Special course on Gaussian processes: Session #4

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30/1-19

Roadmap for today

1. Computational challenges
   - Computational complexity of GP regression
   - Non-Gaussian likelihoods: GP classification

2. Approximate inference
   - Variational inference: scratching the surface
   - Inducing points approximations

Computational complexity of Gaussian process regression

- The key equations for predictions (with Gaussian likelihood)

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p(f_*|\boldsymbol{y}) &= \mathcal{N}\left(f_* \middle| \mu_*, \sigma_*^2\right) \\
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- Recall: If $\boldsymbol{A} \in \mathbb{R}^{N \times M}$ and $\boldsymbol{b} \in \mathbb{R}^M$, then the cost of computing $\boldsymbol{A}\boldsymbol{b}$ is $\mathcal{O}(NM)$
- Recall: If $\boldsymbol{C} \in \mathbb{R}^{N \times N}$, then the cost of computing $\boldsymbol{C}^{-1}$ is $\mathcal{O}\left(N^3\right)$
- What is computational complexity for computing the posterior distribution for 1 test point based on a data set with N observations? What is the dominating operation?

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- $N \leq 1000$: Fine, $N \leq 10000$: Slow, but possible, $N > 10000$: Prohibitively slow

Regression vs classification

- Response variable $\boldsymbol{y}$ is continuous in regression problems

$$y_n \in \mathbb{R}$$

- Response variable $\boldsymbol{y}$ is discrete in classification problems

$$y_n \in \{c_1, c_2, \ldots, c_K\}$$

- Classification problems

$$\begin{aligned}
\boldsymbol{X} &= \text{images}, & y_n &\in \{\text{cat}, \text{dog}\} \\
\boldsymbol{X} &= \text{X-ray scan}, & y_n &\in \{\text{tumor}, \text{no tumor}\} \\
\boldsymbol{X} &= \text{images of digits}, & y_n &\in \{0, 1, 2, \ldots, 9\} \\
\boldsymbol{X} &= \text{emails}, & y_n &\in \{\text{spam}, \text{not spam}\}
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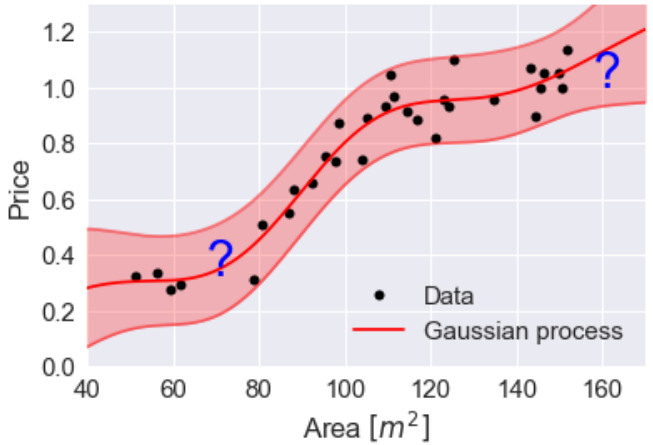

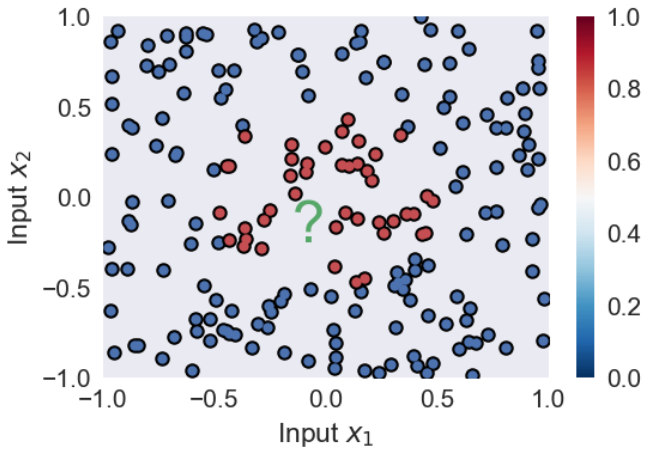

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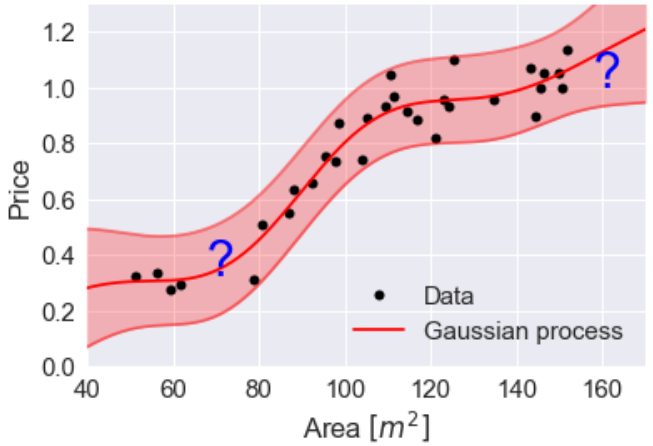
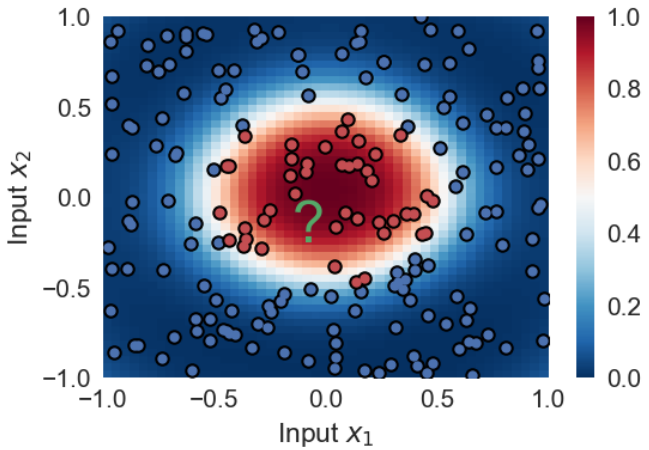
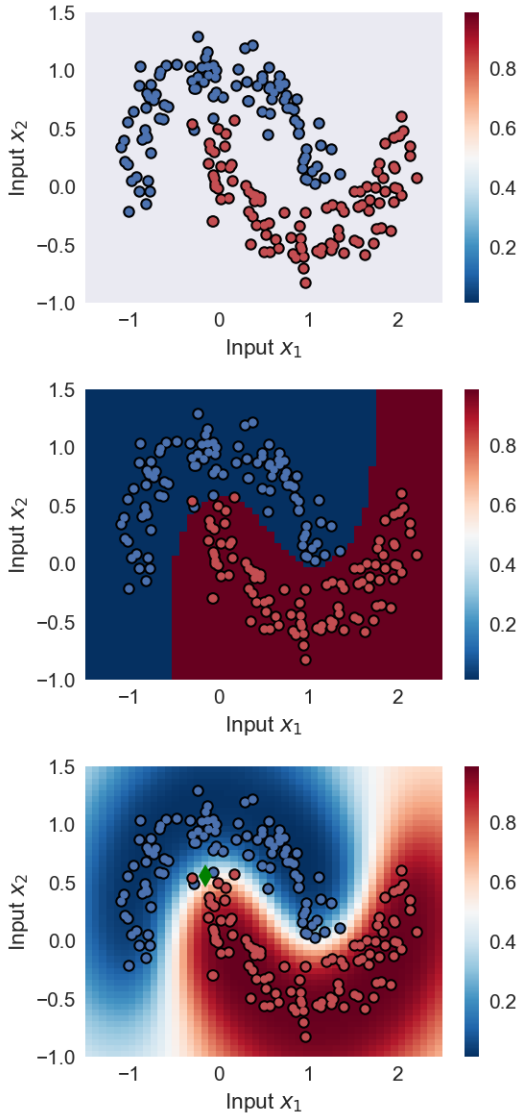




Why Gaussian processes for classification?

- Complex decision boundaries
  1. Non-linear boundary
  2. Can learn complexity of decision boundary from data
- Probabilistic classification
  1. How would you classify the green point?
  2. We want to model the uncertainty



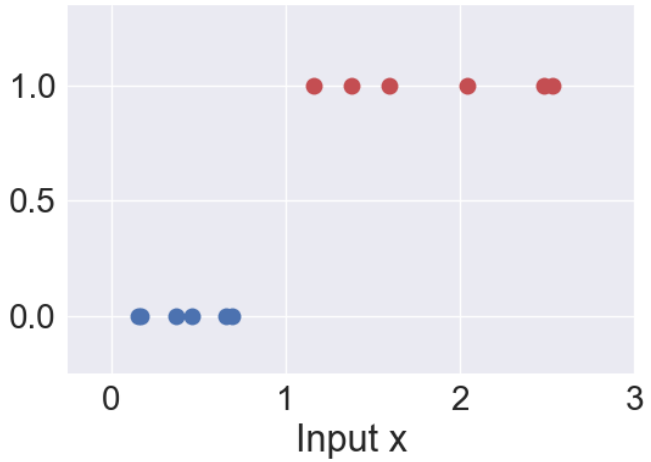
Why don't we use regression models for classification?

- We focus on binary classification: $y_n \in \{0, 1\}$ or $y_n \in \{-1, 1\}$
- We are given a data set $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$ and we want to model

$$p(y_n = +1|\boldsymbol{x}_n)$$

- What's wrong with simply using the GP regression model with labels: $y_n \in \{0, 1\}$:

$$p(y_n = +1|\boldsymbol{x}_n) = f(\boldsymbol{x_n})$$



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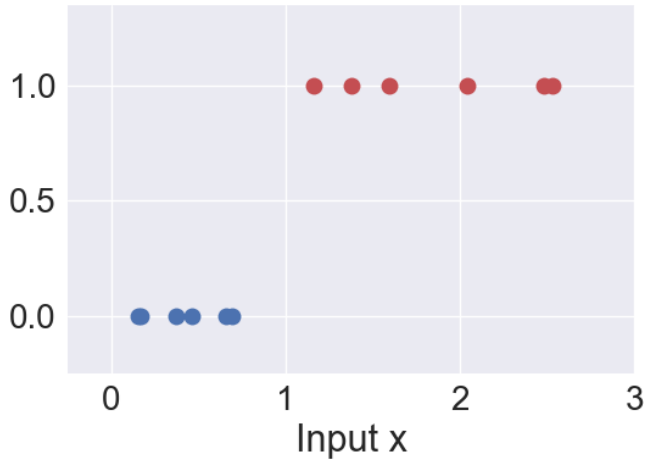

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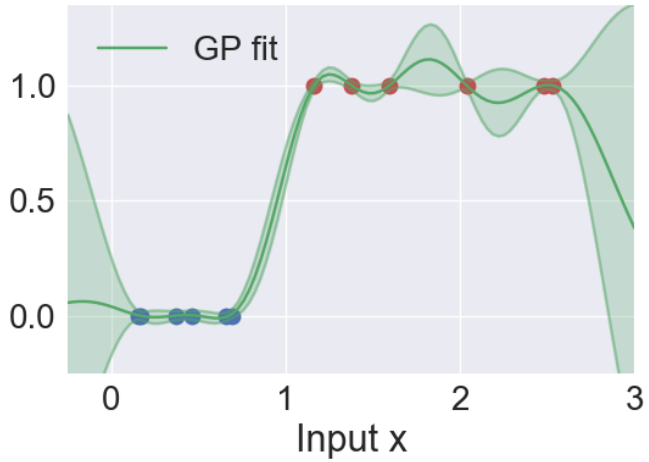


Gaussian process classification setup (I)

- We'll use a 'squashing function' $\phi : \mathbb{R} \to (0, 1)$ with $y_n \in \{-1, 1\}$

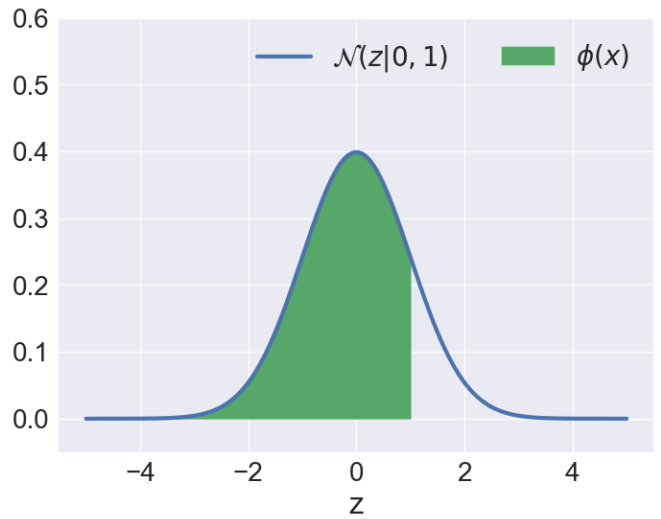
$$p(y_n | \boldsymbol{x}_n) = \phi\left(y_n \cdot f\left(\boldsymbol{x}_n\right)\right) \in (0, 1)$$

- Multiple possible choices for $\phi(\cdot)$, we'll use the standard normal CDF

$$\phi\left(x\right) = \int_{-\infty}^{x} \mathcal{N}\left(z|0, 1\right) \mathrm{d}z$$

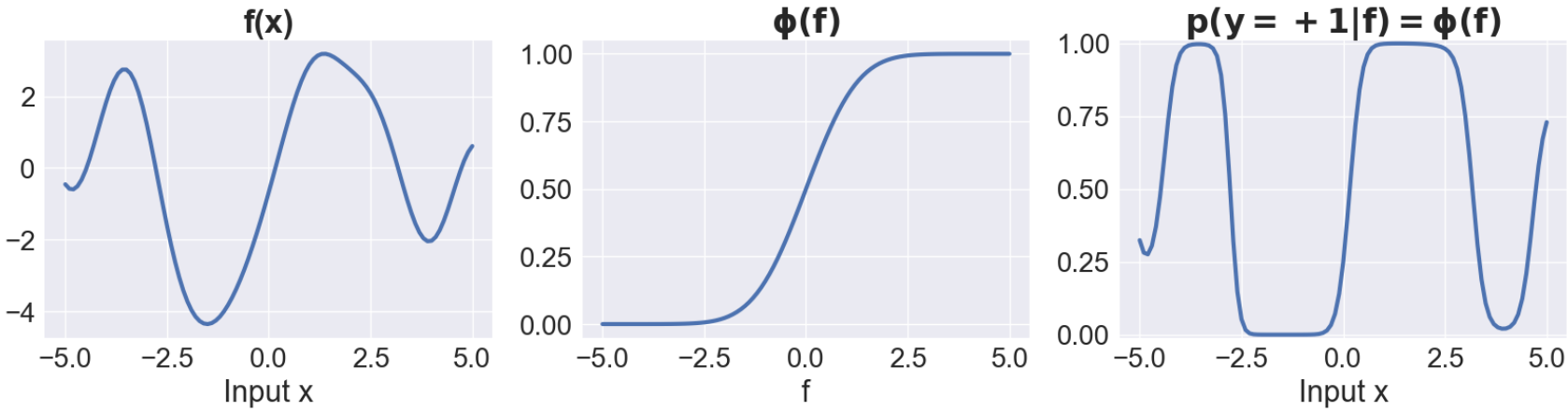
Discuss with your neighbour

1. What is $\phi(0)$?
2. What is $\phi(-\infty)$?
3. What is $\phi(\infty)$?
4. What is $\phi(x) + \phi(-x)$?
5. Is $\phi\left(y_n f\left(\boldsymbol{x}_n\right)\right)$ normalized wrt. y_n?

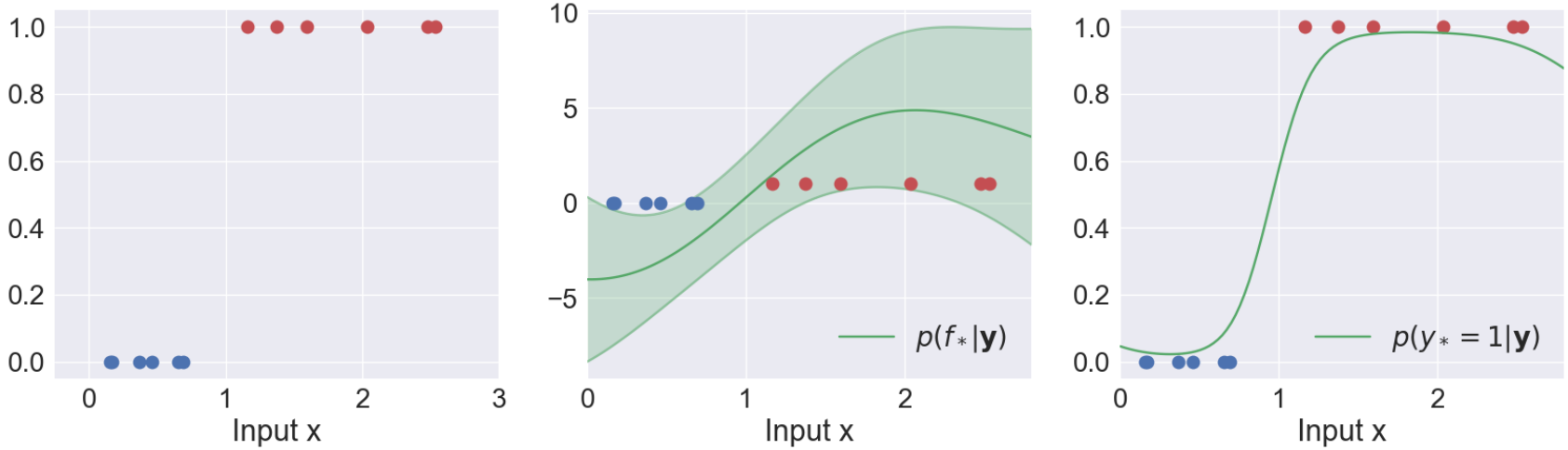


Gaussian process classification setup (II)

- We map the unknown function $f(\boldsymbol{x})$ through the squashing function



- Example re-visited



Gaussian process classification: Inference

Three steps to compute the predictive distribution for a new test point $\boldsymbol{x}_*$

$$p\left(\boldsymbol{y}, \boldsymbol{f}\right) = \prod_{n=1}^{N} p(y_n|f_n)p(\boldsymbol{f}) = \prod_{n=1}^{N} \phi\left(y_n \cdot f_n\right) \mathcal{N}\left(\boldsymbol{f}\middle|\boldsymbol{0}, \boldsymbol{K}\right)$$

- Step 1: Compute posterior distribution of $p(\boldsymbol{f}|\boldsymbol{y})$:

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- Step 2: Compute posterior of f_* for new test point $\boldsymbol{x}_*$:

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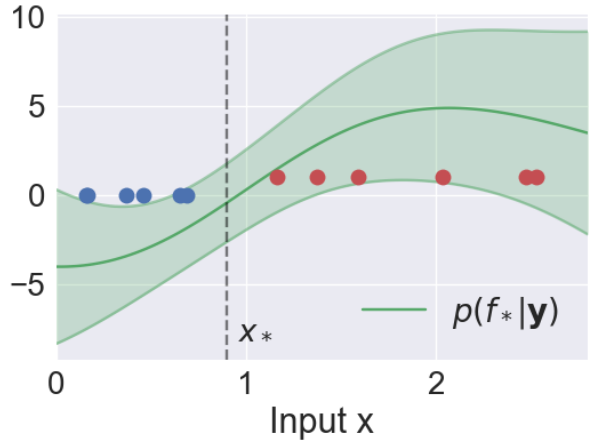

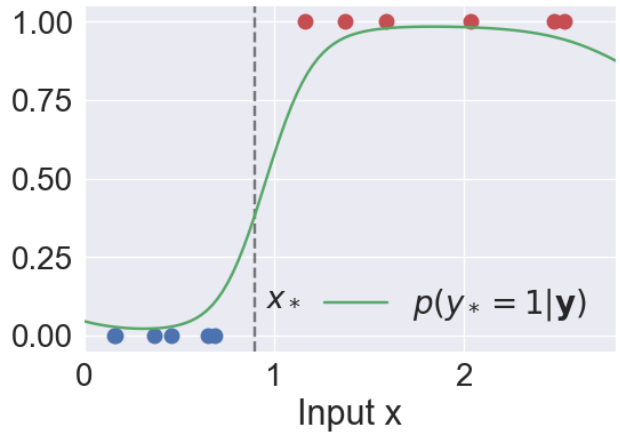

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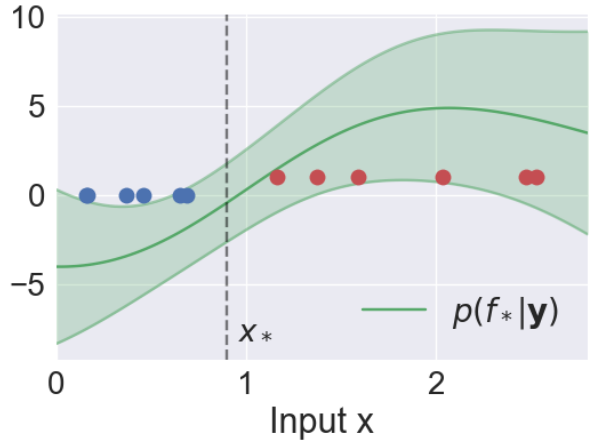
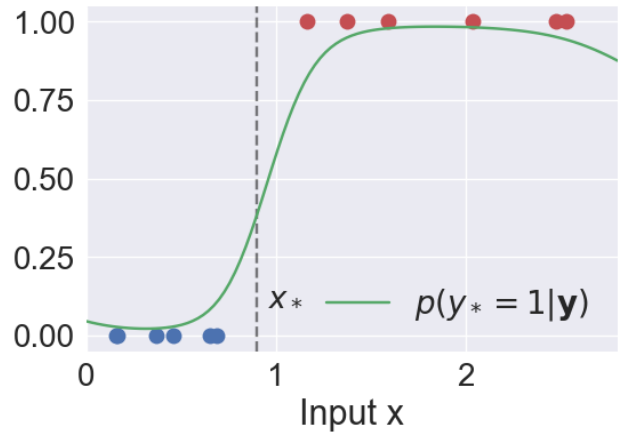
- Unfortunately, these distributions are analytically intractable.





