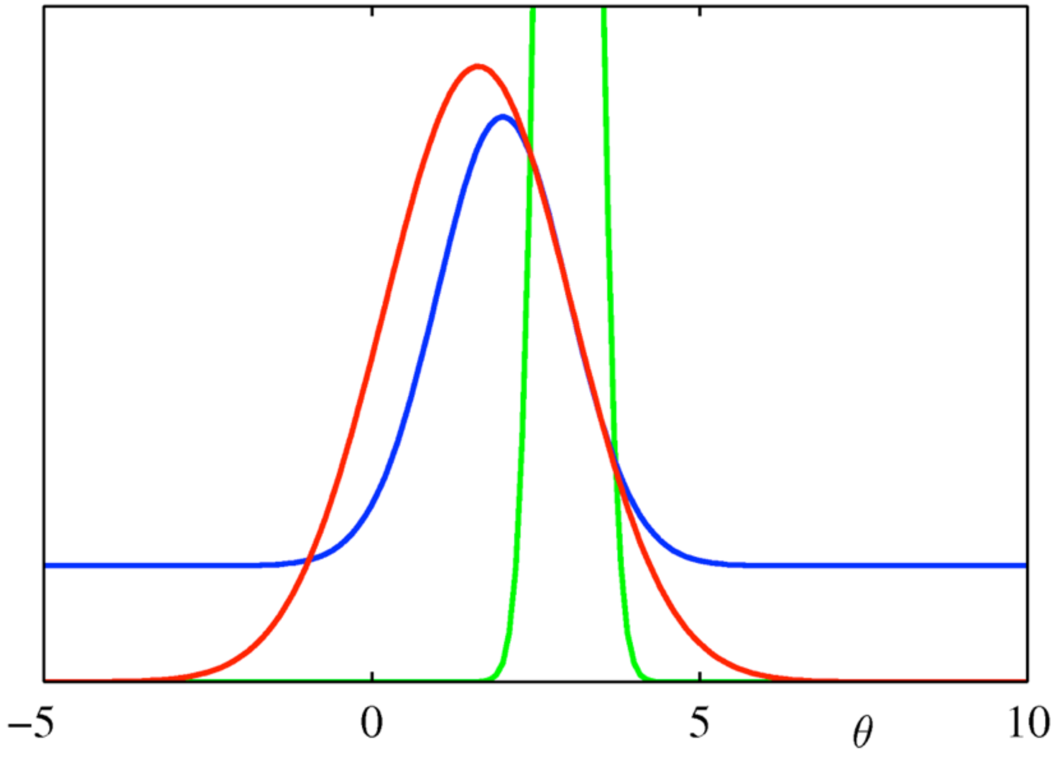
  - Compute the normalization constant:

$$Z_n = \int q_{-n}(\boldsymbol{\theta}) f_n(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

  - Compute mean and variance of $q^{\text{new}} = q_{-n}(\boldsymbol{\theta}) f_n(\boldsymbol{\theta})$
  - Update the factor $\tilde{f}_n(\boldsymbol{\theta}) = Z_n \frac{q^{\text{new}}(\boldsymbol{\theta})}{q_{-n}(\boldsymbol{\theta})}$

# A 1D Example




- blue: true factor $f_n(\boldsymbol{\theta})$
- red: approximate factor $\tilde{f}_n(\boldsymbol{\theta})$
- green: cavity distribution $q_{-n}(\boldsymbol{\theta})$

The form of $q_{-n}(\boldsymbol{\theta})$ controls the range over which $\tilde{f}_n(\boldsymbol{\theta})$ will be a good approximation of $f_n(\boldsymbol{\theta})$

# Summary

- Variational Inference uses approximation of functions so that the KL-divergence is minimal
- In mean-field theory, factors are optimized sequentially by taking the expectation over all other variables
- Variational inference for GMMs reduces the risk of overfitting; it is essentially an EM-like algorithm
- Expectation propagation minimizes the reverse KL-divergence of a single factor by moment matching; factors are in the exp. family