# Non-Gaussian likelihoods for Gaussian Processes

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# Outline

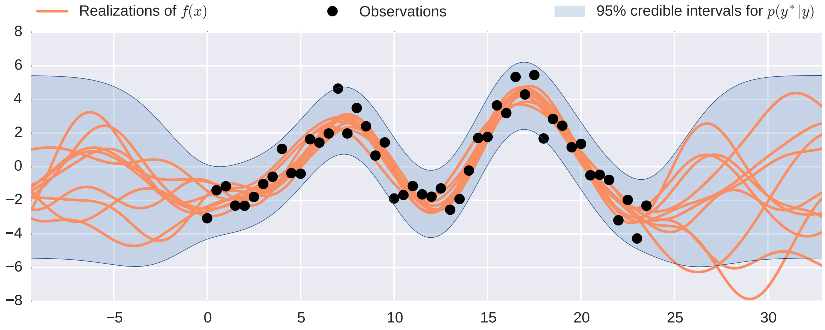
- Motivation
- Laplace approximation
- KL method
- Expectation Propagation
- Comparing approximations

# GP regression

Model the observations as a distorted version of the process $\mathbf{f}_i$:

$$\mathbf{y}_i \sim \mathcal{N}\left(f(\mathbf{x}_i), \sigma^2\right)$$

$f$ is a non-linear function, in our case we assume it is latent, and is assigned a Gaussian process prior.



# GP regression setting

So far we have assumed that the latent values, $\mathbf{f}$, have been corrupted by Gaussian noise. Everything remains analytically tractable.

$$\text{Gaussian Prior:} \qquad \mathbf{f} \sim \mathcal{GP}(\mathbf{0}, \mathbf{K_{ff}}) = p(\mathbf{f})$$

$$\text{Gaussian likelihood:} \qquad \mathbf{y} \sim \mathcal{N}\left(\mathbf{f}, \sigma^2\mathbf{I}\right) = \prod_{i=1}^{n} p(\mathbf{y}_i|\mathbf{f}_i)$$

$$\text{Gaussian posterior:} \qquad p(\mathbf{f}|\mathbf{y}) \propto \mathcal{N}\left(\mathbf{y}|\mathbf{f}, \sigma^2\mathbf{I}\right)\mathcal{N}\left(\mathbf{f}|\mathbf{0}, \mathbf{K_{ff}}\right)$$

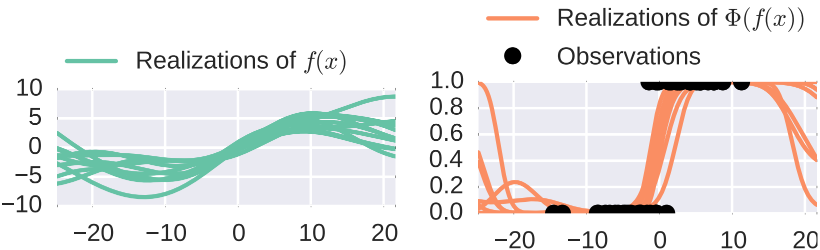
# Likelihood

- $p(\mathbf{y}|\mathbf{f})$ is the probability of the observed data, if we know the latent function values $\mathbf{f}$.
- Can also be seen as the likelihood that the latent function values, $\mathbf{f}$, would give rise to some observed data, $\mathbf{y}$.
- So far assumed that the distortion of the underlying latent function, $\mathbf{f}$, that gives rise to the observed data, $\mathbf{y}$, is independent and Gaussianly distributed.
- This is often not the case, count data, binary data, etc.

# Binary example

- Binary outcomes for $\mathbf{y}_i$, $\mathbf{y}_i \in [0, 1]$.
- Model the probability of $\mathbf{y}_i = 1$ with transformation of GP.
- Probability of 1 must be between 0 and 1, thus use squashing transformation, $\lambda(\mathbf{f}_i) = \Phi(\mathbf{f}_i)$.

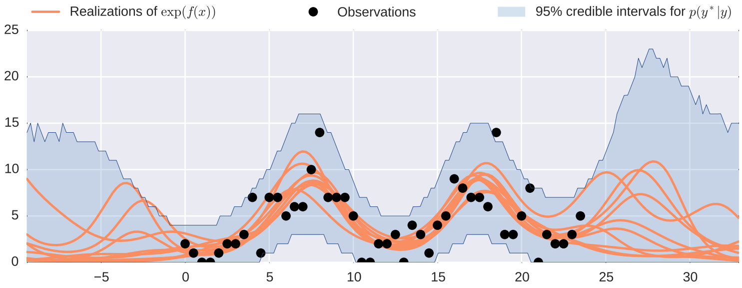
$$\mathbf{y}_i = \begin{cases} 1, & \text{with probability } \lambda(\mathbf{f}_i). \\ 0, & \text{with probability } 1 - \lambda(\mathbf{f}_i). \end{cases}$$



# Count data example

- Non-negative and discrete values only for $\mathbf{y}_i$, $\mathbf{y}_i \in \mathbb{N}$.
- Model the *rate* or *intensity*, $\lambda$, of events with a transformation of a Gaussian process.
- Rate parameter must remain positive, use transformation to maintain positiveness $\lambda(\mathbf{f}_i) = \exp(\mathbf{f}_i)$ or $\lambda(\mathbf{f}_i) = \mathbf{f}_i^2$

$$\mathbf{y}_i \sim \text{Poisson}(\mathbf{y}_i|\lambda_i = \lambda(\mathbf{f}_i)) \qquad \text{Poisson}(\mathbf{y}_i|\lambda_i) = \frac{\lambda_i^{\mathbf{y}_i}}{!\mathbf{y}_i} e^{-\lambda_i}$$