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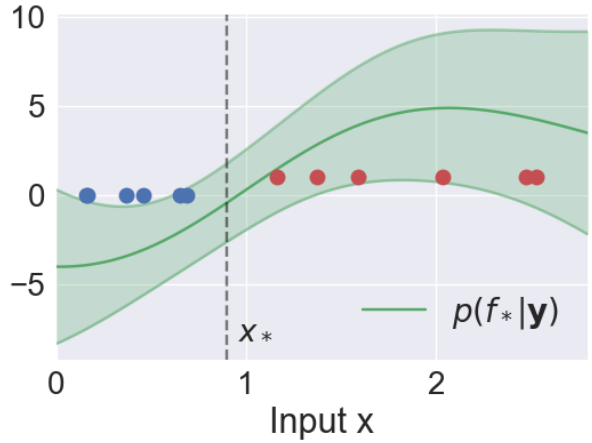

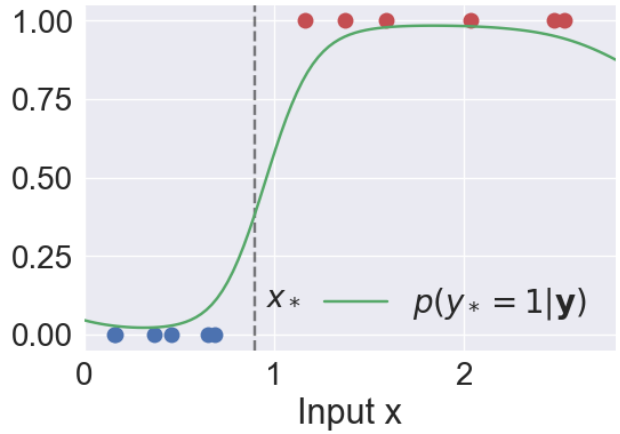

Computational problems

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Variational inference

- General framework for approximate Bayesian inference
- Many recent application in the machine learning literature:
  1. GPs for big data
  2. GPs with non-Gaussian likelihoods
  3. Deep Gaussian processes
  4. Convolutional Gaussian processes
  5. Variational autoencoders (VAEs)
  6. ...

Variational inference: the big picture

Recipe for approximating intractable distribution $p \in \mathcal{P}$

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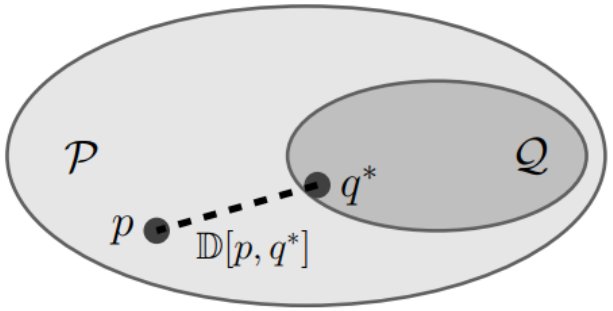

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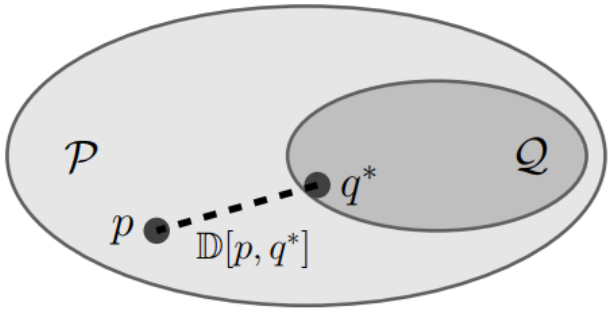

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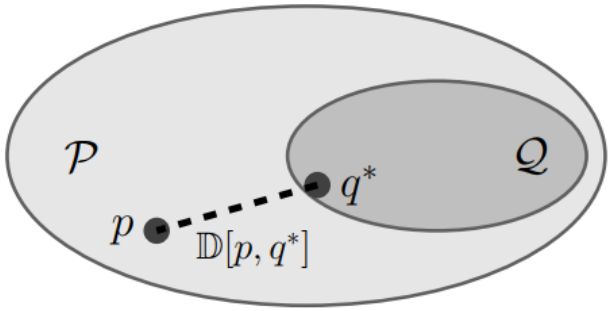

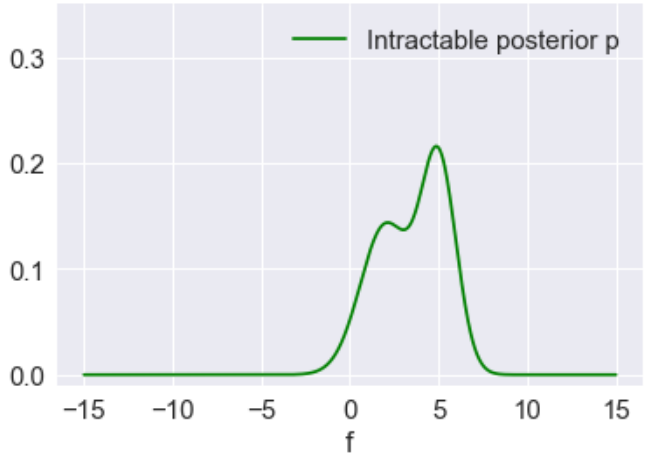

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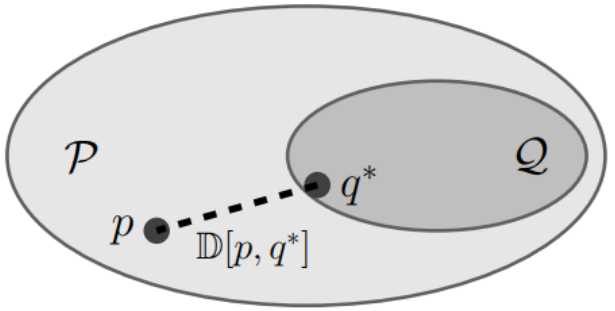

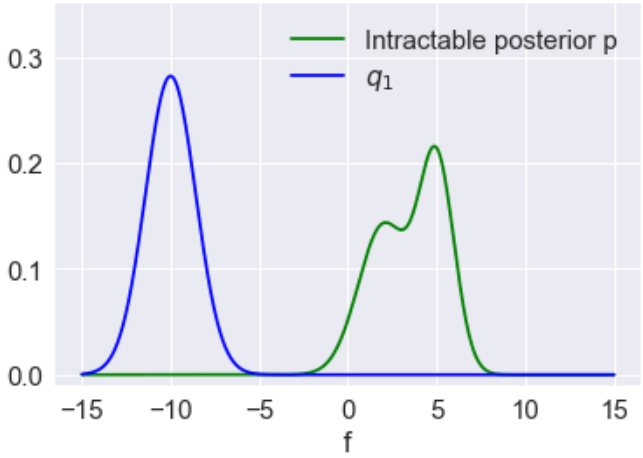

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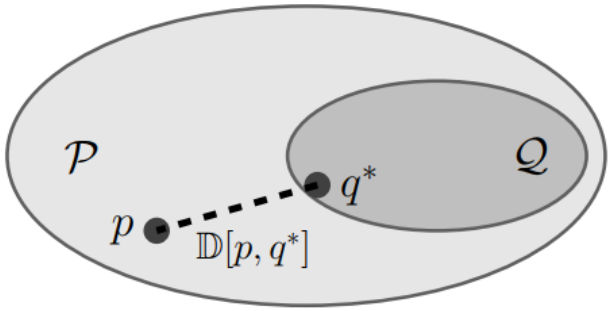

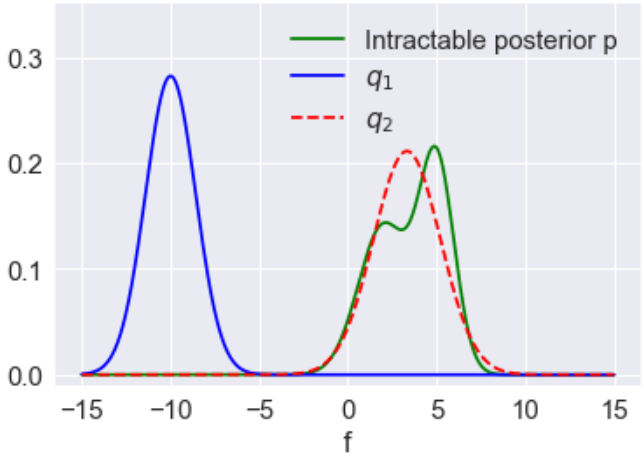

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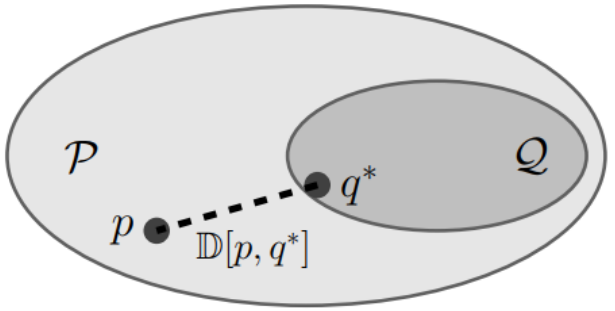
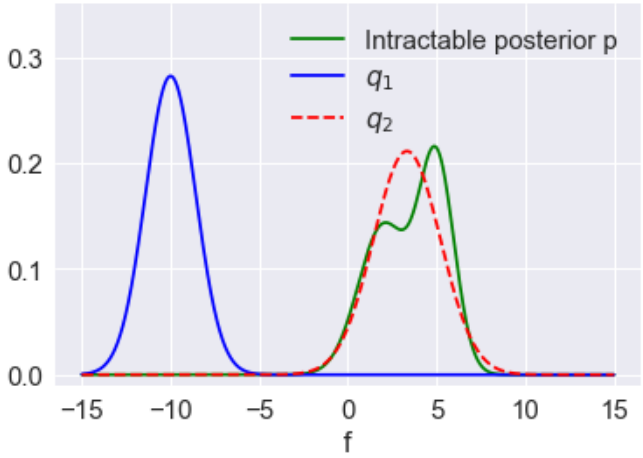
$$\mathbb{D}[q_1, p] > \mathbb{D}[q_2, p]$$





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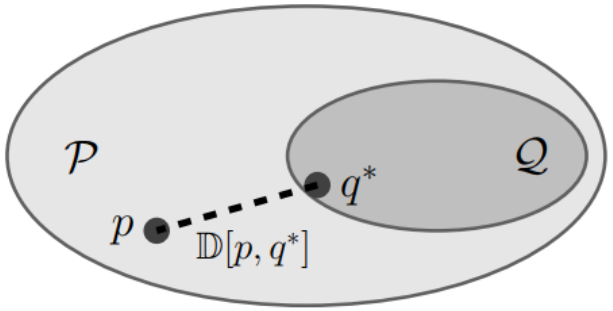
Recipe for approximating intractable distribution $p \in \mathcal{P}$



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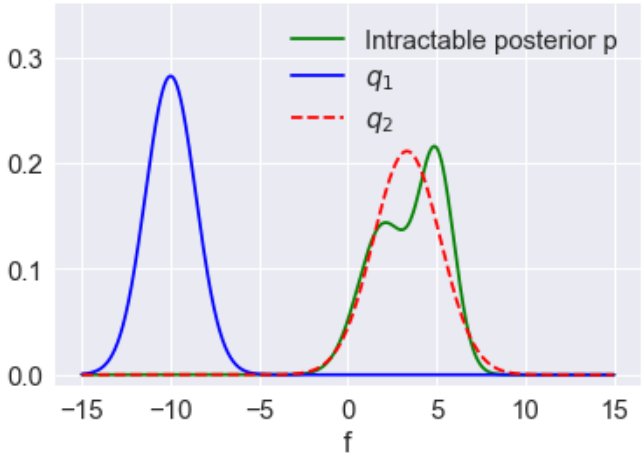
$$\mathbb{D}[q_1, p] > \mathbb{D}[q_2, p]$$



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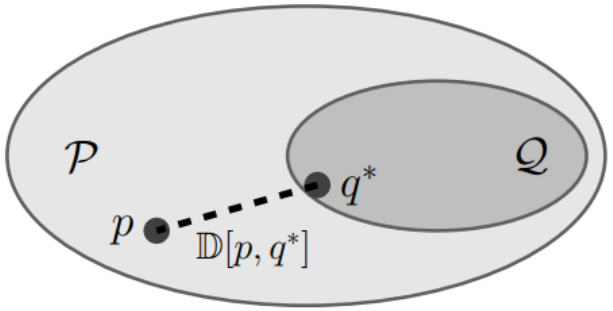

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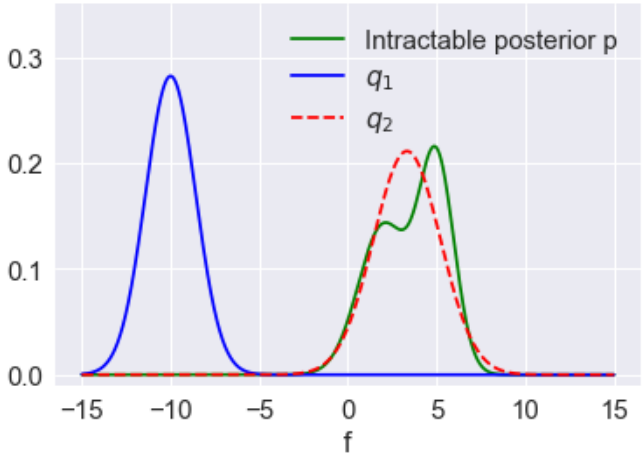

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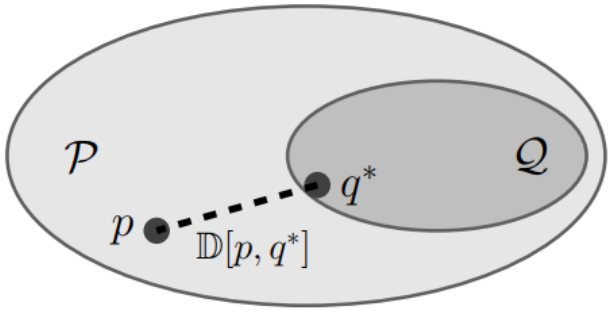

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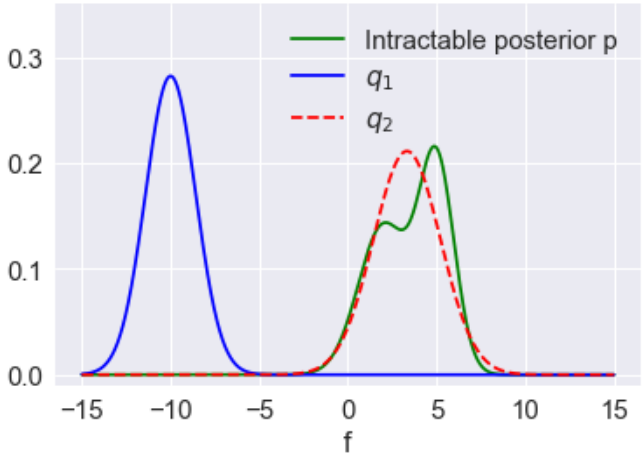

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Here we will always choose $\mathcal{Q}$ to be the set of multivariate Gaussian distributions.

Variational inference I

- We will use to the *Kullback-Leibler divergence* to "measure distances" between distributions

$$\mathbb{D}\left[q||p\right] = \int q(\boldsymbol{f}) \ln \frac{q(\boldsymbol{f})}{p(\boldsymbol{f})} \mathrm{d}\boldsymbol{f} = \mathbb{E}_q \left[\ln \frac{q(\boldsymbol{f})}{p(\boldsymbol{f})} \right]$$

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- Most important properties for our purpose:
  1. Positive definite: $\mathbb{D}\left[q||p\right] \geq 0$
  2. Identity of indiscernibles: $\mathbb{D}\left[q||p\right] = 0 \quad \Longleftrightarrow \quad p = q \quad \text{(a.e.)}$
  3. Not-symmetric: $\mathbb{D}\left[q||p\right] \neq \mathbb{D}\left[p||q\right]$

Variational inference II

Our goal is to minimize the KL divergence between some approximation $q \in \mathcal{Q}$ and some posterior distribution $p(\boldsymbol{f}|\boldsymbol{y})$

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Last term depends on the exact posterior $p(\boldsymbol{f}|\boldsymbol{y})$, which is intractable.

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Using the def. of conditional densities, we can write: $p(\boldsymbol{f}|\boldsymbol{y}) = \frac{p(\boldsymbol{y},\boldsymbol{f})}{p(\boldsymbol{y})}$

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$\mathcal{L}\left[q\right]$ does not depend on the posterior $p(\boldsymbol{f}|\boldsymbol{y})$, but only on the joint density $p(\boldsymbol{y},\boldsymbol{f})$.

