Variational Inference for Gaussian and Determinantal Point Processes

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Motivation

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In this talk: We will present a variational method that has been developed for Gaussian process models and then extend it to determinantal point processes

Gaussian process regression

Inputs $X = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ and outputs $\mathbf{y} = (y_1, \ldots, y_n)$ such that

$$y_i = f(\mathbf{x}_i) + \epsilon_i, \quad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

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Given that we have n data our current "marginal model" is

$$p(\mathbf{y}|\mathbf{f})p(\mathbf{f}) = \mathcal{N}(\mathbf{y}|\mathbf{f}, \sigma^2 I)\mathcal{N}(\mathbf{f}|\mathbf{0}, \mathbf{K}_{ff}), \quad [\mathbf{K}_{ff}]_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

where $\mathbf{f} = (f_1, \ldots, f_n)$ are the parameters

Gaussian process regression

and now the problem appears: as we keep collecting more data the size of $\mathbf{f} = (f_1, f_2, f_3, \ldots)$ increases and the kernel matrix gets bigger and bigger

$$\mathbf{K}_{ff} = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & k(\mathbf{x}_1, \mathbf{x}_2) & k(\mathbf{x}_1, \mathbf{x}_3) & \ldots \\ k(\mathbf{x}_2, \mathbf{x}_1) & k(\mathbf{x}_2, \mathbf{x}_2) & k(\mathbf{x}_2, \mathbf{x}_3) & \ldots \\ k(\mathbf{x}_3, \mathbf{x}_1) & k(\mathbf{x}_3, \mathbf{x}_2) & k(\mathbf{x}_3, \mathbf{x}_3) & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

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Space scales as $O(n^2)$ and time as $O(n^3)$

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Thus GP computations, e.g. learning by maximizing the marginal likelihood

$$p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f})d\mathbf{f} = \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_{ff} + \sigma^2 I)$$

are not feasible for very large n

Inducing variables

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- it could grow if the computational capacity increase in future

Obviously how $\mathbf{u}$ is going to be defined and optimized is crucial

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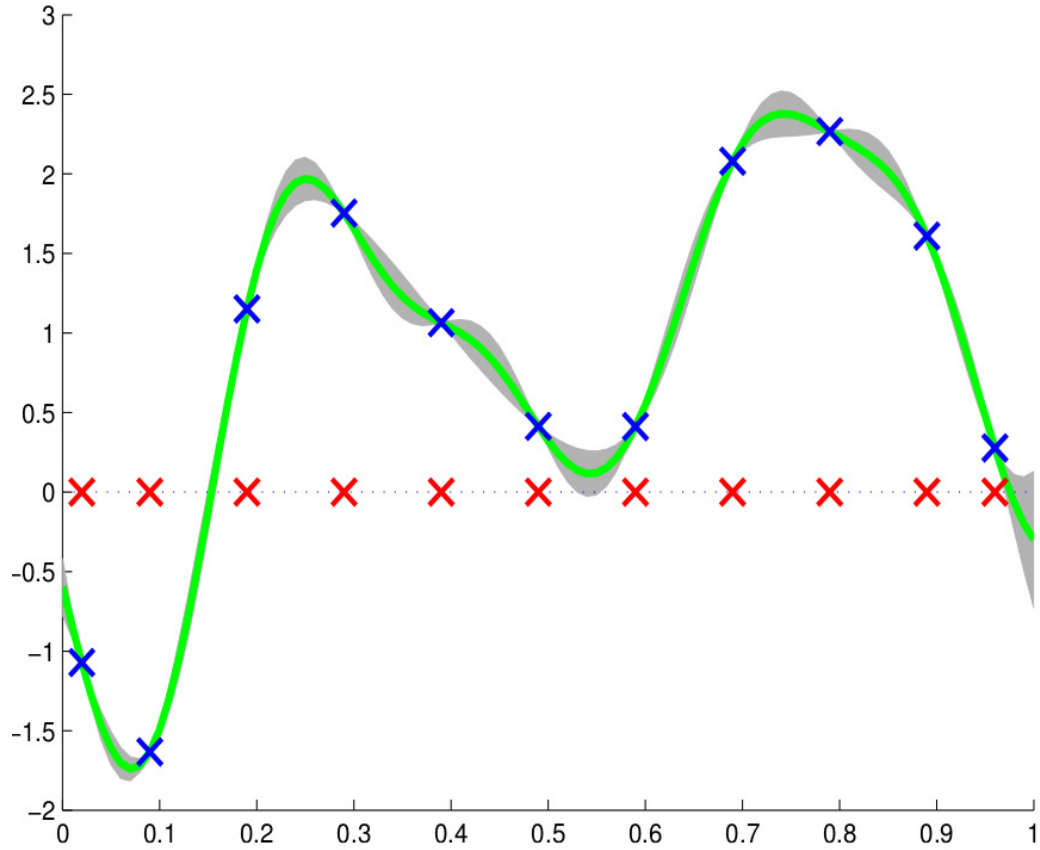