# Non-Gaussian posteriors

- Exact computation of posterior is no longer analytically tractable due to non-conjugate Gaussian process prior to non-Gaussian likelihood, $p(\mathbf{y}|\mathbf{f})$.

$$p(\mathbf{f}|\mathbf{y}) = \frac{p(\mathbf{f}) \prod_{i=1}^{n} p(\mathbf{y}_i|\mathbf{f}_i)}{\int p(\mathbf{f}) \prod_{i=1}^{n} p(\mathbf{y}_i|\mathbf{f}_i)\, d\mathbf{f}}$$

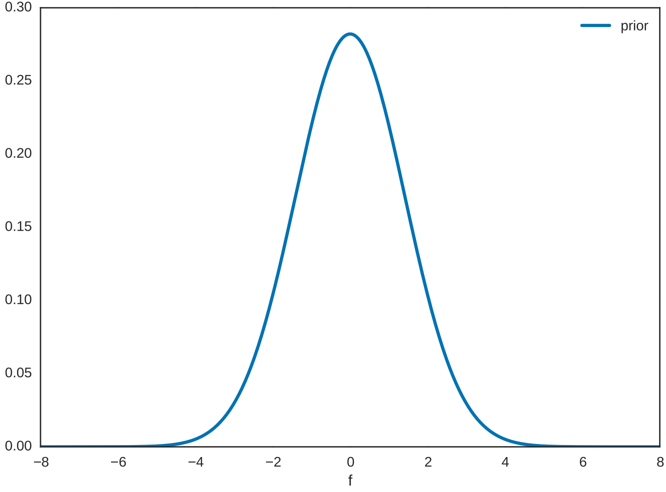
- Various methods to make a Gaussian approximation, $q(\mathbf{f}) \approx p(\mathbf{f}|\mathbf{y})$.
- Allows simple predictions

$$\begin{aligned} p(\mathbf{f}^*|\mathbf{y}) &= \int p(\mathbf{f}^*|\mathbf{f}) p(\mathbf{f}|\mathbf{y}) d\mathbf{f} \\ &\approx \int p(\mathbf{f}^*|\mathbf{f}) q(\mathbf{f}) d\mathbf{f} \end{aligned}$$

# Laplace approximation

- Find the mode of the true log posterior, via Newton's method.
- Use second order Taylor expansion around this modal value.
  - i.e obtain curvature at this point.
- Form Gaussian approximation setting the mean equal to the posterior mode, $\hat{\mathbf{f}}$, and matching the curvature.
- $p(\mathbf{f}|\mathbf{y}) \approx q(\mathbf{f}|\boldsymbol{\mu}, \boldsymbol{C}) = \mathcal{N}\left(\mathbf{f}|\hat{\mathbf{f}}, (\mathbf{K}_{\mathbf{ff}}^{-1} + \boldsymbol{W})^{-1}\right)$
- $\boldsymbol{W} \triangleq -\frac{d^2 \log p(\mathbf{y}|\hat{\mathbf{f}})}{d\hat{\mathbf{f}}^2}$.
- For factorizing likelihoods (most), $\boldsymbol{W}$ is diagonal.

# Visualization of Laplace



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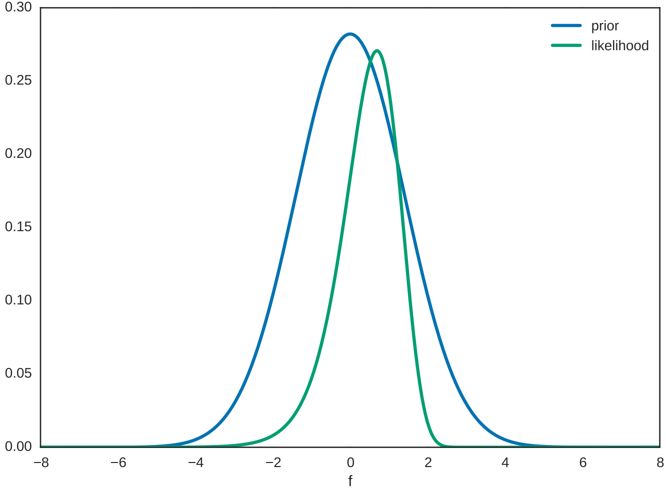

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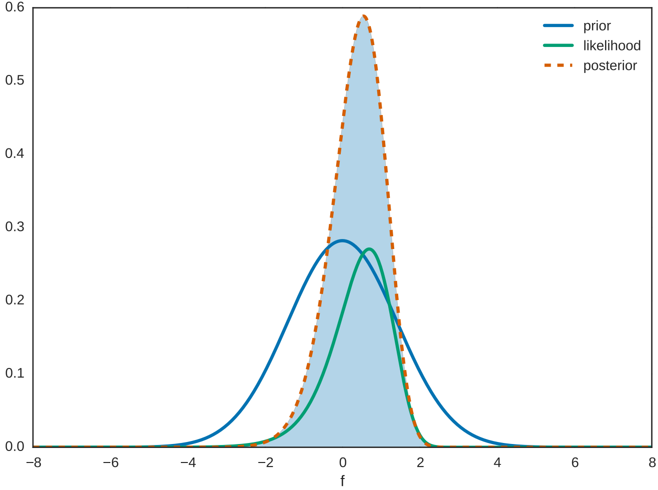