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Key take-away: we can fit the variational approx. q by optimizing $\mathcal{L}$

Variational inference V

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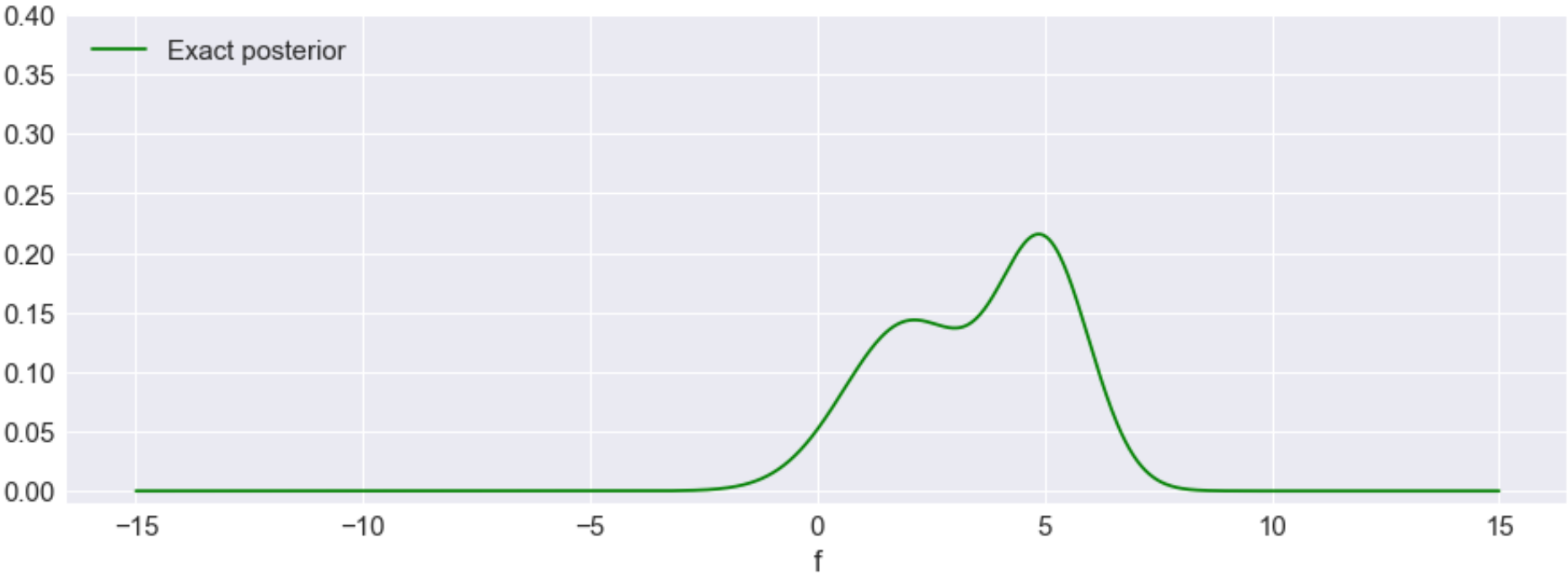
- In practice, we optimize $\mathcal{L}\left[\boldsymbol{\lambda}\right]$ using gradient-based methods

1D Toy example I

- Assume we have some model $p(y, f)$ that gives rise to some intractable posterior $p(f|y)$
- We want to approximate $p(f|y)$ using a variational approximation
- In 1D: $\mathcal{Q}$ is the the set of univariate Gaussian, i.e. $q_\lambda(x) = \mathcal{N}(x|m, v)$, where we denote $\boldsymbol{\lambda} = \{m, v\}$
- We initialize our approximation as $q(f) = \mathcal{N}(f|0, 1)$



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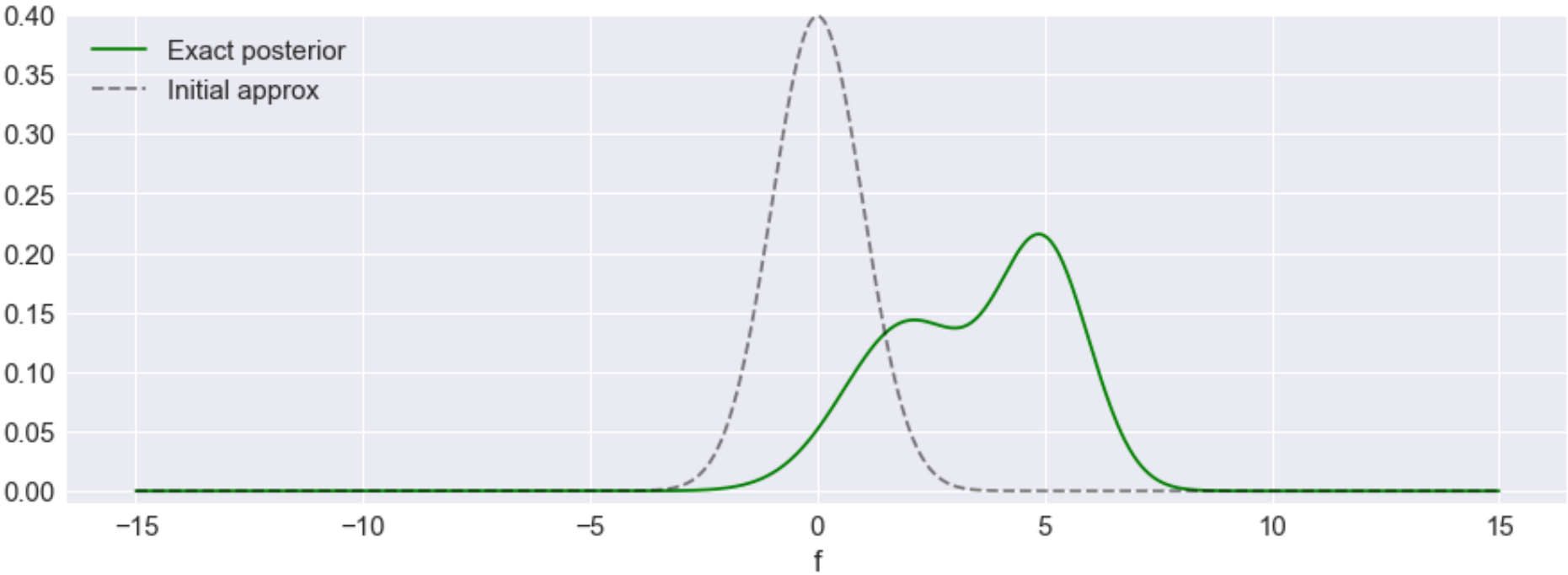

1D Toy example II

- Gradient ascent: $\boldsymbol{\lambda}_{i+1} = \boldsymbol{\lambda}_i + \eta \nabla_{\boldsymbol{\lambda}} \mathcal{L}[\boldsymbol{\lambda}]$
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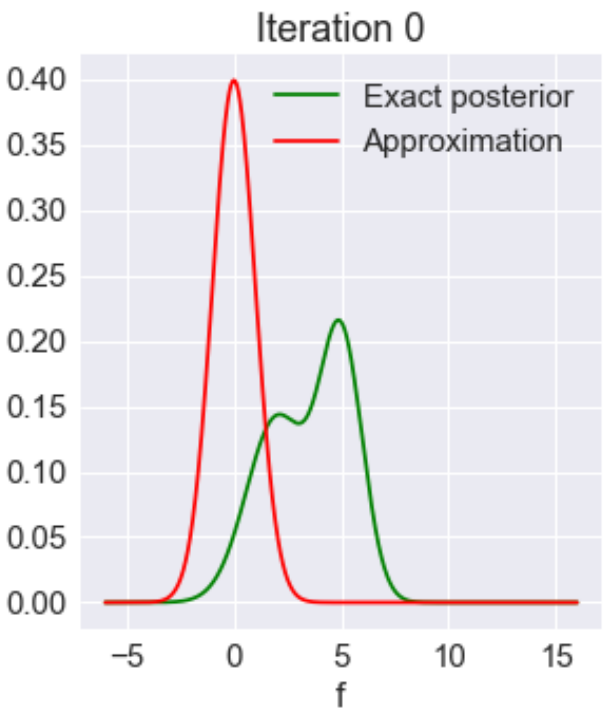

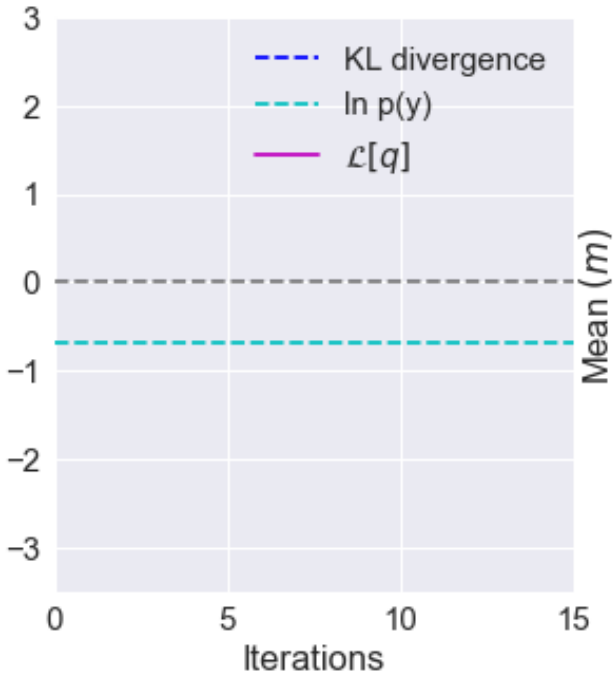

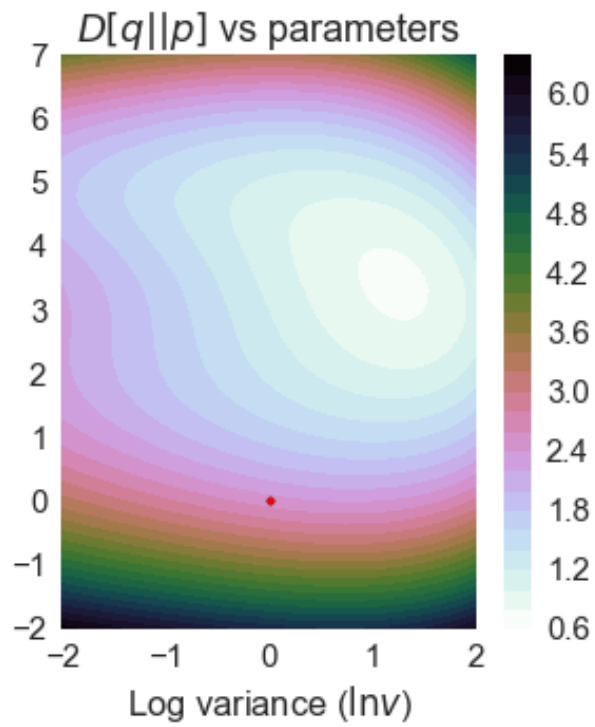

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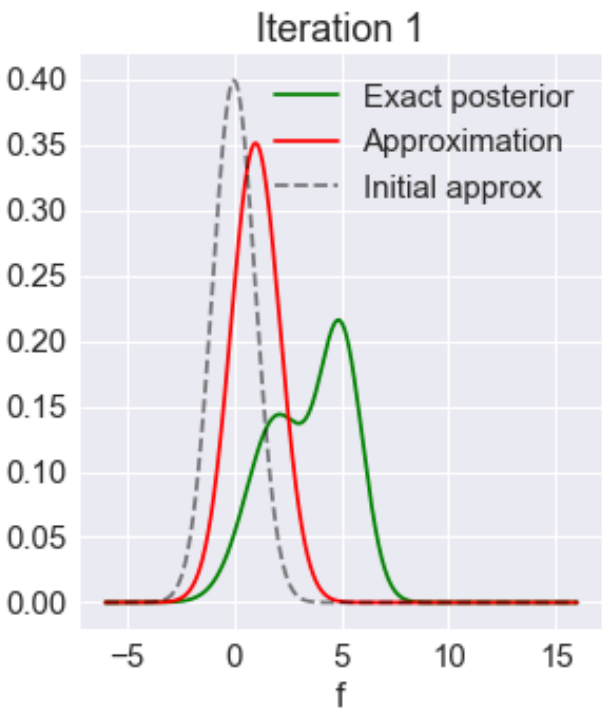

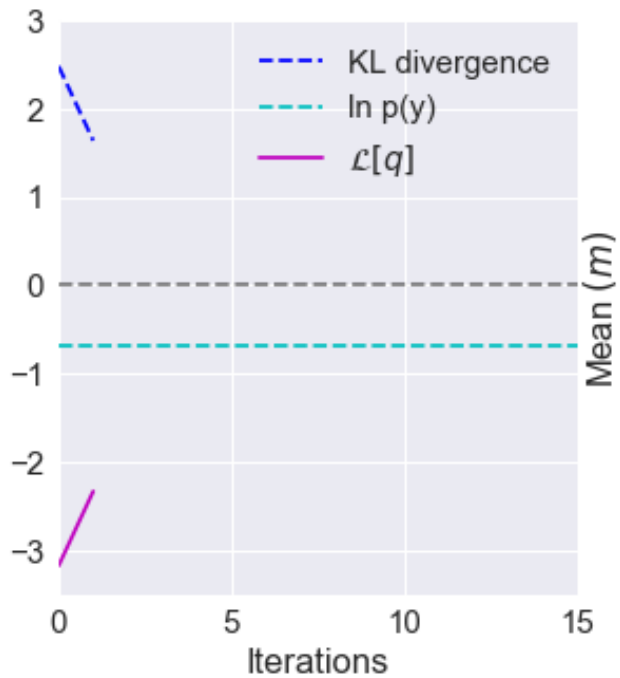

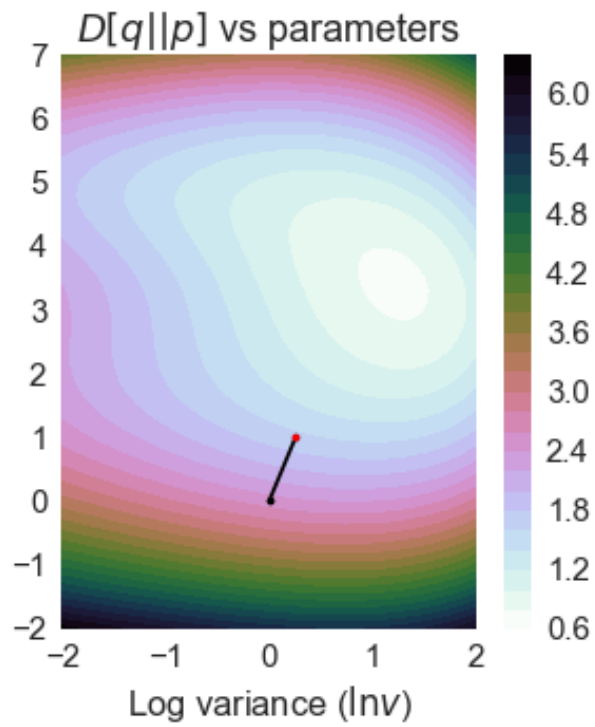

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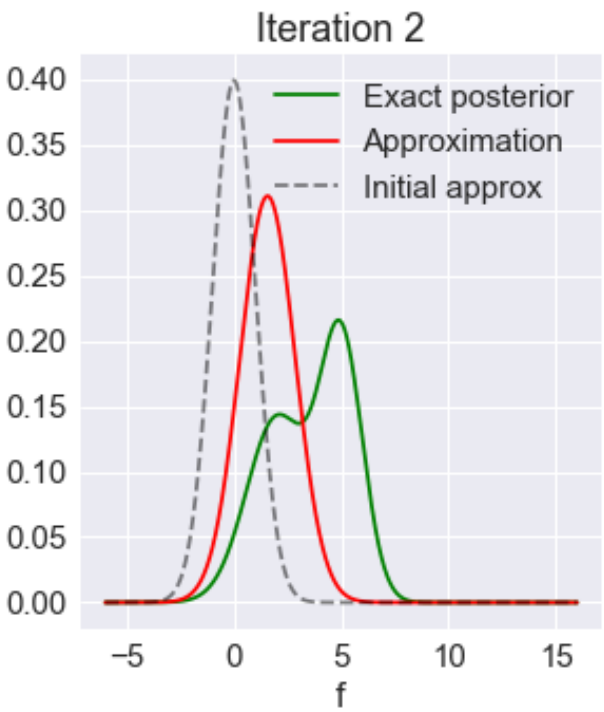

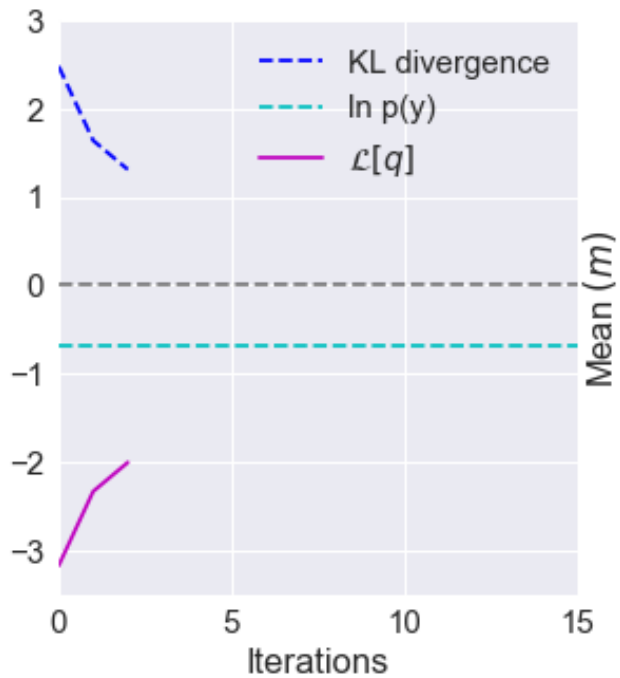

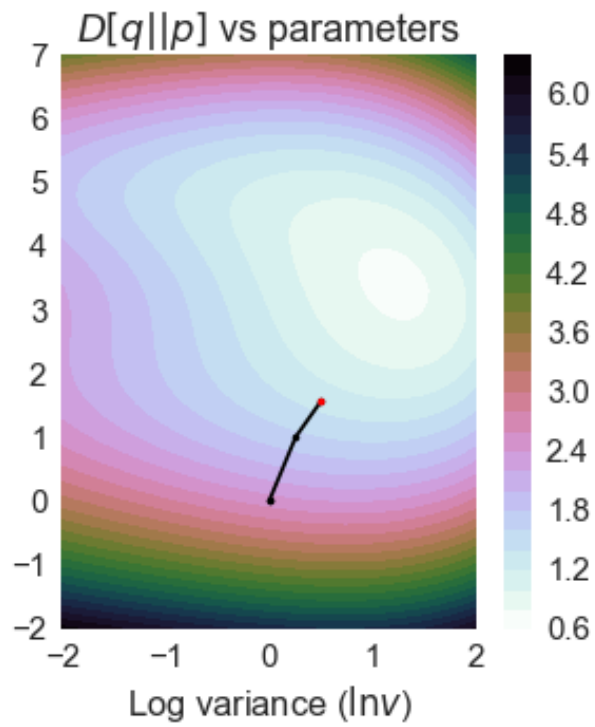

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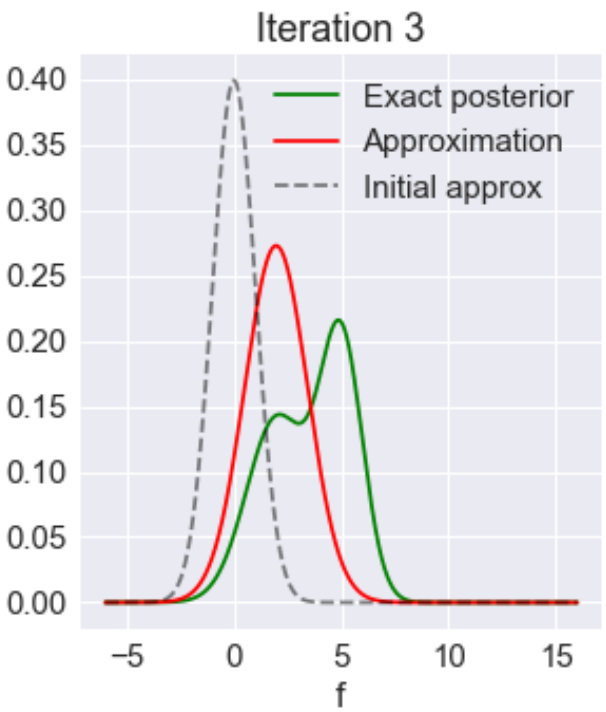

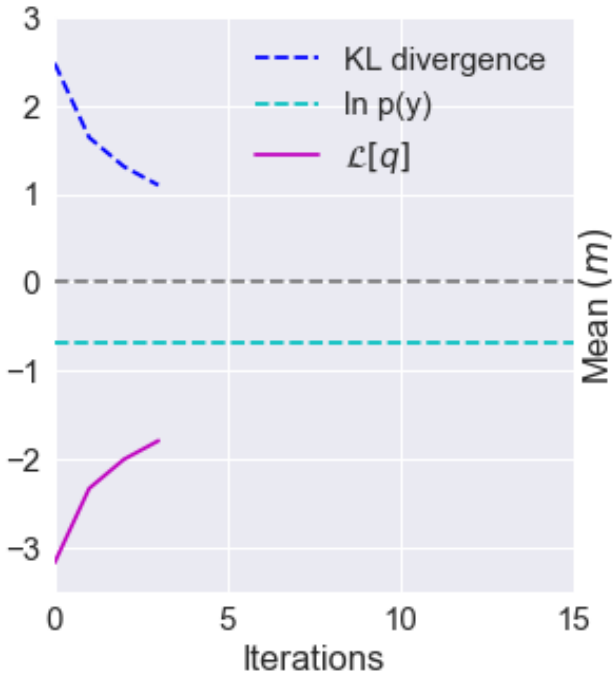

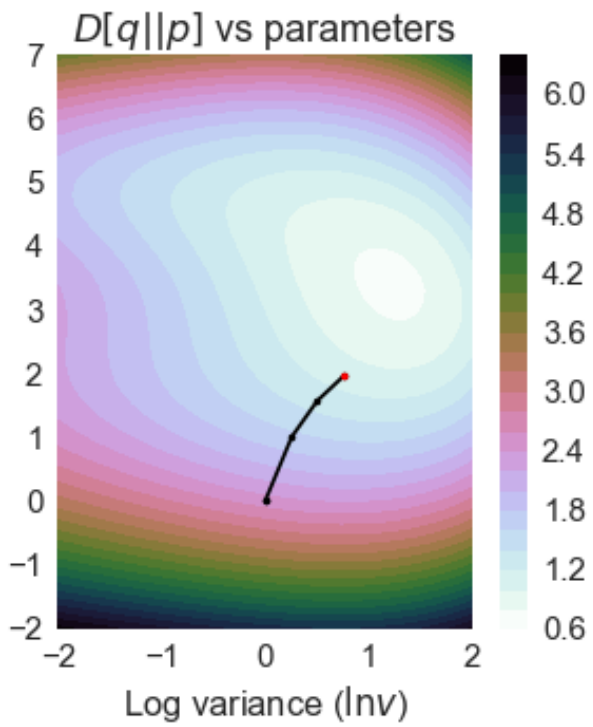

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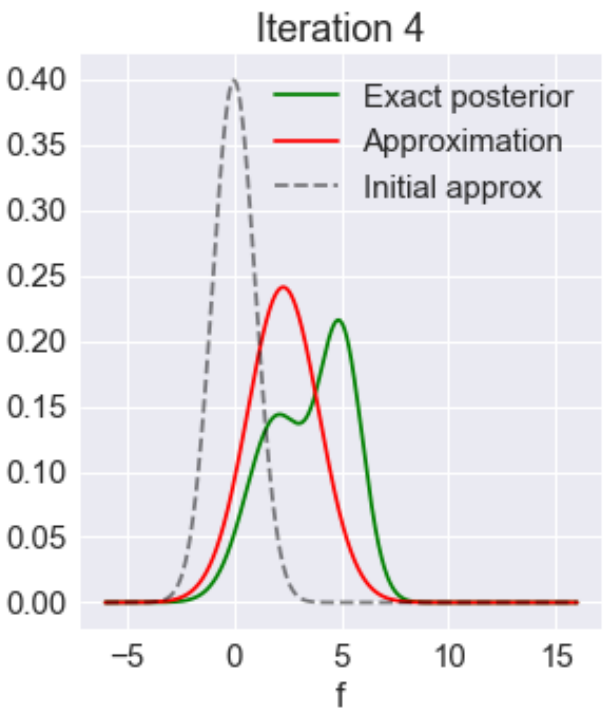

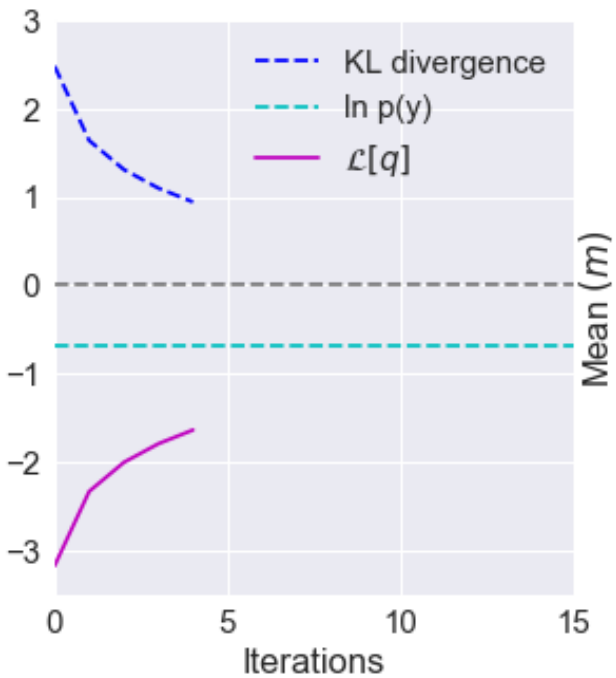

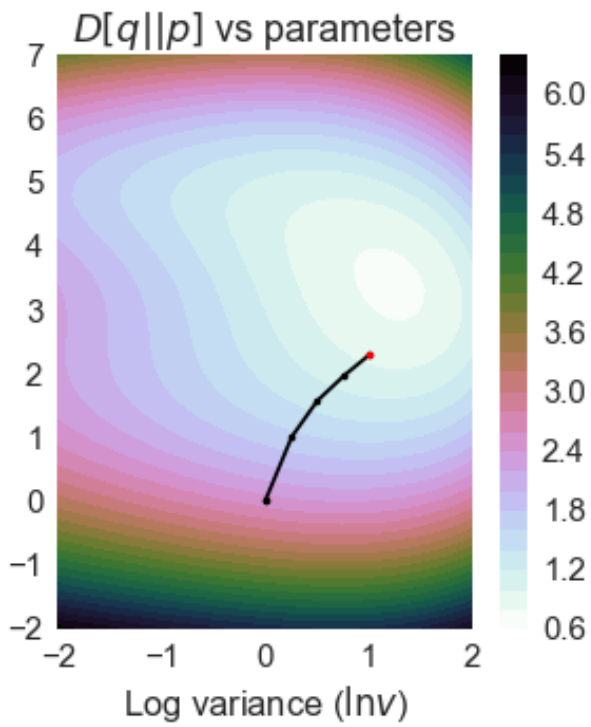

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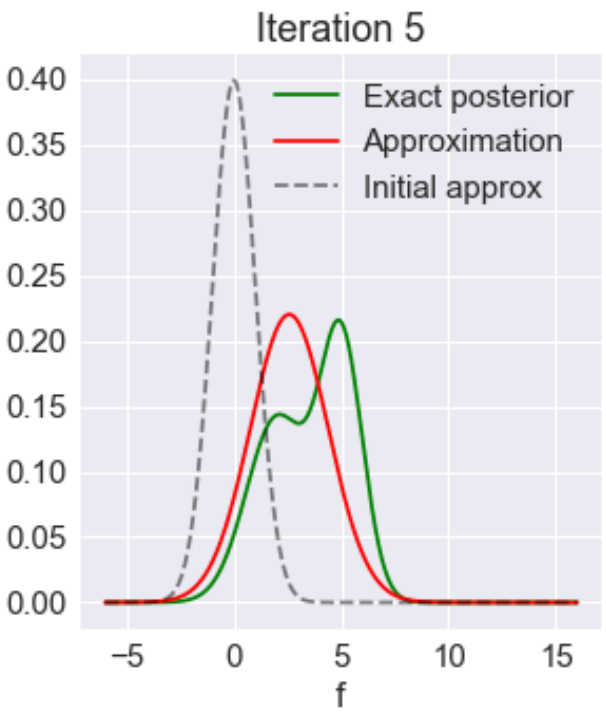

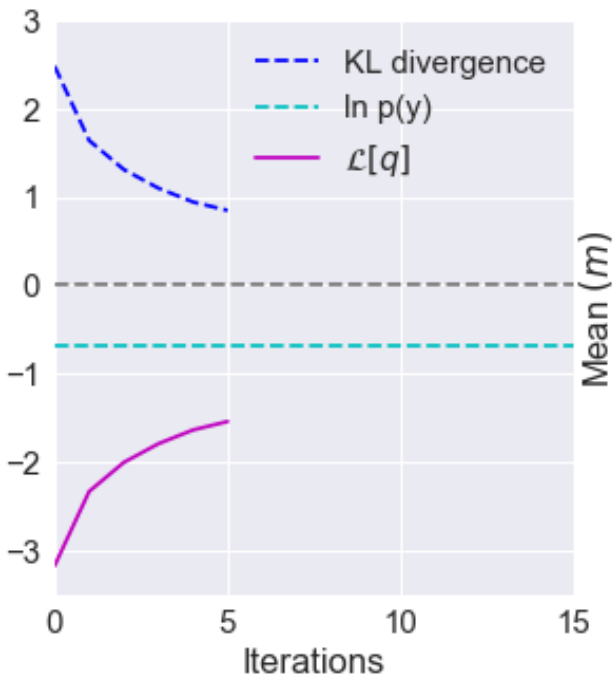

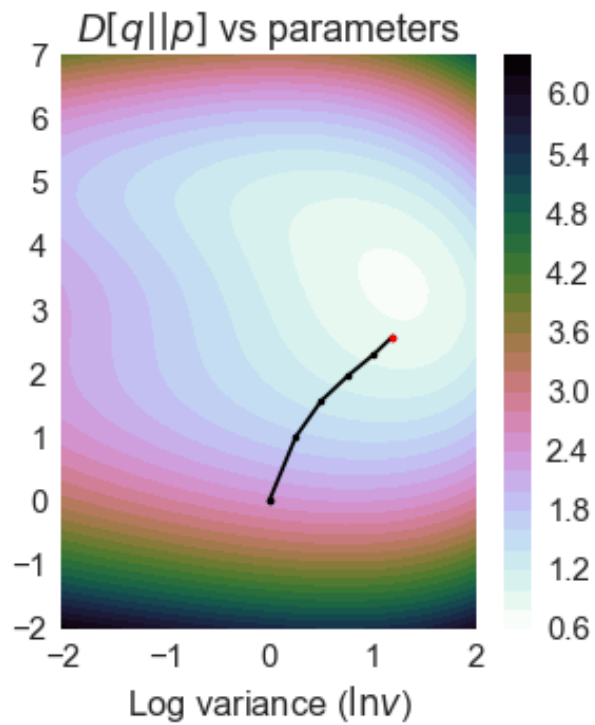

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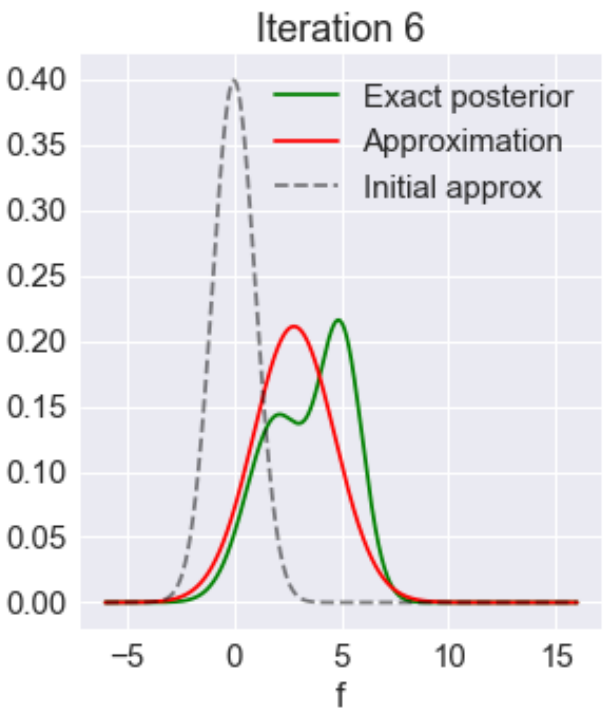

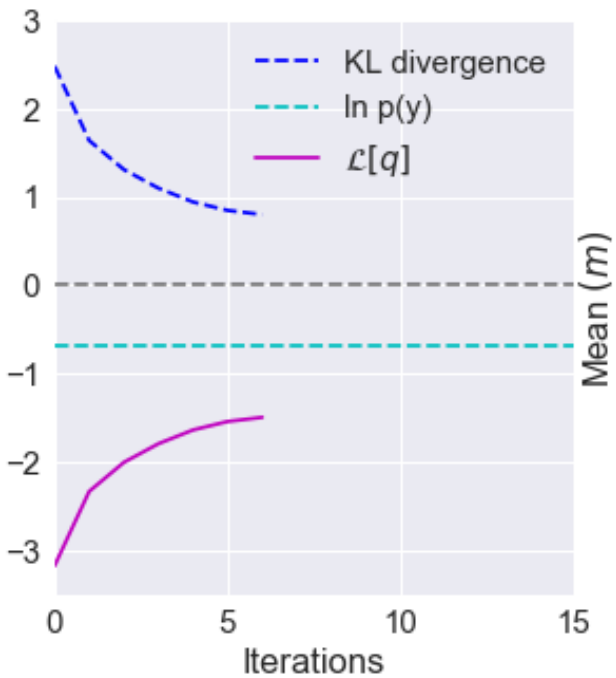

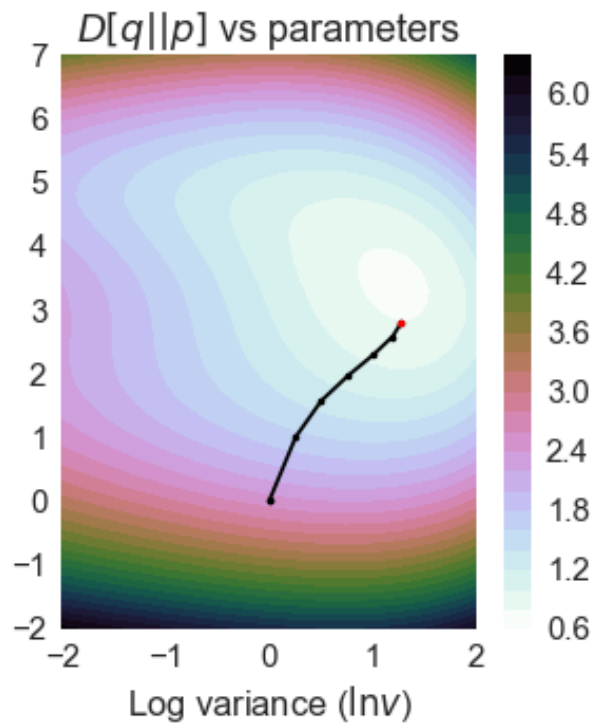

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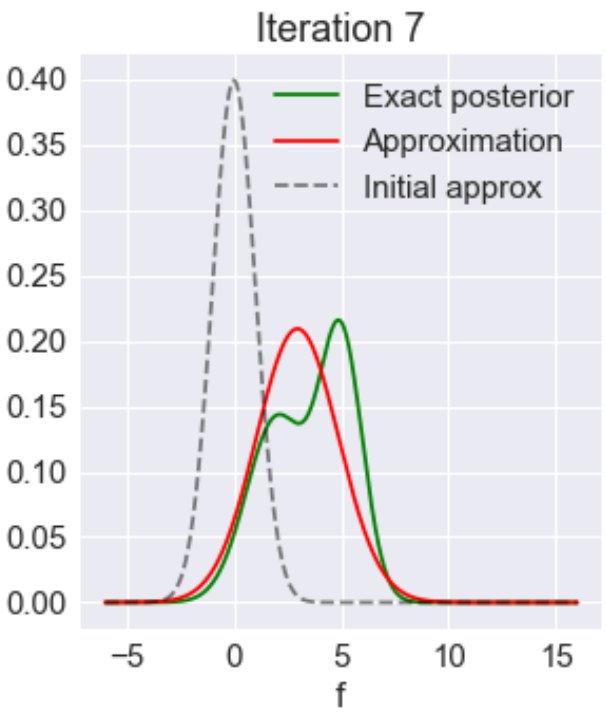

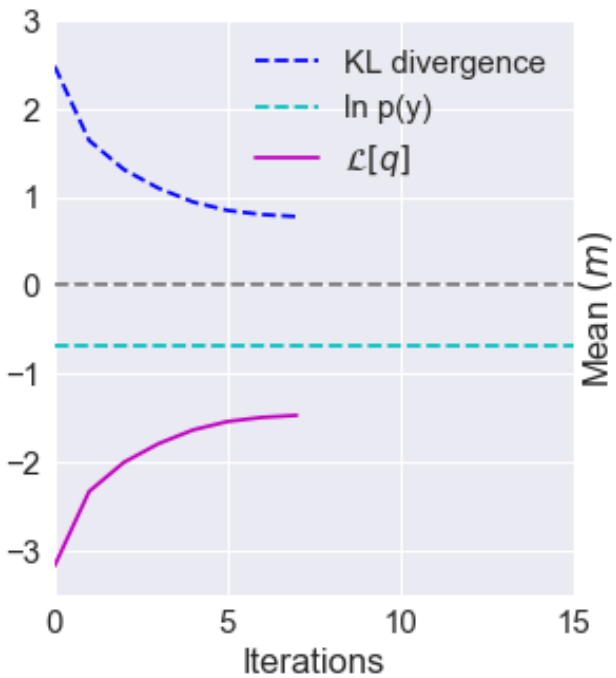

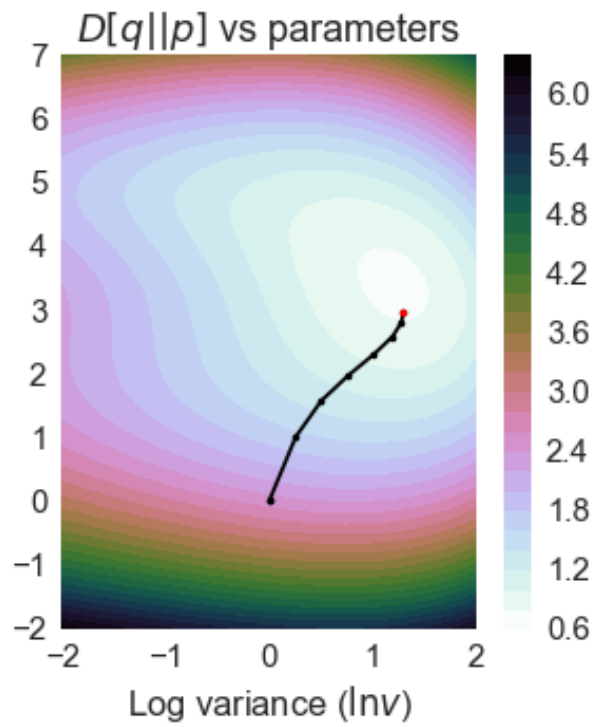

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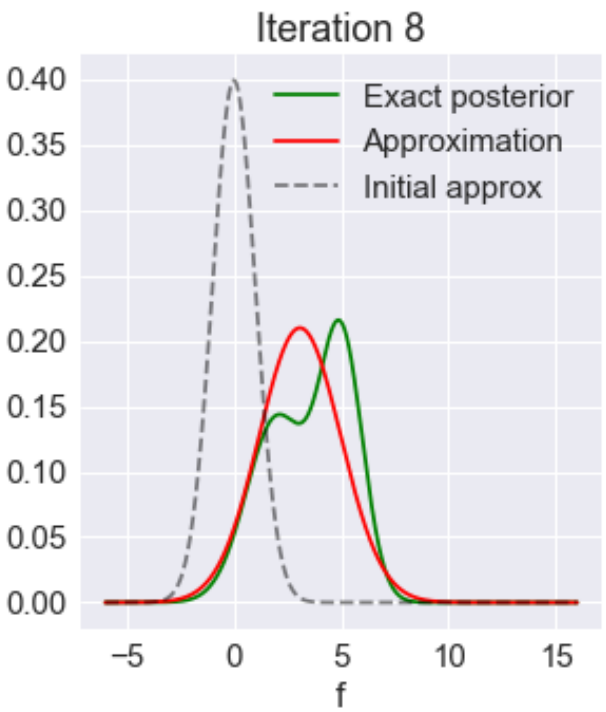