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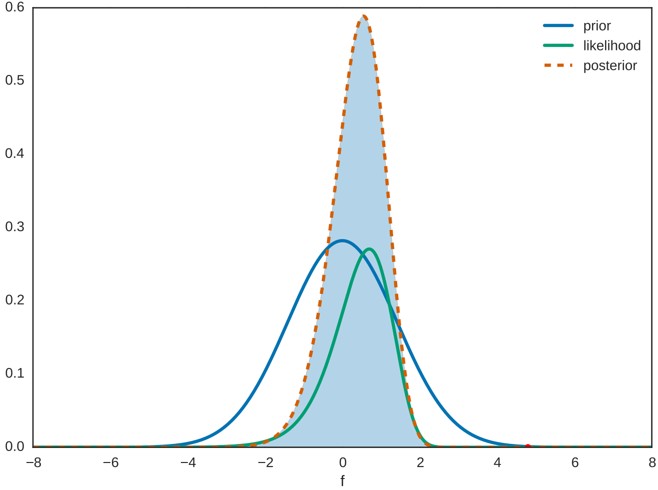

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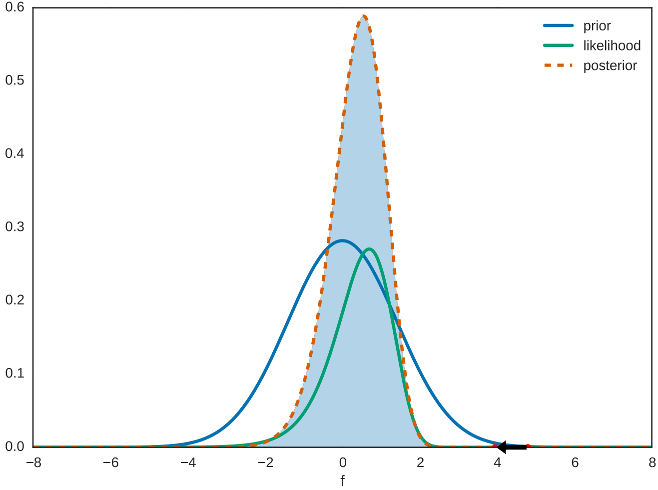

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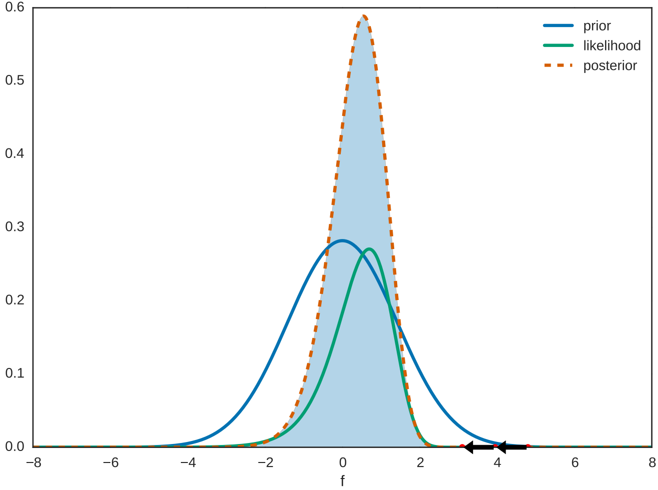

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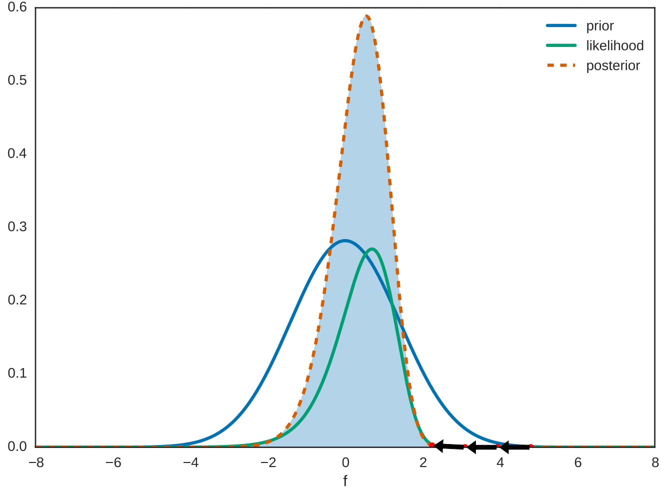

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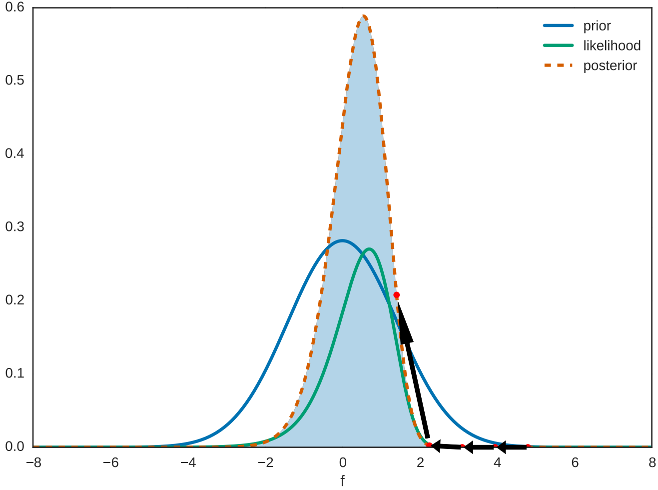

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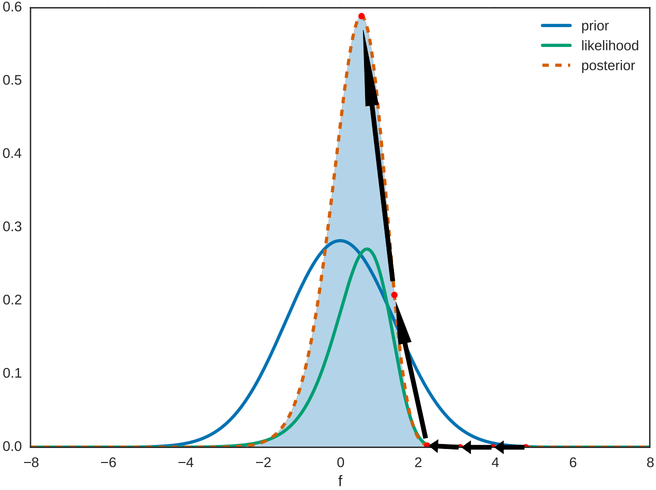

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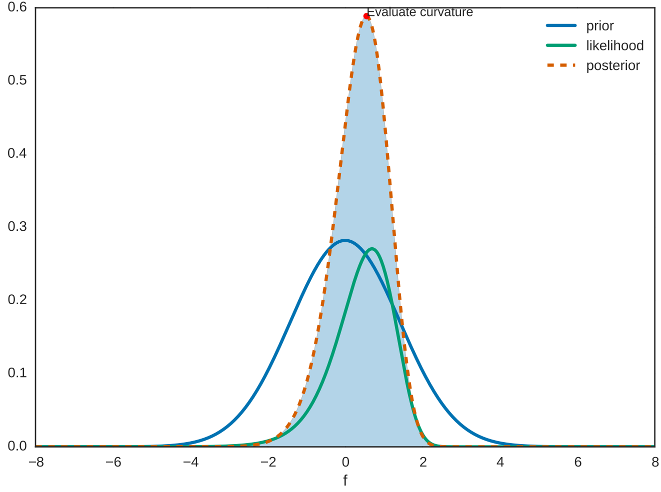

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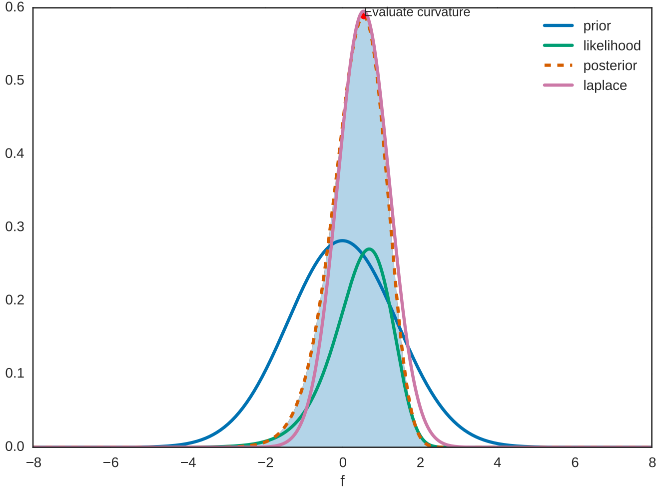


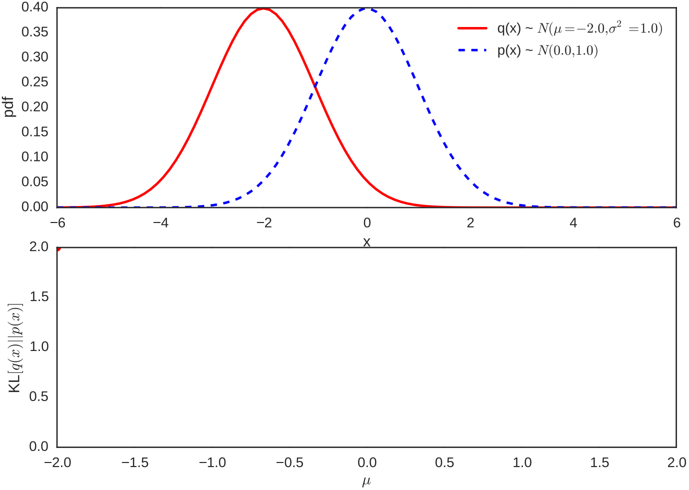
# KL-method

- Make a Gaussian approximation, $q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\boldsymbol{\mu}, \boldsymbol{C})$, as similar possible to true posterior, $p(\mathbf{f}|\mathbf{y})$.
- Treat $\boldsymbol{\mu}$ and $\boldsymbol{C}$ as variational parameters, effecting quality of approximation.
- Define a divergence measure between two distributions, KL divergence, $\mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f}|\mathbf{y})\right)$.
- Minimize this divergence between the two distributions (Nickisch and Rasmussen, 2008).

# KL divergence

- General for any two distributions $q(\mathbf{x})$ and $p(\mathbf{x})$.
- $\mathrm{KL}\left(q(\mathbf{x}) \,\|\, p(\mathbf{x})\right)$ is the average additional amount of information required to specify the values of $\mathbf{x}$ as a result of using an approximate distribution $q(\mathbf{x})$ instead of the true distribution, $p(\mathbf{x})$.
- $\mathrm{KL}\left(q(\mathbf{x}) \,\|\, p(\mathbf{x})\right) = \left\langle \log \frac{q(\mathbf{x})}{p(\mathbf{x})} \right\rangle_{q(\mathbf{x})}$
- Always 0 or positive, not symmetric.
- Lets look at how it changes with response to changes in the approximating distribution.