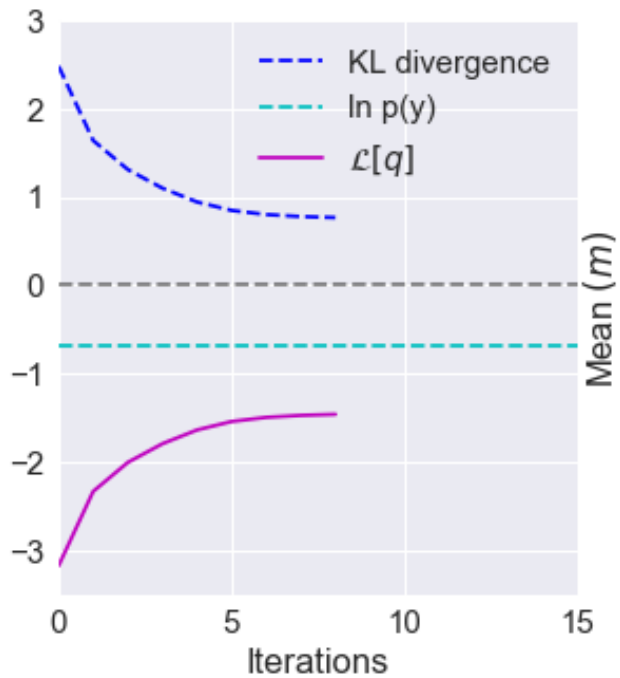

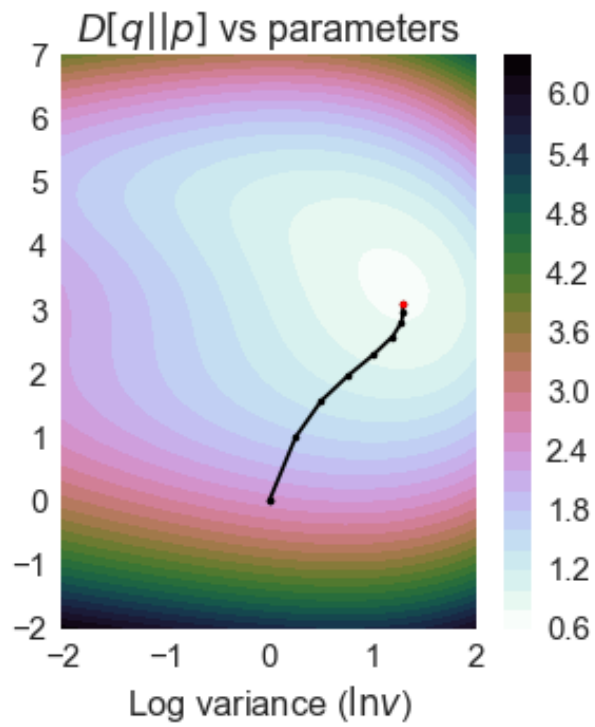

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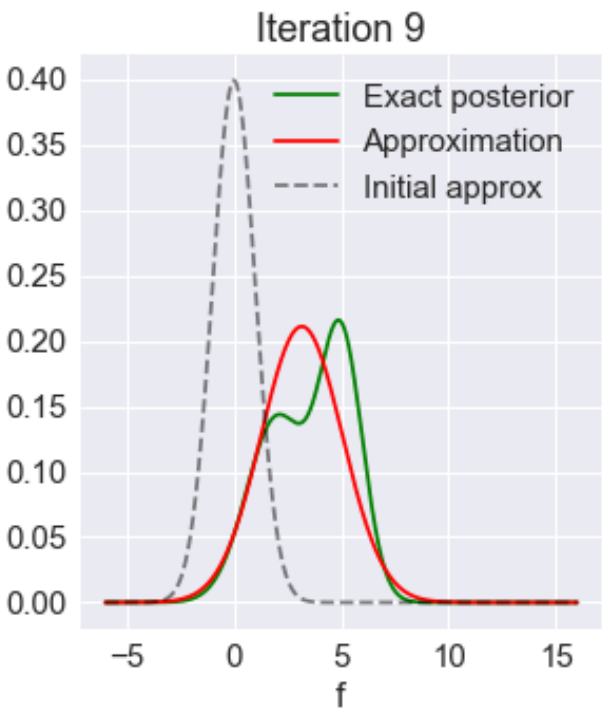

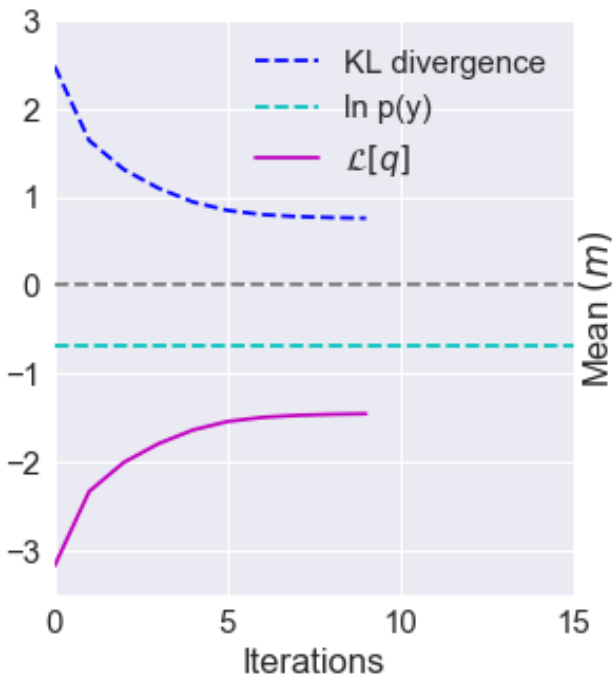

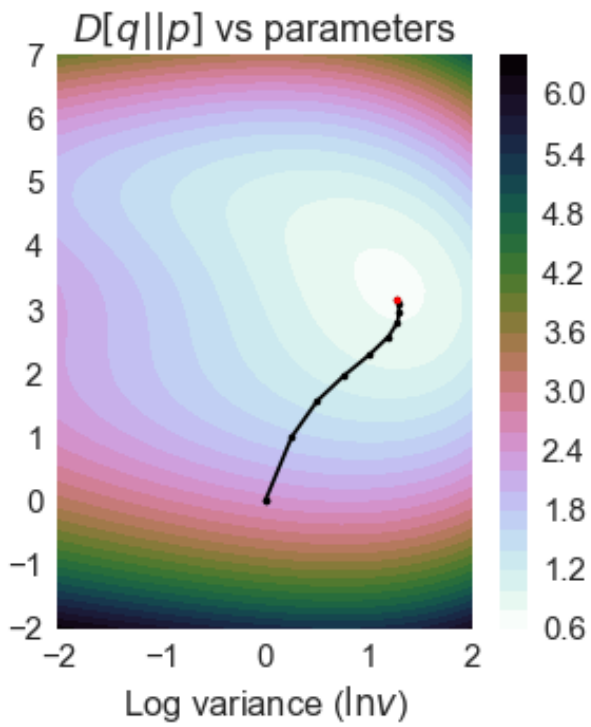

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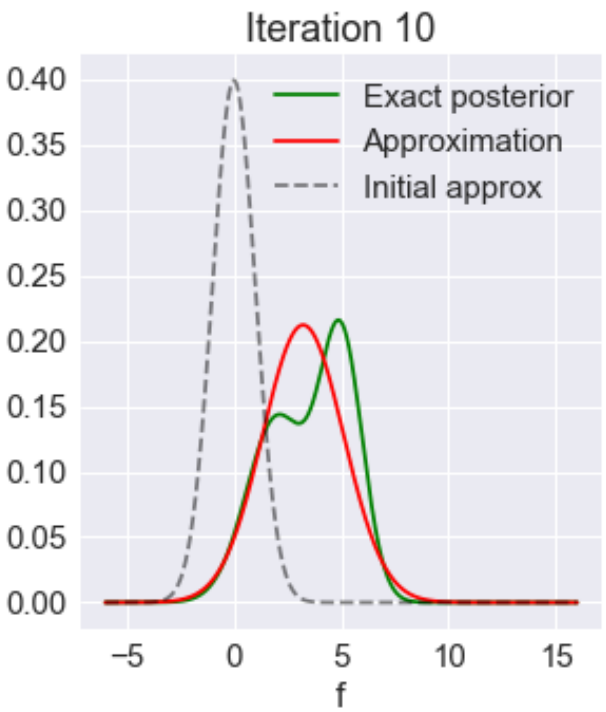

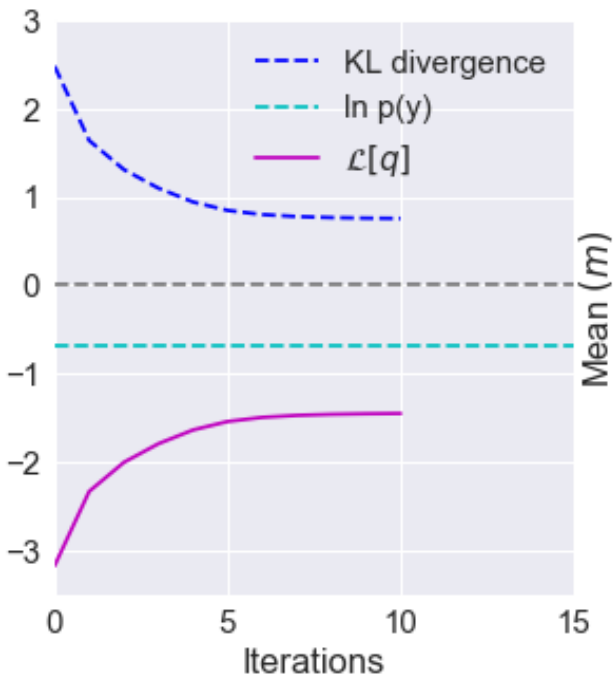

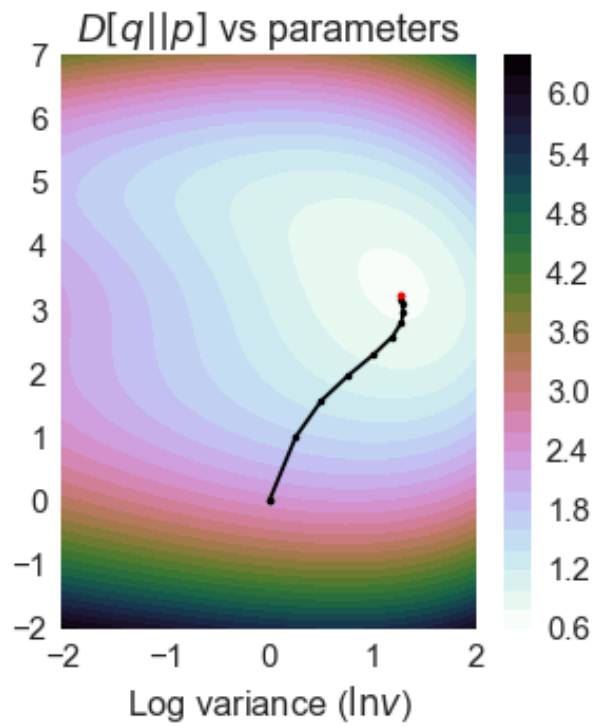

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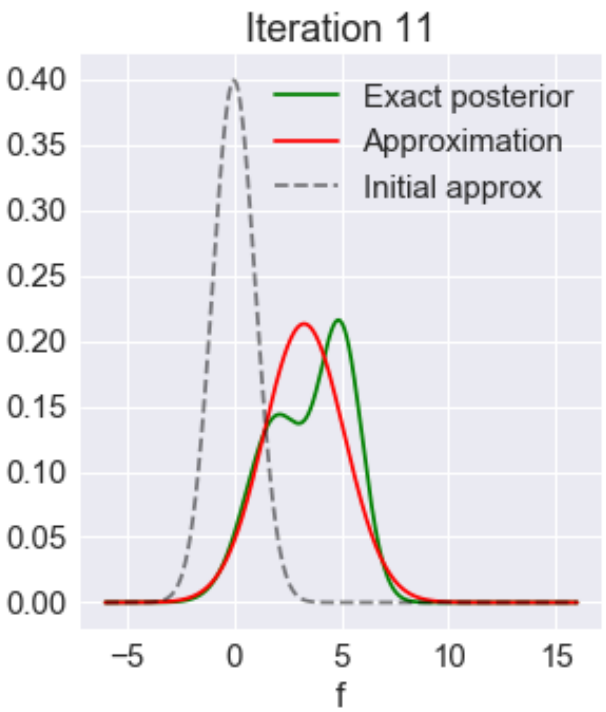

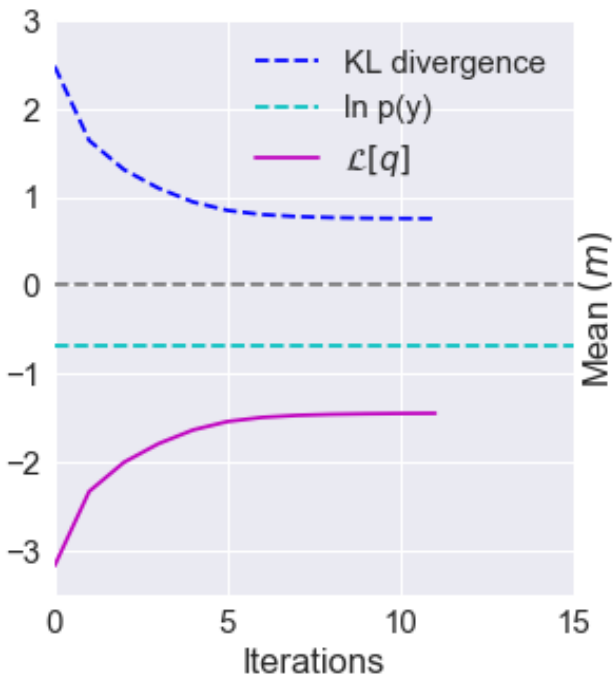

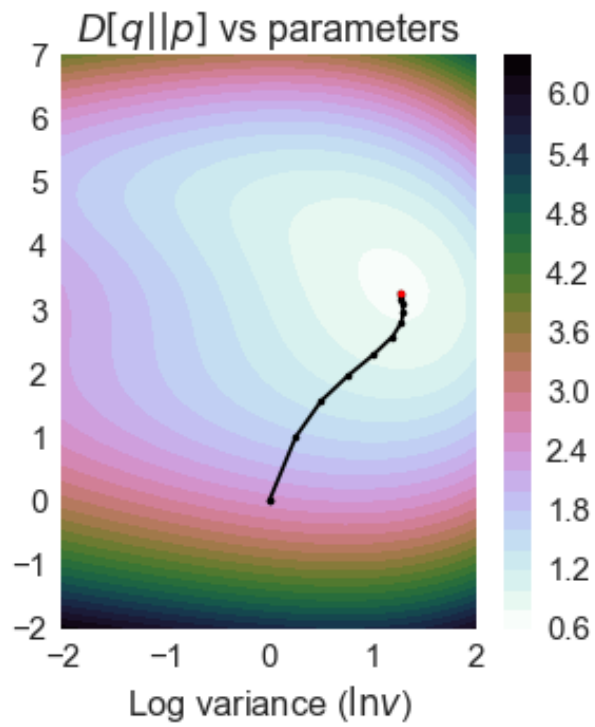

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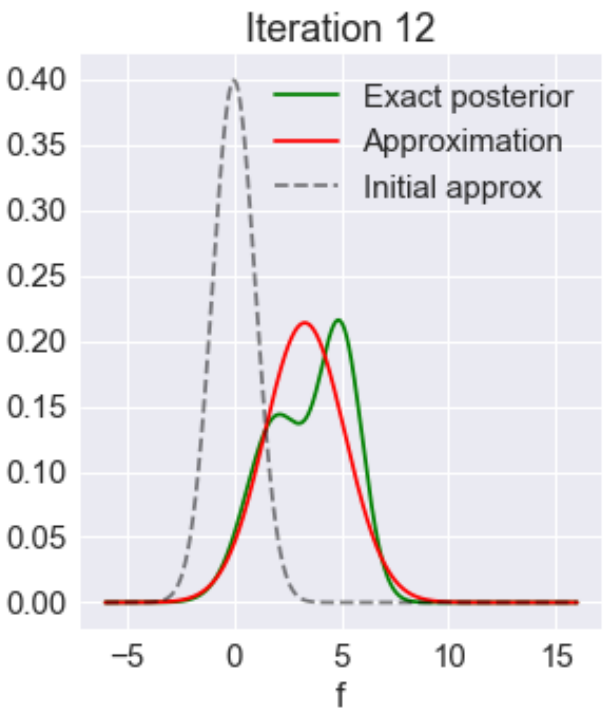

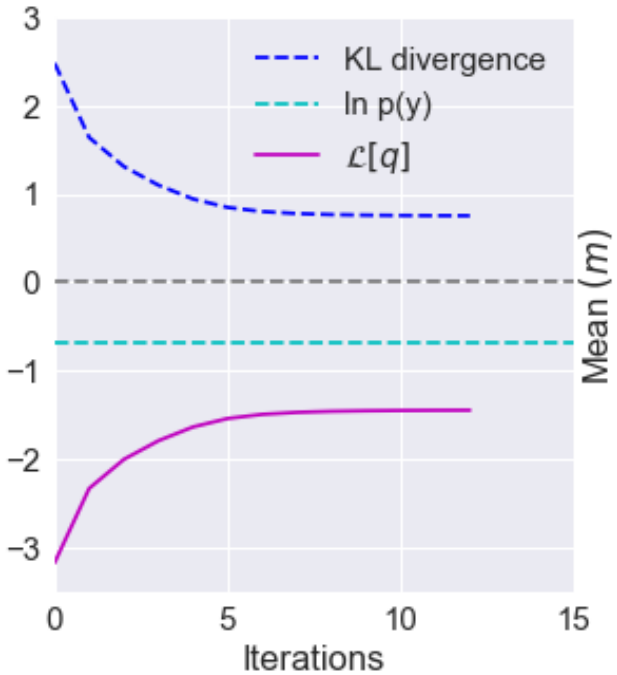

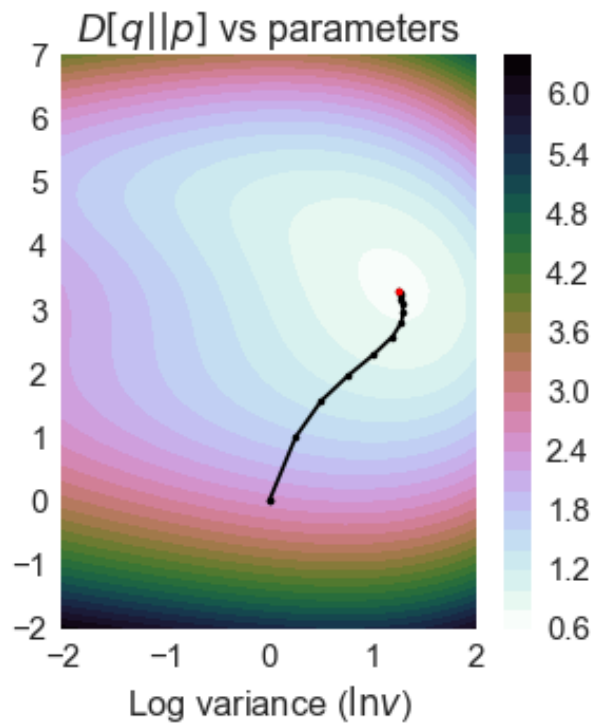

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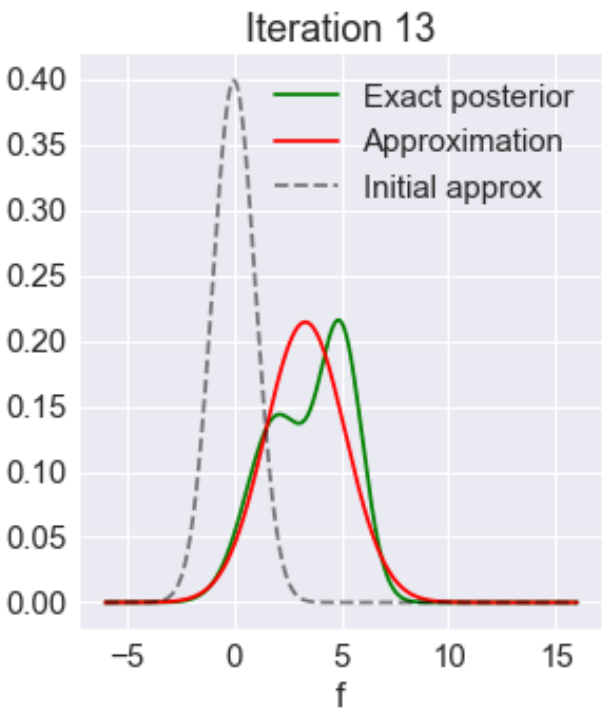