# KL varying mean



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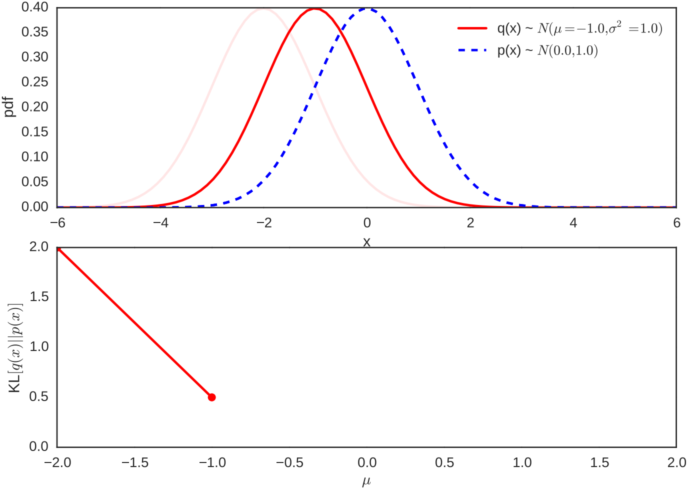

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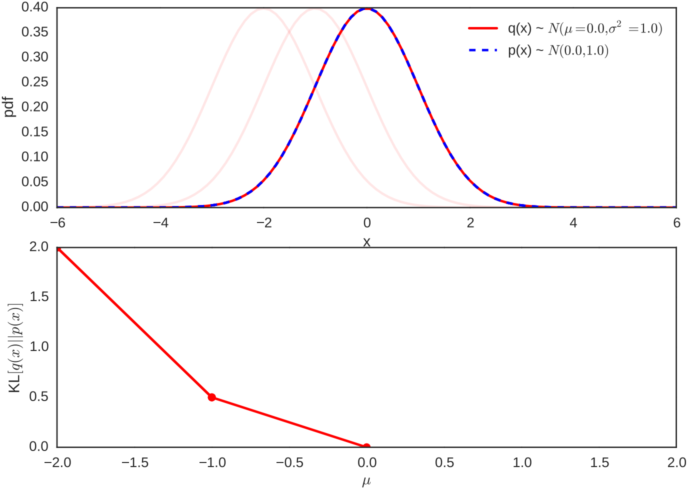

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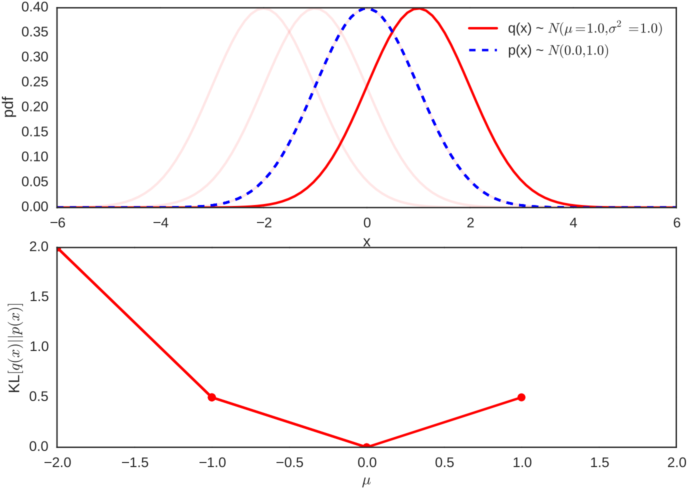

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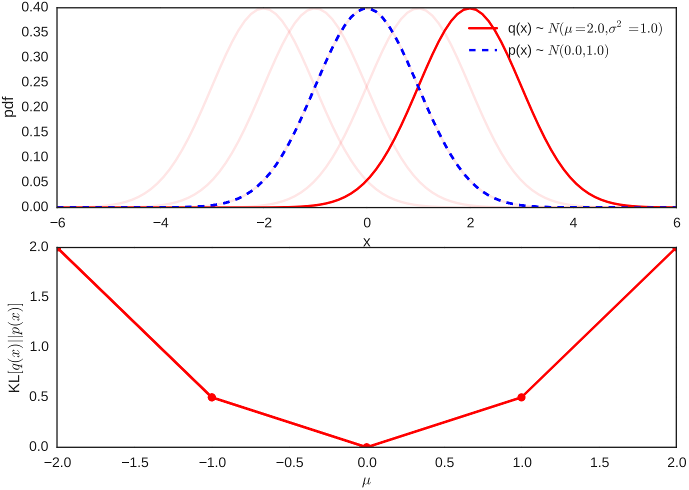
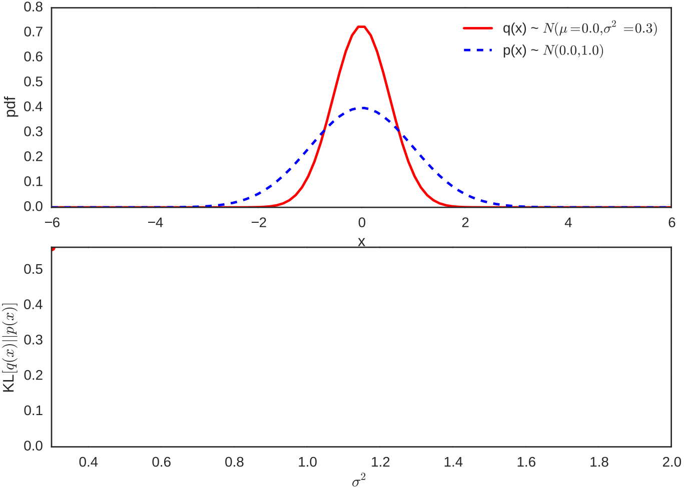


# KL varying variance



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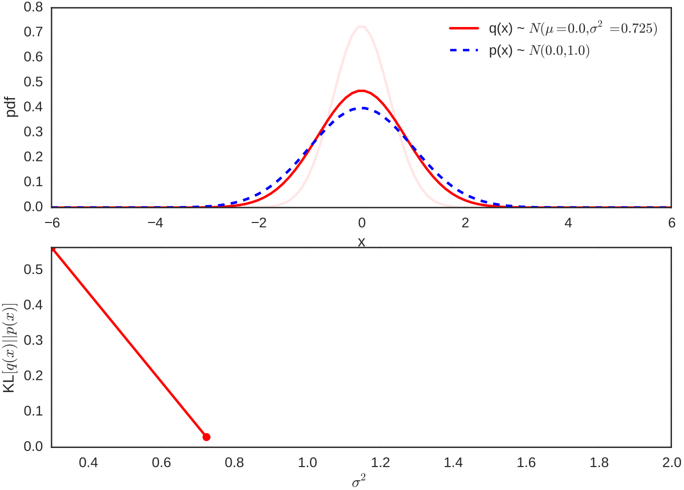

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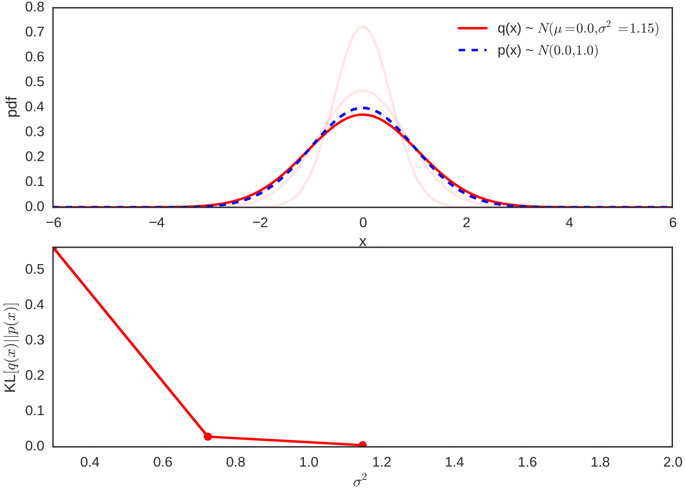

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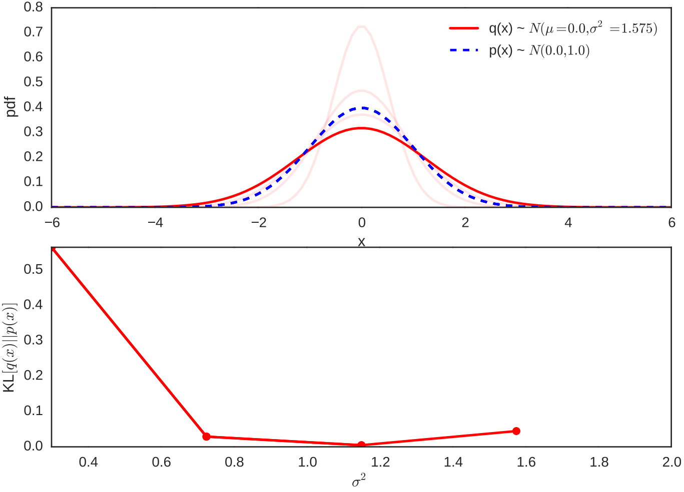

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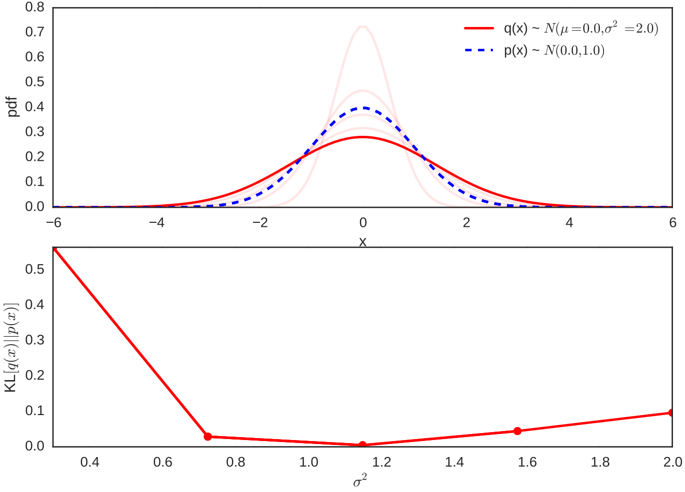


# KL-method derivation

- Assume Gaussian approximate posterior, $q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\boldsymbol{\mu}, \boldsymbol{C})$.
- True posterior using Bayes rule, $p(\mathbf{f}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{f})p(\mathbf{f})}{p(\mathbf{y})}$.
- Cannot compute the KL divergence as we cannot compute the true posterior, $p(\mathbf{f}|\mathbf{y})$.

$$
\begin{aligned}
\mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f}|\mathbf{y})\right) &= \left\langle \log \frac{q(\mathbf{f})}{p(\mathbf{f}|\mathbf{y})} \right\rangle_{q(\mathbf{f})} \\
&= \left\langle \log \frac{q(\mathbf{f})}{p(\mathbf{f})} - \log p(\mathbf{y}|\mathbf{f}) + \log p(\mathbf{y}) \right\rangle_{q(\mathbf{f})} \\
&= \mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f})\right) - \left\langle \log p(\mathbf{y}|\mathbf{f}) \right\rangle_{q(\mathbf{f})} + \log p(\mathbf{y}) \\
\log p(\mathbf{y}) &= \left\langle \log p(\mathbf{y}|\mathbf{f}) \right\rangle_{q(\mathbf{f})} - \mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f})\right) + \mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f}|\mathbf{y})\right)
\end{aligned}
$$

# KL-method derivation

$$\begin{aligned}\log p(\mathbf{y}) &= \left\langle \log p(\mathbf{y}|\mathbf{f}) \right\rangle_{q(\mathbf{f})} - \mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f})\right) + \mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f}|\mathbf{y})\right) \\ &\geq \left\langle \log p(\mathbf{y}|\mathbf{f}) \right\rangle_{q(\mathbf{f})} - \mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f})\right)\end{aligned}$$

- Tractable terms give lower bound on $\log p(\mathbf{y})$ as $\mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f}|\mathbf{y})\right)$ always positive.
- Adjust variational parameters $\boldsymbol{\mu}$ and $\boldsymbol{C}$ to make tractable terms as large as possible, thus $\mathrm{KL}\left(q(\mathbf{f}) \,\|\, p(\mathbf{f}|\mathbf{y})\right)$ as small as possible.
- $\left\langle \log p(\mathbf{y}|\mathbf{f}) \right\rangle_{q(\mathbf{f})}$ with factorizing likelihood can be done with a series of $n$ 1 dimensional integrals.
- In practice, can reduce the number of variational parameters by reparameterizing $\boldsymbol{C} = (\mathbf{K}_{\mathbf{ff}} - 2\Lambda)^{-1}$ by noting that the bound is constant in off diagonal terms of $\boldsymbol{C}$.