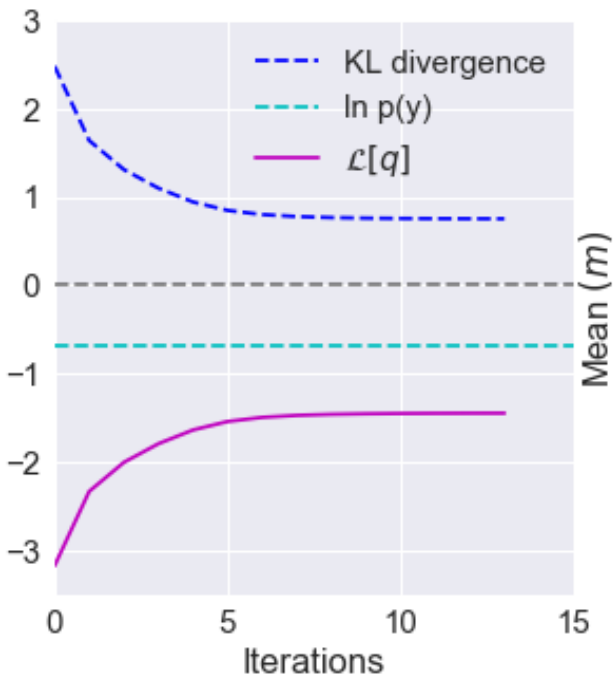

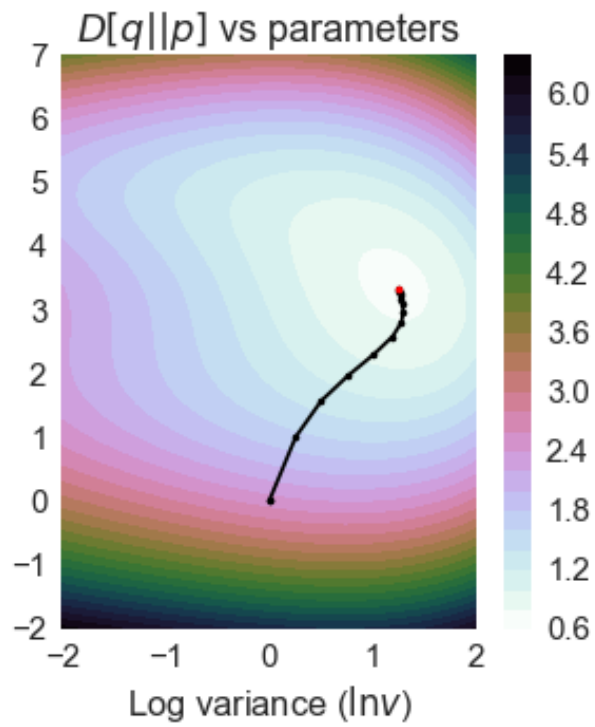

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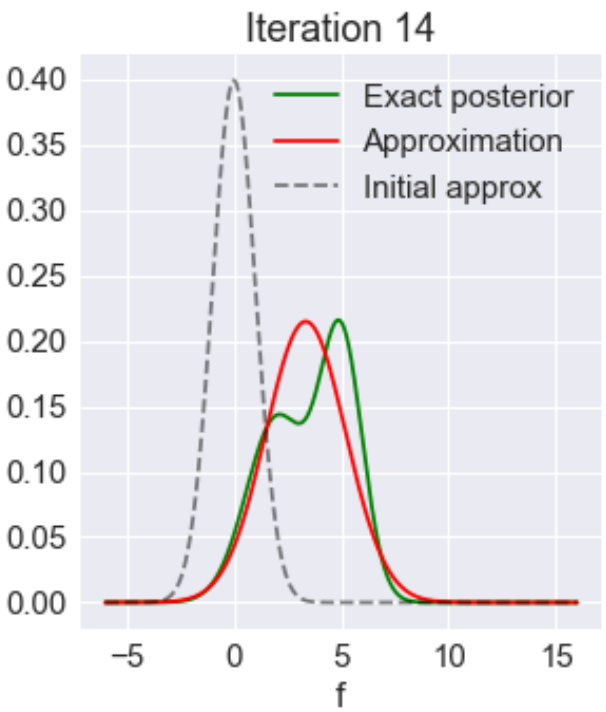

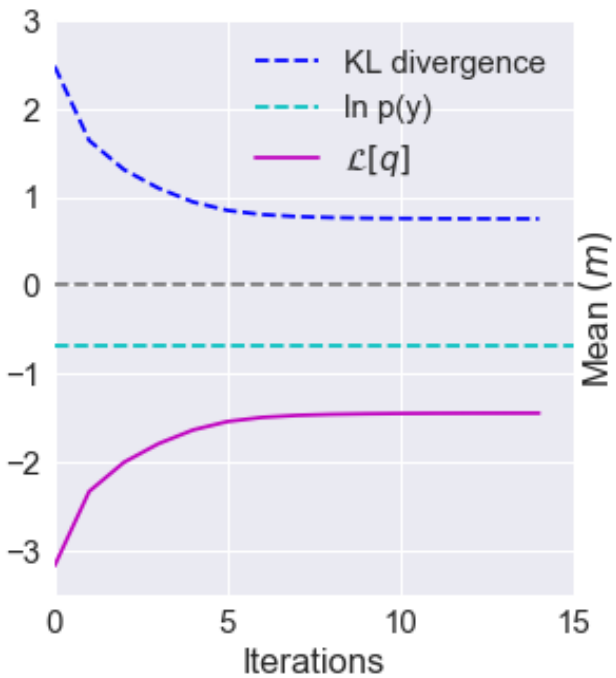

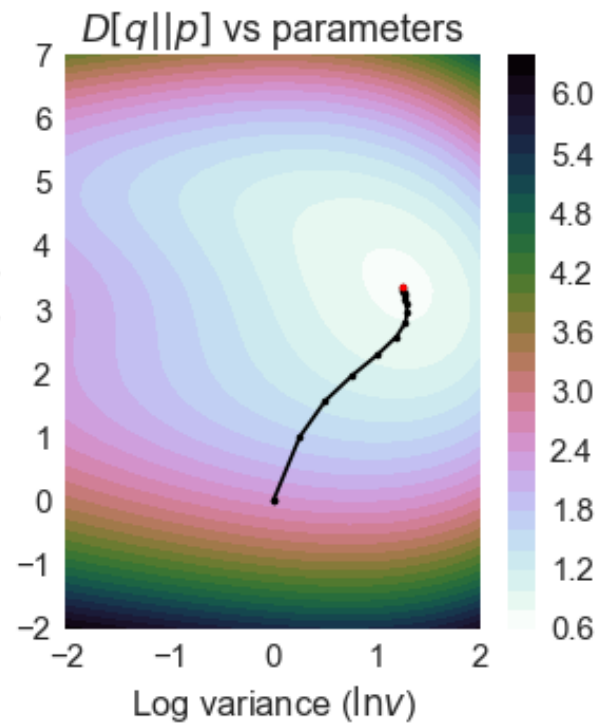

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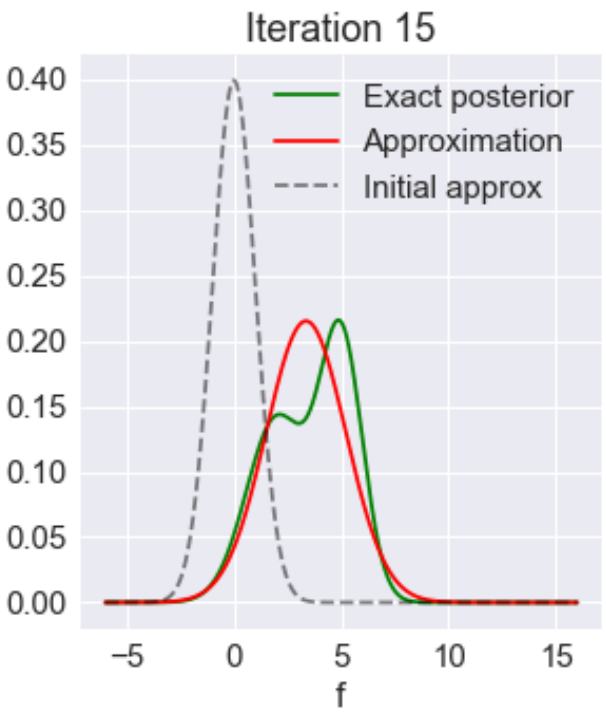

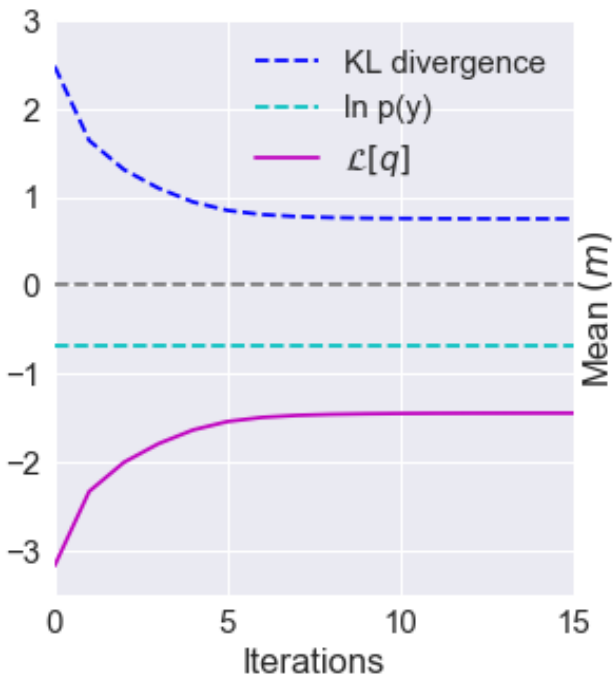

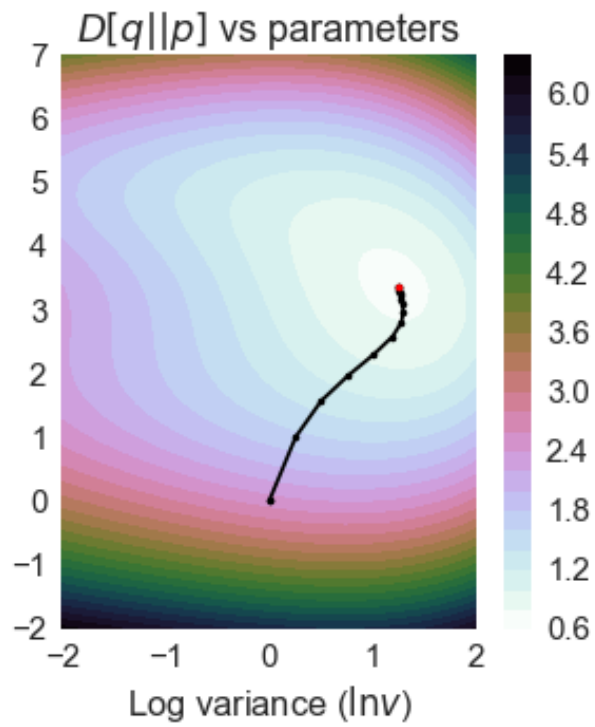

Computational challenges

- Let's see how we can use combine the ideas from variational inference with inducing points methods to solve the two computational problems:

1. The computational complexity of GPs is $\mathcal{O}(N^3)$
2. How to handle non-Gaussian likelihoods

Solution: Inducing point methods

- The main idea is to "represent" the information from the full dataset using a smaller "virtual" dataset

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- The main idea is to "represent" the information from the full dataset using a smaller "virtual" dataset
- Recall our GP model:

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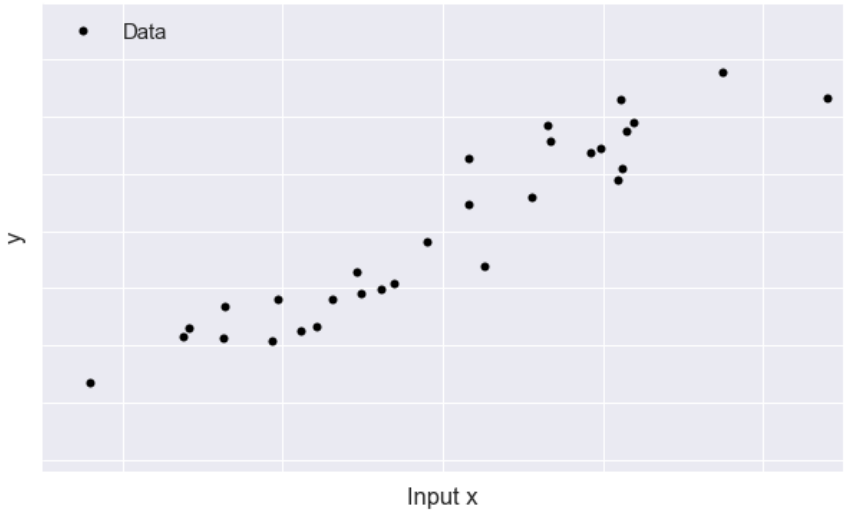
- Let u_m denote the value of the function f evaluated at each $\boldsymbol{z}_m$, i.e. $u_m = f(\boldsymbol{z}_m)$
- ... and $\boldsymbol{u} = [f(\boldsymbol{z}_1), f(\boldsymbol{z}_2), \ldots, f(\boldsymbol{z}_M)]$

Inducing point methods



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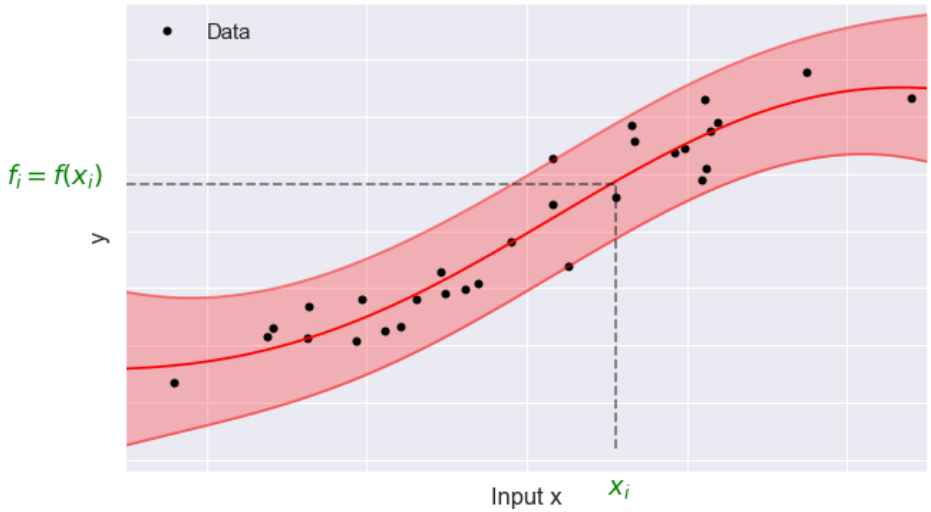

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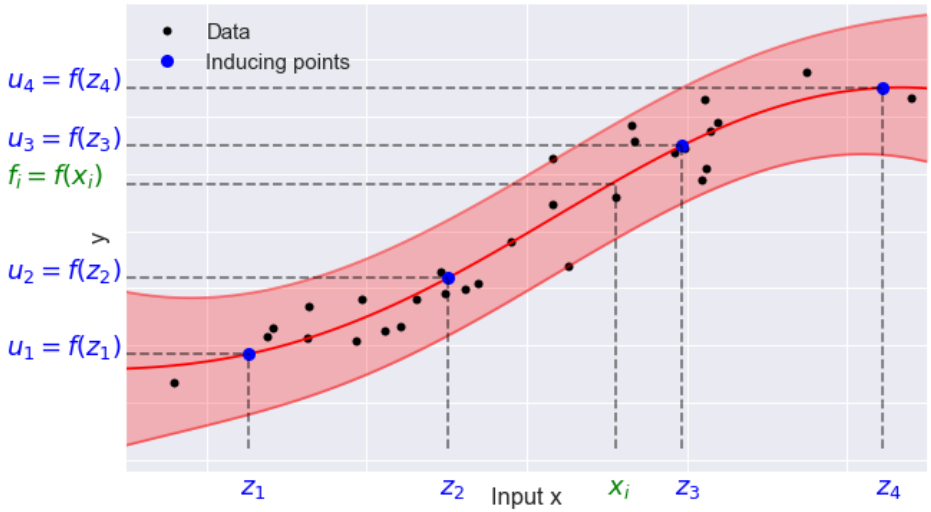

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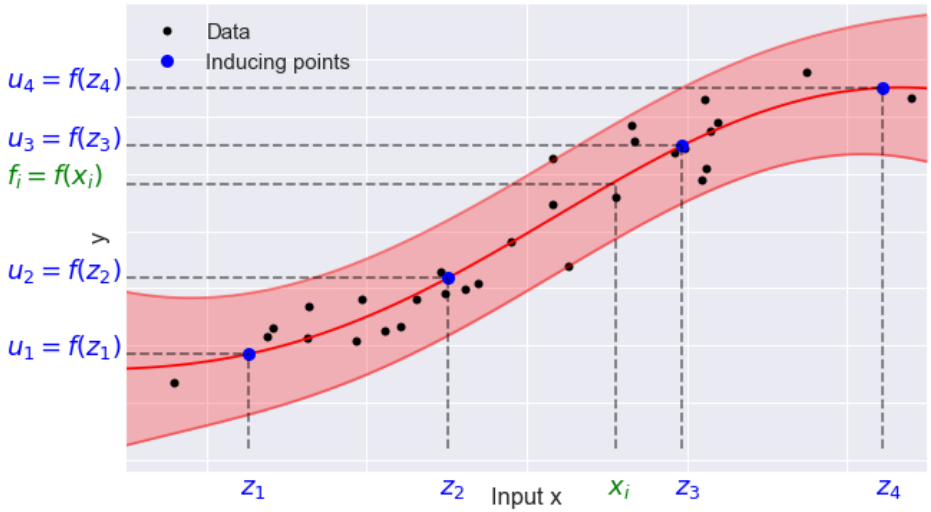