# Expectation Propagation

$$p(\mathbf{f}|\mathbf{y}) \propto p(\mathbf{f}) \prod_{i=1}^{n} p(\mathbf{y}_i|\mathbf{f}_i)$$

$$q(\mathbf{f}|\mathbf{y}) \triangleq \frac{1}{Z_{ep}} p(\mathbf{f}) \prod_{i=1}^{n} t_i(\mathbf{f}_i|\tilde{Z}_i, \tilde{\mu}_i, \tilde{\sigma}_i^2) = \mathcal{N}(\mathbf{f}|\boldsymbol{\mu}, \Sigma)$$

$$t_i \triangleq \tilde{Z}_i \mathcal{N}\left(\mathbf{f}_i|\tilde{\boldsymbol{\mu}}_i, \tilde{\boldsymbol{\sigma}}_i^2\right)$$

- Individual likelihood terms, $p(\mathbf{y}_i|\mathbf{f}_i)$, replaced by independent local likelihoods, $t_i$.
- Uses an iterative algorithm to update $t_i$'s.

# Expectation Propagation

1. From the current posterior, $q(\mathbf{f}|\mathbf{y})$, leave out one of the local likelihoods, $t_i$, then marginalize out $\mathbf{f}_{j\neq i}$, giving rise to the *cavity distribution*, $q_{-i}(\mathbf{f}_i)$.
2. Combine cavity distribution, $q_{-i}(\mathbf{f}_i)$, with exact likelihood contribution, $p(\mathbf{y}_i|\mathbf{f}_i)$, giving non-Gaussian un-normalized distribution, $\hat{q}(\mathbf{f}_i) \triangleq p(\mathbf{y}_i|\mathbf{f}_i)q_{-i}(\mathbf{f}_i)$.
3. Choose a un-normalized Gaussian approximation to this distribution, $\mathcal{N}\left(\mathbf{f}_i|\hat{\boldsymbol{\mu}}_i, \hat{\boldsymbol{\sigma}}_i^2\right)\hat{Z}_i$, by finding moments of $\hat{q}(\mathbf{f}_i)$.
4. Replace parameters of $t_i$ with those that produce the same moments as this approximation.
5. Choose another $i$ and start again. Repeat to convergence.

# Expectation Propagation - in math

Step 1. First choose a marginal, $i$, to focus on, then

$$q(\mathbf{f}|\mathbf{y}) \propto p(\mathbf{f}) \prod_{j=1}^{n} t_j(\mathbf{f}_j) \rightarrow \frac{p(\mathbf{f}) \prod_{j=1}^{n} t_j(\mathbf{f}_j)}{t_i(\mathbf{f}_i)} \rightarrow p(\mathbf{f}) \prod_{j \neq i} t_j(\mathbf{f}_j)$$

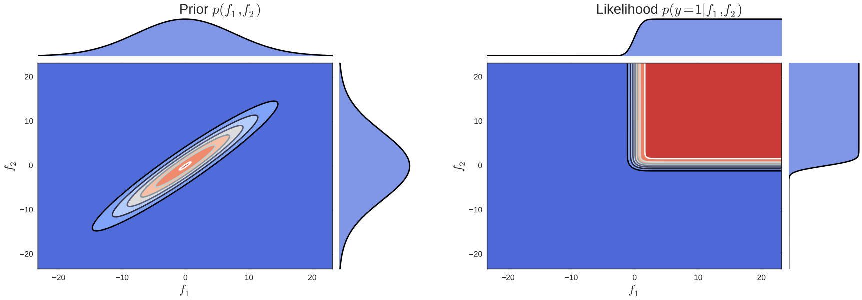
$$\rightarrow \int p(\mathbf{f}) \prod_{j \neq i} t_j(\mathbf{f}_j)\, d\mathbf{f}_{j \neq i} \triangleq q_{-i}(\mathbf{f}_i)$$

Step 2. $p(\mathbf{y}_i|\mathbf{f}_i) q_{-i}(\mathbf{f}_i) \triangleq \hat{q}(\mathbf{f}_i)$

Step 3. $\hat{q}(\mathbf{f}_i) \approx \mathcal{N}\left(\mathbf{f}_i|\hat{\boldsymbol{\mu}}_i, \hat{\boldsymbol{\sigma}}_i^2\right) \hat{Z}_i$

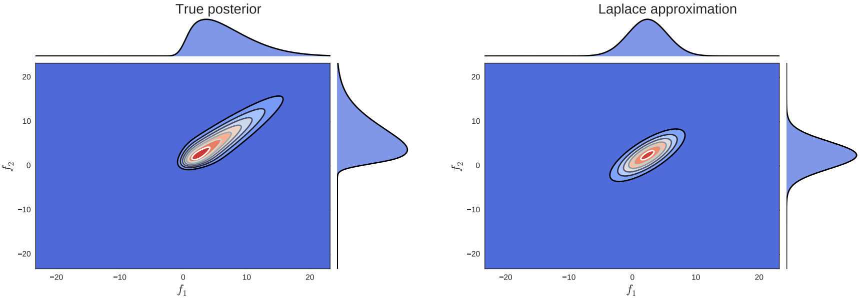
Step 4: Compute parameters of $t_i(\mathbf{f}_i|\tilde{Z}_i, \tilde{\mu}_i, \tilde{\sigma}_i^2)$ making moments of $q(\mathbf{f}_i)$ match those of $\hat{Z}_i \mathcal{N}\left(\mathbf{f}_i|\hat{\boldsymbol{\mu}}_i, \hat{\boldsymbol{\sigma}}_i^2\right)$.