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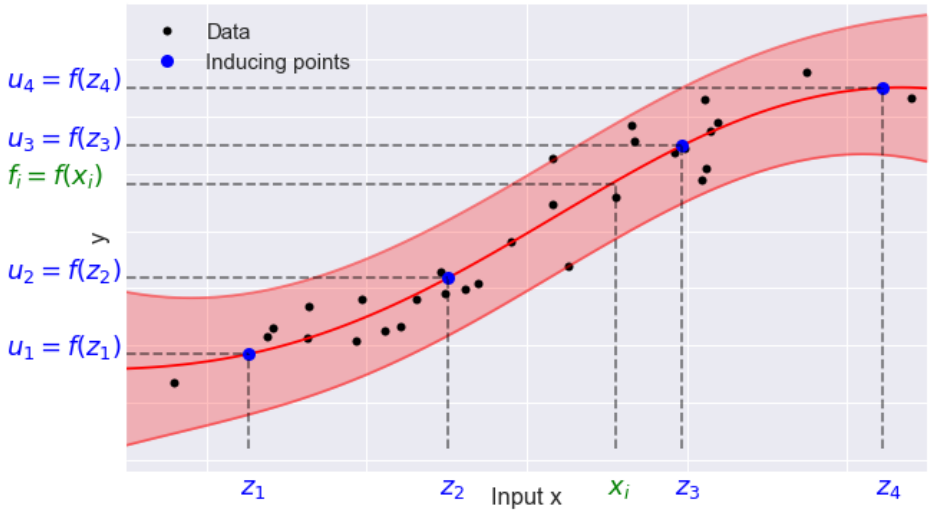

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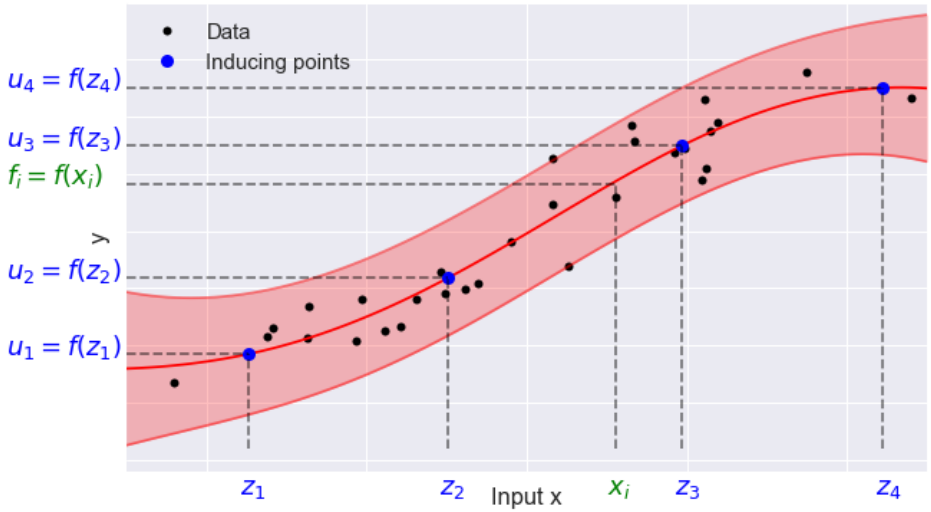

- Goal: choose the set of inducing points such that it contains the same information as the full dataset
- Remember: Both $u_j = f(\boldsymbol{z}_j)$ and $f_i = f(\boldsymbol{x}_i)$ are random variables
- Next step: Formulate joint model $p(\boldsymbol{y}, \boldsymbol{f}, \boldsymbol{u})$

Inducing point methods: the joint model

- The augmented model

$$p(\boldsymbol{y}, \boldsymbol{f}, \boldsymbol{u}) = p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}, \boldsymbol{u})$$

- Let's decompose the "augmented" model as follows

$$p(\boldsymbol{y}, \boldsymbol{f}, \boldsymbol{u}) = p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}|\boldsymbol{u})p(\boldsymbol{u})$$

- We can get back to the original model by marginalizing over $\boldsymbol{u}$

$$p(\boldsymbol{y}, \boldsymbol{f}) = \int p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}, \boldsymbol{u})\mathrm{d}\boldsymbol{u} = p(\boldsymbol{y}|\boldsymbol{f}) \int p(\boldsymbol{f}, \boldsymbol{u})\mathrm{d}\boldsymbol{u} = p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f})$$

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$$\ln p(\boldsymbol{y}) = \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln p(\boldsymbol{y}|\boldsymbol{f})\right] + \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln p(\boldsymbol{u})\right] - \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln q(\boldsymbol{u})\right] + \mathbb{D}\left[q||p\right]$$

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&\geq \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln p(\boldsymbol{y}|\boldsymbol{f})\right] + \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln p(\boldsymbol{u})\right] - \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln q(\boldsymbol{u})\right] \equiv \mathcal{L}_3
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The inducing points approximation

- **Take-away #1**: We can now tractably optimize the lower bound wrt. $\boldsymbol{m}$, $\boldsymbol{S}$, and even $\boldsymbol{z}$

$$\ln p(\boldsymbol{y}) \geq \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln p(\boldsymbol{y}|\boldsymbol{f})\right] + \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln p(\boldsymbol{u})\right] - \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln q(\boldsymbol{u})\right] \equiv \mathcal{L}_3$$

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- Let's have a closer look at the first term

$$\begin{aligned}
\mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln p(\boldsymbol{y}|\boldsymbol{f})\right] &= \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln \prod_{i=1}^{N} p(y_i|f_i)\right] = \sum_{i=1}^{N} \mathbb{E}_{q(\boldsymbol{u},\boldsymbol{f})}\left[\ln p(y_i|f_i)\right] \\
&= \sum_{i=1}^{N} \int\int q(\boldsymbol{u},\boldsymbol{f}) \ln p(y_i|f_i) \mathrm{d}\boldsymbol{u}\mathrm{d}\boldsymbol{f} \\
&= \sum_{i=1}^{N} \int\int p(f_i|\boldsymbol{u}) \mathcal{N}\left(\boldsymbol{u}|\boldsymbol{m},\boldsymbol{S}\right) \ln p(y_i|f_i) \mathrm{d}\boldsymbol{u}\mathrm{d}f_i \\
&= \sum_{i=1}^{N} \int\int p(f_i|\boldsymbol{u}) \mathcal{N}\left(\boldsymbol{u}|\boldsymbol{m},\boldsymbol{S}\right) \mathrm{d}\boldsymbol{u} \ln p(y_i|f_i) \mathrm{d}f_i
\end{aligned}$$

Decomposing the likelihood term

- Let's define the univariate distribution

$$q(f_i) \equiv \int p(f_i|\boldsymbol{u})\mathcal{N}\left(\boldsymbol{u}|\boldsymbol{m},\boldsymbol{S}\right)\mathrm{d}\boldsymbol{u} = \mathcal{N}\left(f_i|\boldsymbol{k}_{im}\boldsymbol{K}_{mm}^{-1}\boldsymbol{m}, \tilde{K}_{ii} + \boldsymbol{k}_{im}\boldsymbol{K}_{mm}^{-1}\boldsymbol{S}\boldsymbol{K}_{mm}^{-1}\boldsymbol{k}_{mi}\right)$$

- then we can write

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- Thus, the "likelihood term" decomposes into a sum over 1D integrals
- Can be solved analytically for Gaussian likelihoods and some classification likelihoods
- But it is fast to approximate 1D integrals using numerical integration for other likelihoods
- **Take away #2**: We can tractably optimize the bound even with non-Gaussian likelihoods

The resulting bound

- Substituting back into $\mathcal{L}_3$

$$\ln p(\boldsymbol{y}) \geq \mathcal{L}_3 = \sum_{i=1}^{N} \int q(f_i) \ln p(y_i|f_i) \mathrm{d}f_i + \mathbb{E}_{q(\boldsymbol{u})} \left[\ln p(\boldsymbol{u})\right] - \mathbb{E}_{q(\boldsymbol{u})} \left[\ln q(\boldsymbol{u})\right]$$

- We want to optimize $\mathcal{L}_3$ wrt. $\boldsymbol{\lambda} = \{\boldsymbol{m}, \boldsymbol{S}, \boldsymbol{z}\}$ using gradient-based methods

$$\nabla_{\boldsymbol{\lambda}} \mathcal{L}_3 = \nabla_{\boldsymbol{\lambda}} \sum_{i=1}^{N} \int q(f_i) \ln p(y_i|f_i) \mathrm{d}f_i + \nabla_{\boldsymbol{\lambda}} \mathbb{E}_{q(\boldsymbol{u})} \left[\ln p(\boldsymbol{u})\right] - \nabla_{\boldsymbol{\lambda}} \mathbb{E}_{q(\boldsymbol{u})} \left[\ln q(\boldsymbol{u})\right]$$

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- We can approximate the gradient as follows (mini-batching)

$$\nabla_{\boldsymbol{\lambda}} \sum_{i=1}^{N} \int q(f_i) \ln p(y_i|f_i) \mathrm{d}f_i \approx \frac{N}{|S|} \sum_{i \in S} \nabla_{\boldsymbol{\lambda}} \int q(f_i) \ln p(y_i|f_i) \mathrm{d}f_i$$

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- We can approximate the gradient as follows (mini-batching)

$$\nabla_{\boldsymbol{\lambda}} \sum_{i=1}^{N} \int q(f_i) \ln p(y_i|f_i) \mathrm{d}f_i \approx \frac{N}{|S|} \sum_{i \in S} \nabla_{\boldsymbol{\lambda}} \int q(f_i) \ln p(y_i|f_i) \mathrm{d}f_i$$

- **Take away #3**: Because it decomposes as a sum over the data points, the bound becomes amendable to stochastic gradient descent (mini-batching) and hence, we can scale the method to really really large datasets!

Example from the paper

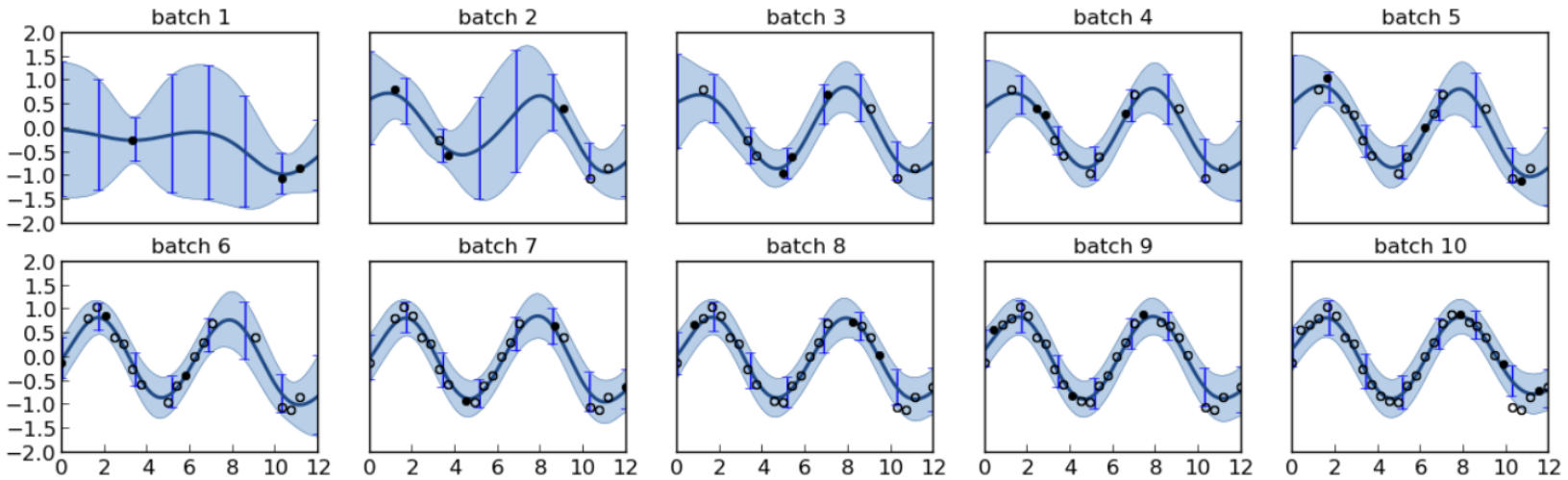


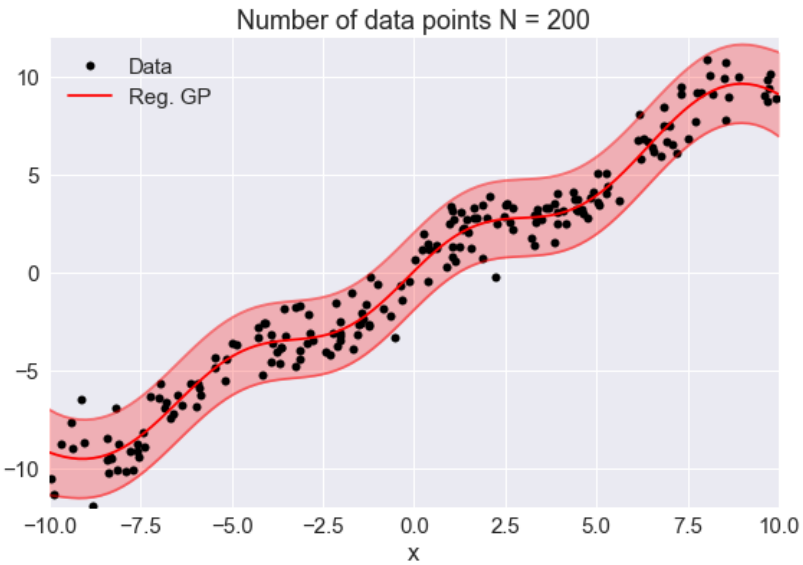
Figure 2: Stochastic variational inference on a trivial GP regression problem. Each pane shows the posterior of the GP after a batch of data, marked as solid points. Previoulsy seen (and discarded) data are marked as empty points, the distribution $q(\mathbf{u})$ is represented by vertical errorbars.

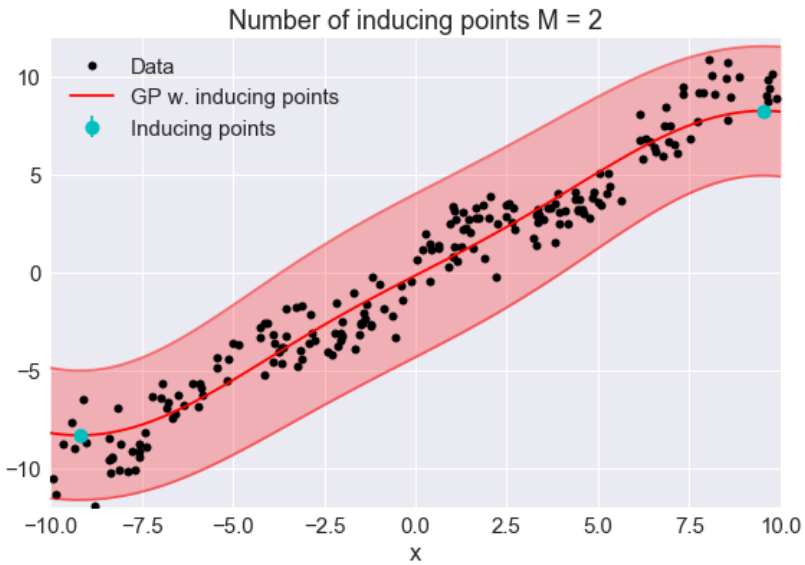
(from Hensman et al: Gaussian processes for big data)

Inducing points method summary

- The inducing point approximation allows us to
  - ... scale Gaussian processes to big data
  - ... use non-Gaussian likelihoods
- It reduces the computational complexity from $\mathcal{O}(N^3)$ to $\mathcal{O}(M^3)$, where $M \ll N$
- It's implemented in most GP toolboxes, e.g. GPy (numpy) and gpflow (tensorflow)

Example: Number of inducing points





- We can think of the number of inducing points as a parameter that trades off speed for accuracy

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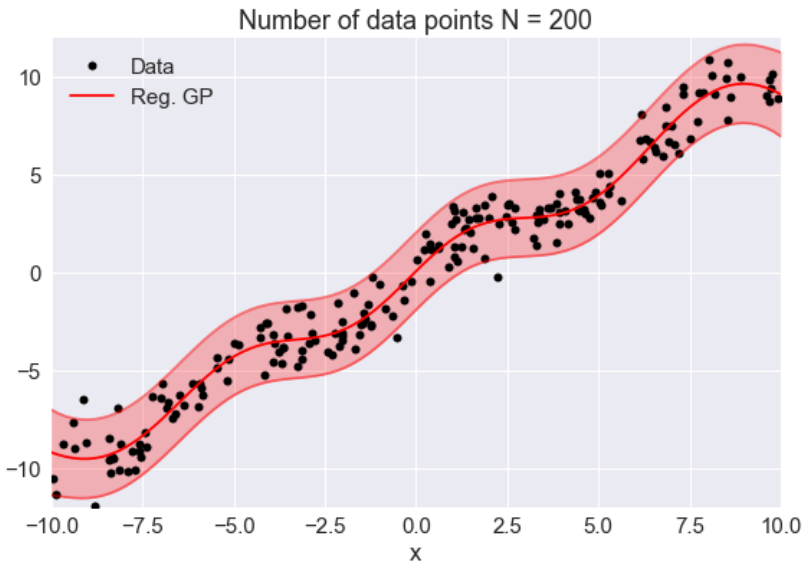

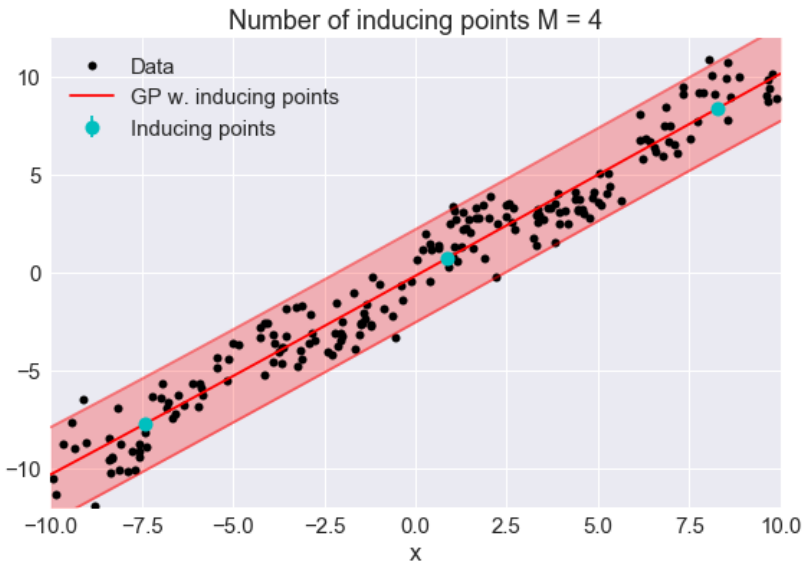

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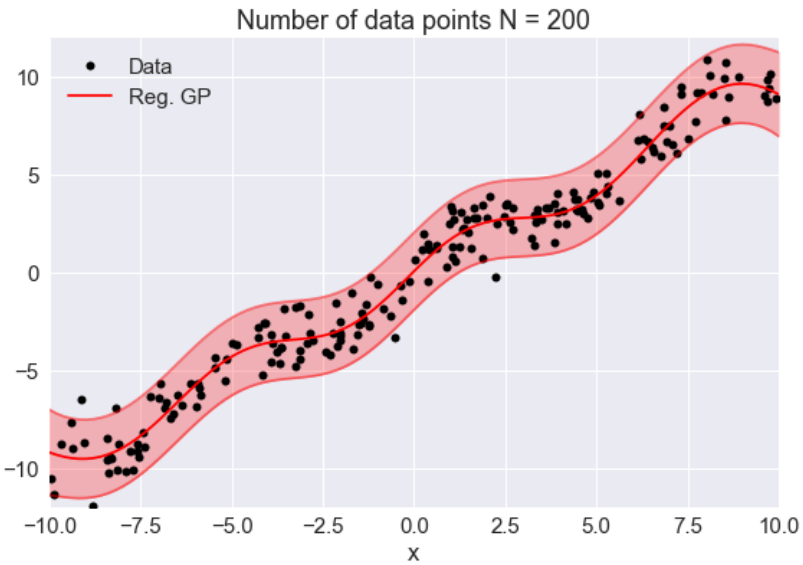