# Comparing posterior approximations



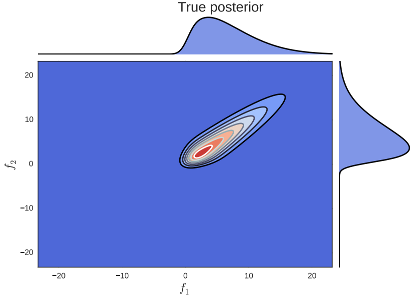

- Gaussian prior between two function values $\{\mathbf{f}_1, \mathbf{f}_2\}$, at $\{\mathbf{x}_1, \mathbf{x}_2\}$ respectively.
- Bernoulli likelihood, $\mathbf{y}_1 = 1$ and $\mathbf{y}_2 = 1$.

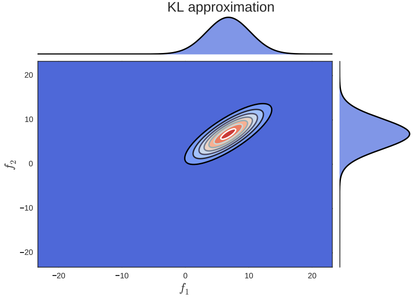
# Comparing posterior approximations




- True posterior is non-Gaussian.
- Laplace approximates with a Gaussian at the mode of the posterior.

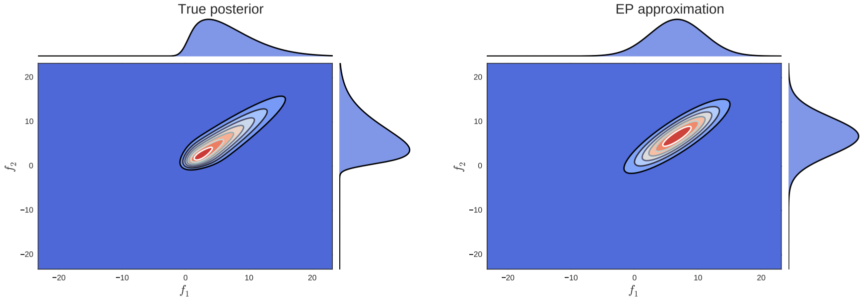
# Comparing posterior approximations



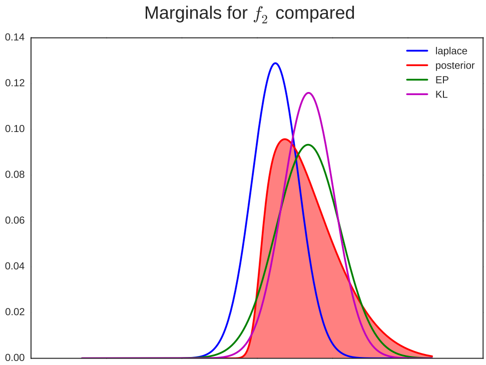

- True posterior is non-Gaussian.
- KL approximate with a Gaussian that has minimal KL divergence, $\mathrm{KL}\left(q(\mathbf{f})\,\|\,p(\mathbf{f}|\mathbf{y})\right)$.
- This leads to distributions that avoid regions in which $p(\mathbf{f}|\mathbf{y})$ is small.
- It has a large penality for assigning density where there is none.

# Comparing posterior approximations




- True posterior is non-Gaussian.
- EP tends to try and put density where $p(\mathbf{f}|\mathbf{y})$ is large
- Cares less about assigning density density where there is none. Contrasts to KL method.

# Comparing posterior marginal approximations




- Laplace: Poor approximation.
- KL: Avoids assigning density to areas where there is none, at the expense of areas where there is some (right tail).
- EP: Assigns density to areas with density, at the expense of areas where there is none (left tail).

# Pros - Cons - When - Laplace

Laplace approximation

- Pros
  - Very fast.
- Cons
  - Poor approximation if the mode does not well describe the posterior, for example Bernoulli likelihood (probit).
- When
  - When the posterior *is* well characterized by its mode, for example Poisson.

# Pros - Cons - When - KL

KL method

- Pros
  - Principled in that it we are directly optimizing a measure of divergence between an approximation and true distribution.
  - Can be relatively quick, and lends it self to sparse approximations (Hensman et al., 2015).
- Cons
  - Requires factorizing likelihoods to avoid $n$ dimensional integral.
- When
  - Likelihood is not Bernoulli, and Laplace approximation poor.

# Pros - Cons - When - EP

EP method

- Pros
  - Very effective for certain likelihoods (classification).
- Cons
  - Slow though possible to extend to sparse case.
  - Convergence issues for certain likelihoods.
  - Must be able to match moments.
- When
  - Binary data (Nickisch and Rasmussen, 2008; Kuß, 2006), perhaps with truncated likelihood (censored data) (Vanhatalo et al., 2015).

# Pros - Cons - When - MCMC

MCMC methods

- Pros
  - Theoretical limit gives true distribution
- Cons
  - Can be very slow
- When
  - If time is not an issue, but exact accuracy is.
  - If you are unsure whether a different approximation is appropriate, can be used as a “ground truth”

# Questions

Thanks for listening.

Any questions?

# References I

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