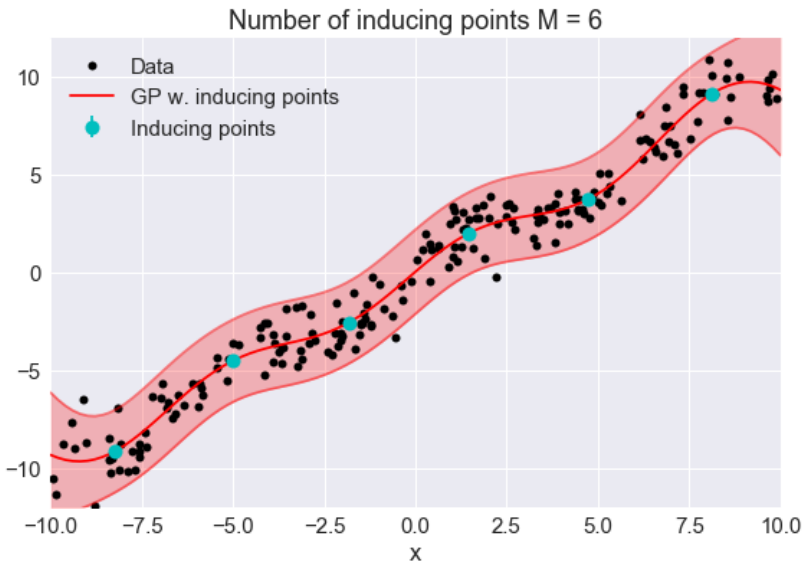

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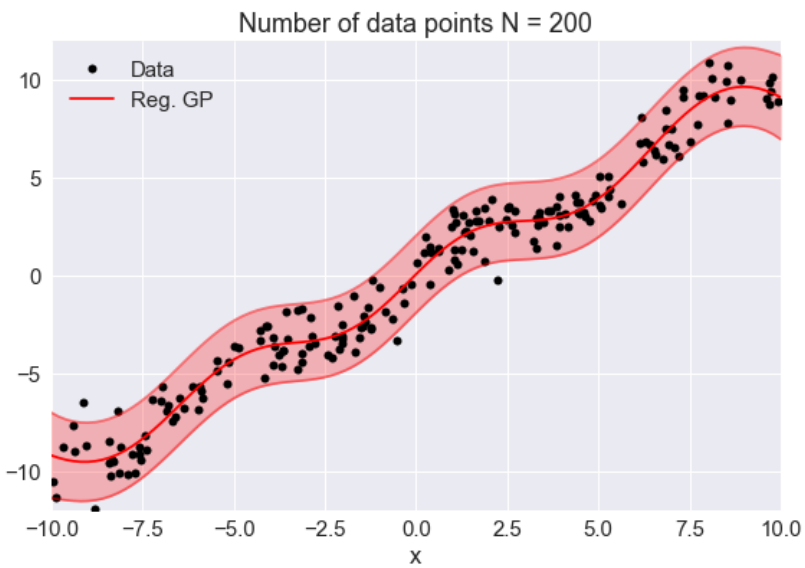

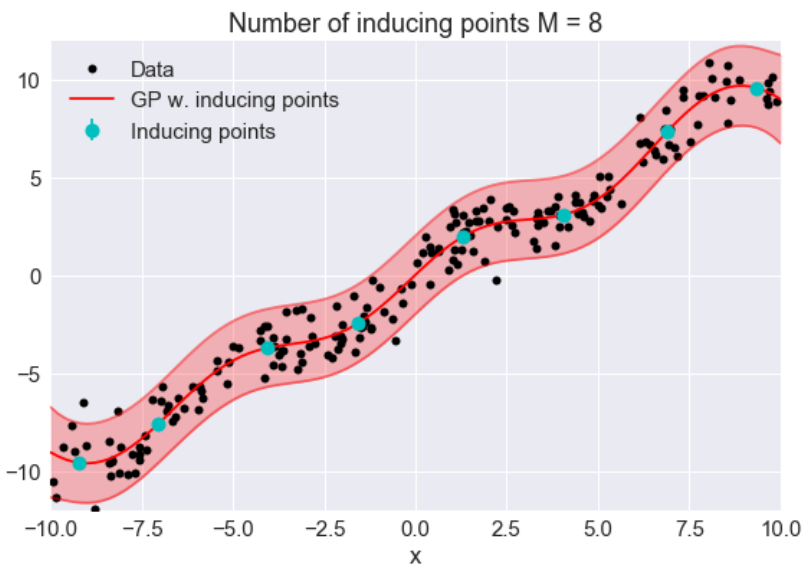

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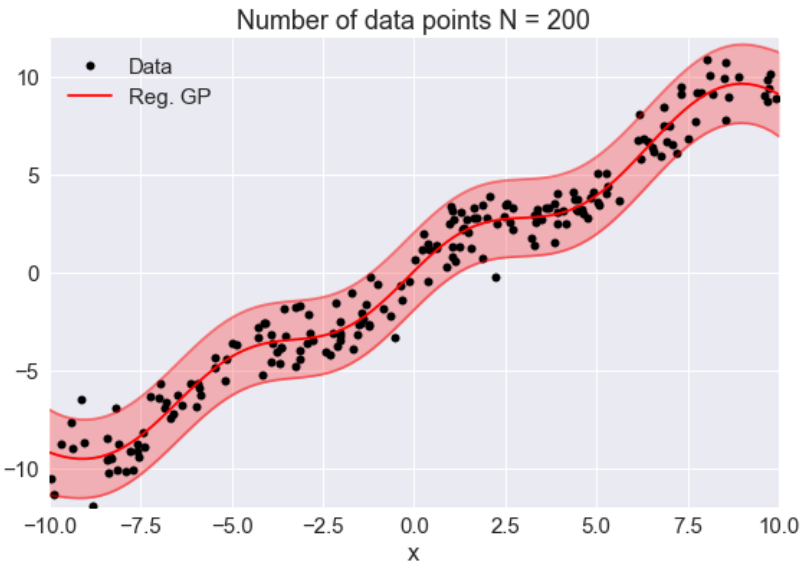

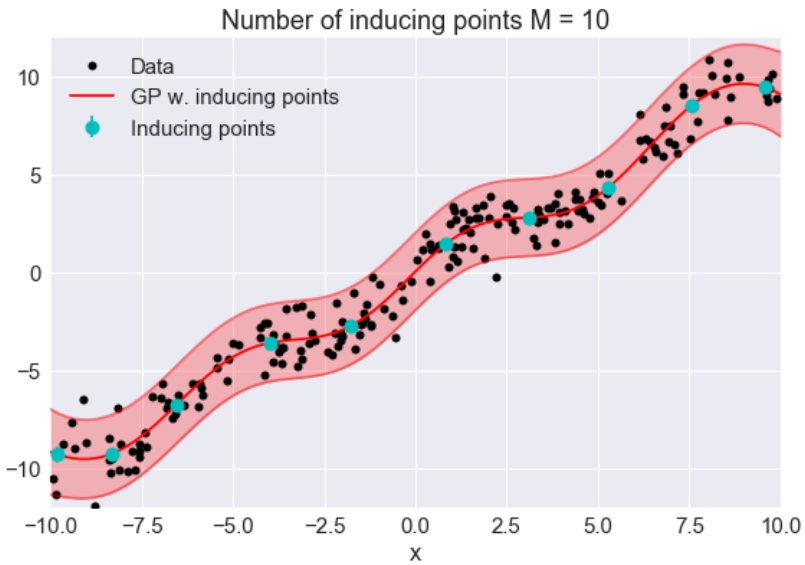

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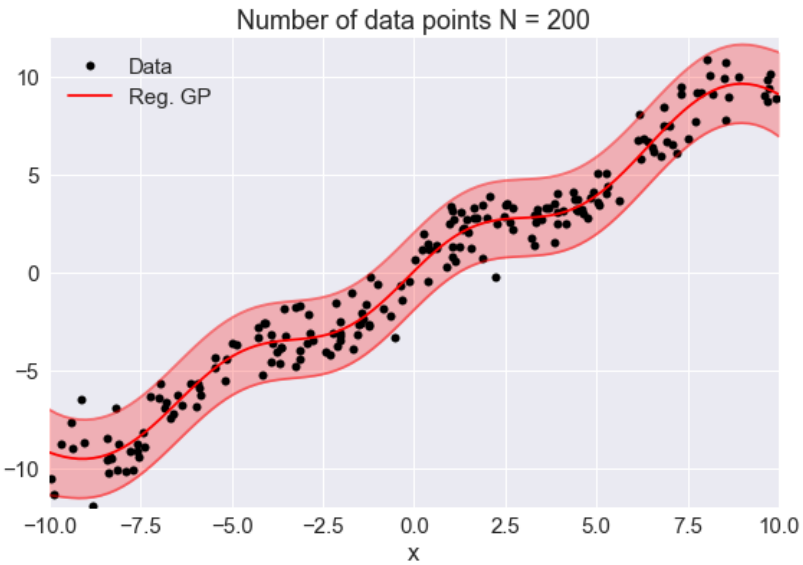
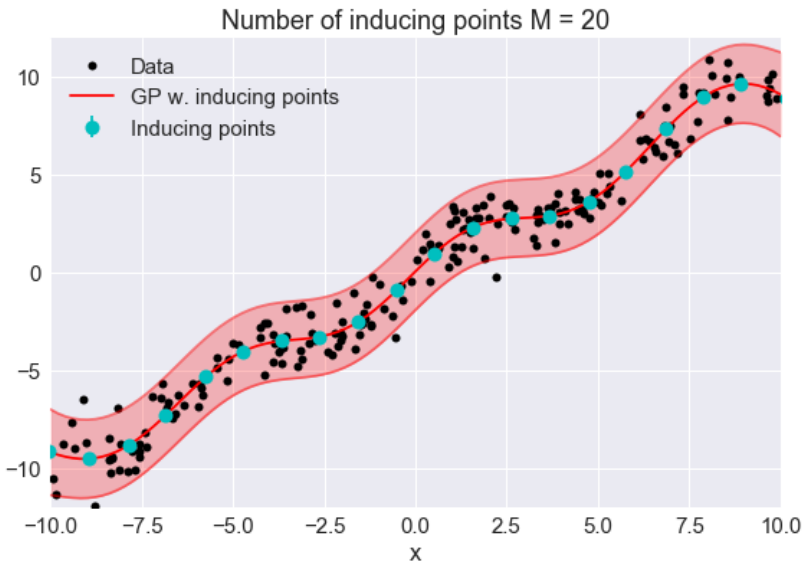


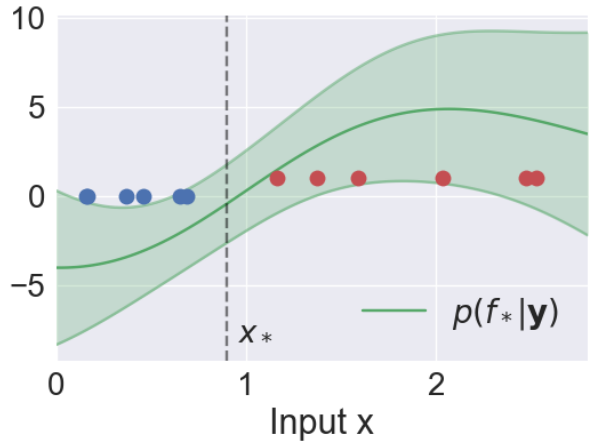


- We can think of the number of inducing points as a parameter that trades off speed for accuracy

Gaussian process classification: Inference

Three steps to compute the predictive distribution for a new test point $\boldsymbol{x}_*$

$$p\left(\boldsymbol{y}, \boldsymbol{f}\right) = \prod_{n=1}^{N} p(y_n|f_n)p(\boldsymbol{f}) = \prod_{n=1}^{N} \phi\left(y_n \cdot f_n\right) \mathcal{N}\left(\boldsymbol{f}\middle|\boldsymbol{0}, \boldsymbol{K}\right)$$

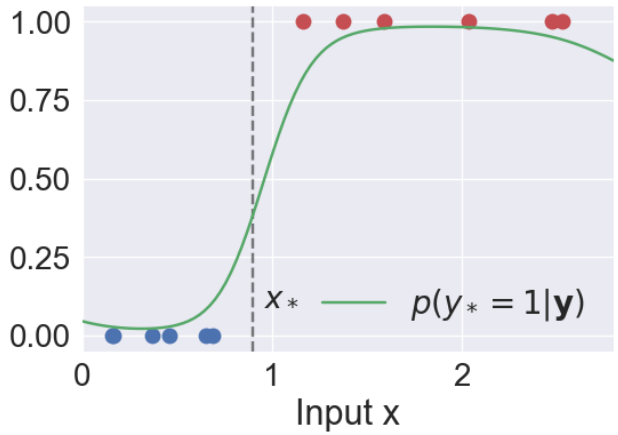


- Step 1: Compute posterior distribution of $p(\boldsymbol{f}|\boldsymbol{y})$:

$$p(\boldsymbol{f}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f})}{p(\boldsymbol{y})} \approx q(\boldsymbol{f})$$

- Step 2: Compute posterior of f_* for new test point $\boldsymbol{x}_*$:

$$p(f_*\left|\boldsymbol{y}\right) = \int p\left(f_*|\boldsymbol{f}\right) p\left(\boldsymbol{f}\middle|\boldsymbol{y}\right) \mathrm{d}\boldsymbol{f} \approx \int p\left(f_*|\boldsymbol{f}\right) q\left(\boldsymbol{f}\right) \mathrm{d}\boldsymbol{f}$$



- Step 3: Compute predictive distribution

$$p(y_*|\boldsymbol{y}) = \int \phi\left(y_* \cdot f_*\right) p(f_*\left|\boldsymbol{y}\right)\mathrm{d}f_*$$

Predictive distribution

- Using the (approximate) posterior $q(f_*)$, we can compute $p(y_*|\boldsymbol{y})$

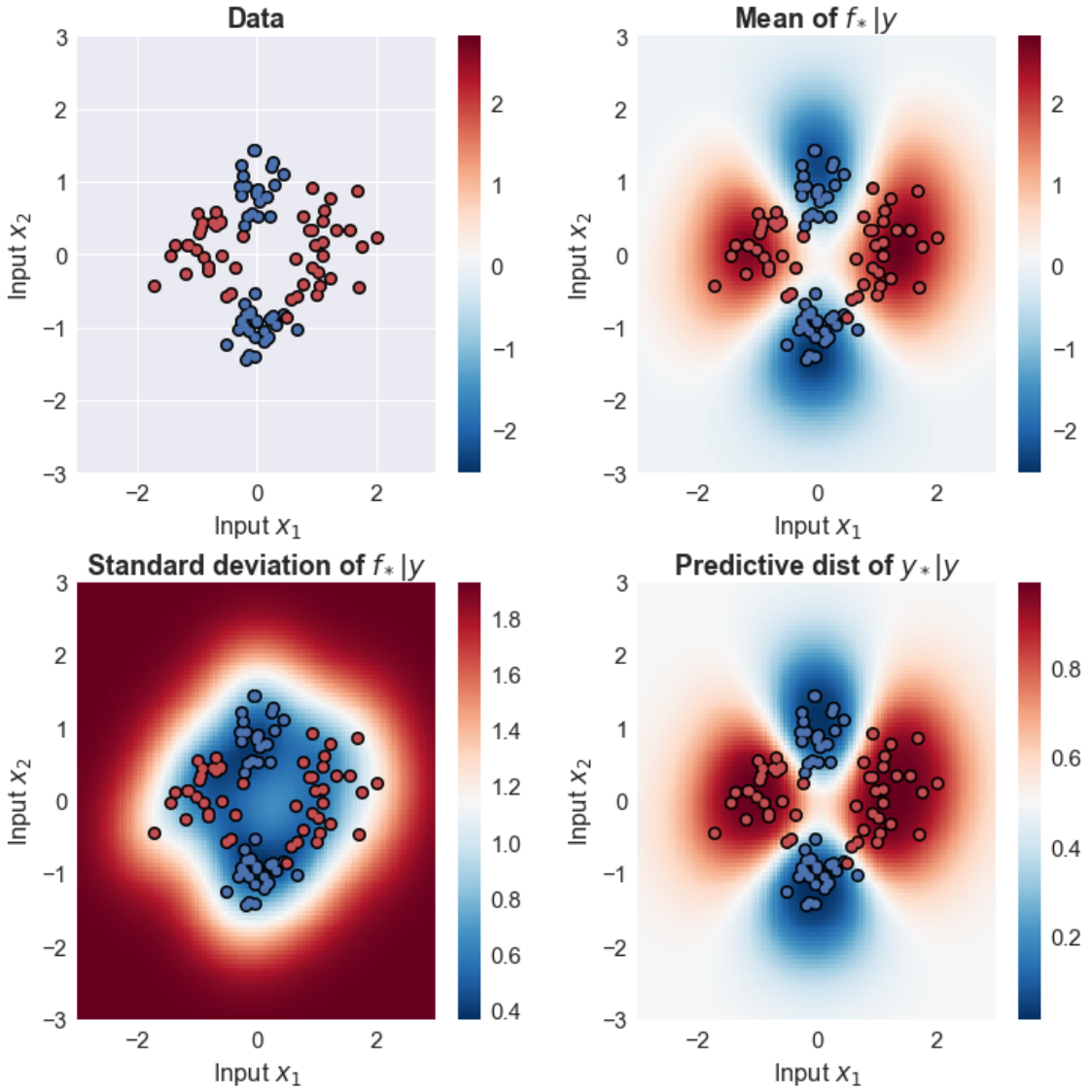
$$
\begin{aligned}
p(y_* = 1|\boldsymbol{y}) &= \int p(y_*|f_*)p(f_*\big|\boldsymbol{y})\mathrm{d}f_* \\
&= \int \phi\left(y_* \cdot f_*\right) p(f_*\big|\boldsymbol{y})\mathrm{d}f_* \\
&\approx \int \phi\left(y_* \cdot f_*\right) q\left(f_*\right) \mathrm{d}f_* \\
&= \int \phi\left(y_* \cdot f_*\right) \mathcal{N}\left(f_*\big|\mu_*, \sigma_*^2\right) \mathrm{d}f_* \\
&= \phi\left(\frac{\mu_*}{\sqrt{1+\sigma_*^2}}\right)
\end{aligned}
$$

Discuss with your neighbor

- What can we say about the predictive distributions for y_* when μ_* is positive? or negative?
- How does the uncertainty of the posterior distribution of f_* influence the predictions for y_*? What happens as σ_*^2 approaches ∞?

Gaussian process classification example

- Non-linear classification problem
- $N = 100$ data points
- Squared exponential kernel
- Hyperparameters are chosen by optimizing $\mathcal{L}_3$



End of todays lecture

- This will be my last lecture
- Markus Heinonen, Arno Solin and Aki Vehtari will handle the rest of the course
- Next time: Markus Heinonen will give a lecture about spectral kernels
- In two weeks: Arno Solin will give a lecture about spatio-temporal modelling
- Now time for questions and assignment #2