A realization of a full (infinite) GP function/sample path

Summarize with a discrete set of function values $\mathbf{u} = (u_1, \ldots, u_m)$

and some uncertainty for the intermediate points

Inducing variables

Inducing variables $\mathbf{u}$ form a vector of user-controllable size that augments the GP prior:

$$p(\mathbf{f}, \mathbf{u}) = \mathcal{N}\left(\begin{bmatrix} \mathbf{f} \\ \mathbf{u} \end{bmatrix} \middle| \mathbf{0}, \begin{bmatrix} \mathbf{K}_{ff} & \mathbf{K}_{fu} \\ \mathbf{K}_{uf} & \mathbf{K}_{uu} \end{bmatrix} \right), \; \mathbf{K}_{fu} = \mathbb{E}[\mathbf{f}\mathbf{u}^T], \; \mathbf{K}_{uu} = \mathbb{E}[\mathbf{u}\mathbf{u}^T]$$

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$\mathbf{u}$ can be:

- a subset of $\mathbf{f}$
- values of $f(\mathbf{x})$ at arbitrary "pseudo-inputs"
- arbitrary linear functionals, e.g. $u = z_i f(\mathbf{x}_i) + z_j f(\mathbf{x}_j)$

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The augmentation with $\mathbf{u}$ adds some parameters Z

- indices that specify the subset in $\mathbf{f}$, pseudo-inputs, weights etc
- $\mathbf{K}_{fu}$ and $\mathbf{K}_{uu}$ depend on those parameters

Inducing variables

We have

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where

$$p(\mathbf{f}|\mathbf{u}) = \mathcal{N}(\mathbf{f}|\mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{u}, \mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}) \quad \text{conditional GP prior}$$

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We can marginalize out $\mathbf{u}$ and recover back $p(\mathbf{f})$:

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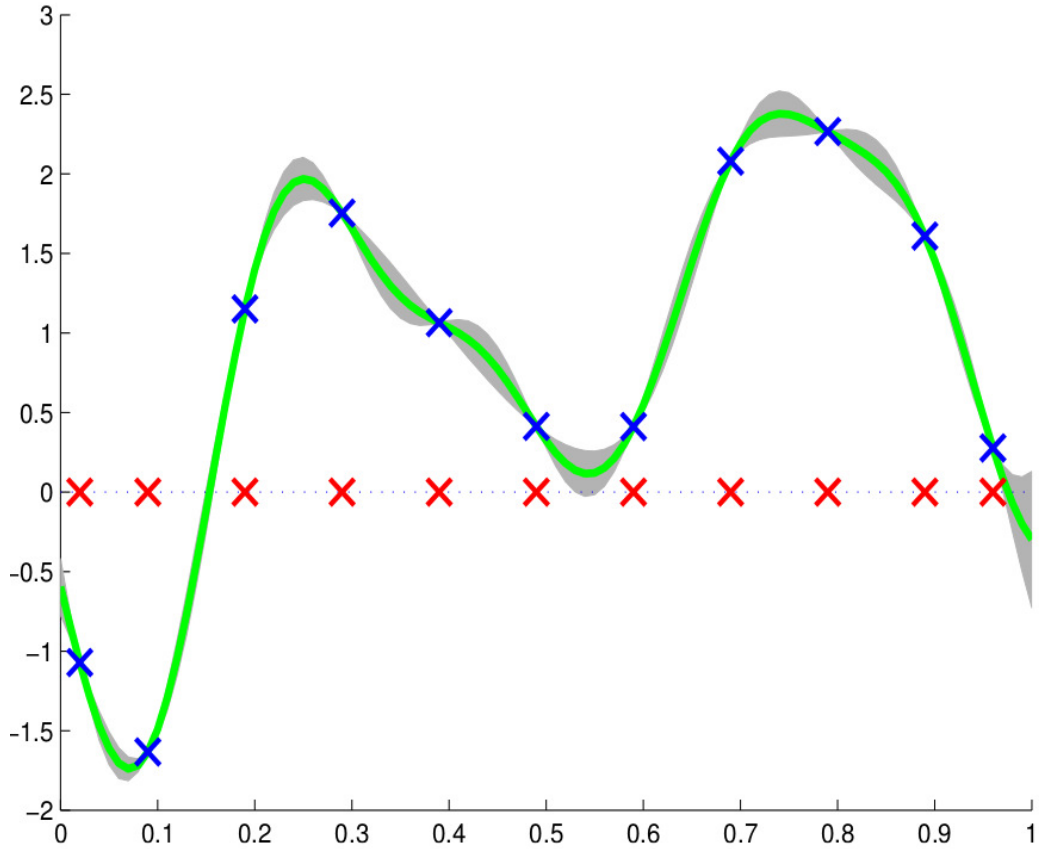
An efficient construction of $\mathbf{u}$ and selection of values for Z should be such that $\mathbf{u}$ correlates strongly with $\mathbf{f}$

- i.e. $p(\mathbf{f}|\mathbf{u})$ is sharply picked

Inducing variables



A realized value for $\mathbf{f}$

Realized values for the inducing variables $\mathbf{u} = (u_1, \ldots, u_m)$, $u_i = f(\mathbf{z}_i)$

The augmentation parameters are the **inducing inputs** $Z = (\mathbf{z}_1, \ldots, \mathbf{z}_m)$

Conditional prior $p(\mathbf{f}|\mathbf{u})$

Inducing variables

The whole purpose of adding **u** is to help us obtain an approximation to our Bayesian non-parametric model (**without changing its non-parametric nature... as will be discussed shortly**) that will scale better computationally

Inducing variables

The whole purpose of adding $\mathbf{u}$ is to help us obtain an approximation to our Bayesian non-parametric model (**without changing its non-parametric nature... as will be discussed shortly**) that will scale better computationally

The big question now is how do we "turn around" $\mathbf{u}$ in order to make it the basis of our approximation? Further, how do we learn the augmentation parameters Z?

Variational learning of inducing variables

Augmented joint

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

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Marginal likelihood is invariant to the augmentation parameters Z

$$p(\mathbf{y}) = \int p(\mathbf{y}|\mathbf{f})p(\mathbf{f}|\mathbf{u})p(\mathbf{u})d\mathbf{f}d\mathbf{u}$$

and the marginal posterior $p(\mathbf{f}|\mathbf{y})$ is also invariant to Z

- **I.e. Z is not model parameter**
- **$\Rightarrow$ we can turn it into variational parameter by lower bounding**

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This choice encourages $\mathbf{u}$ to become approximate sufficient statistic

if $p(\mathbf{f}|\mathbf{u}) \approx p(\mathbf{f}|\mathbf{u}, \mathbf{y})$, then $\mathbf{u}$ summarizes well the data

Variational learning of inducing variables

Minimize KL $[q(\mathbf{f}, \mathbf{u})||p(\mathbf{f}, \mathbf{u}|\mathbf{y})]$ or equivalently maximize the bound on the log marginal likelihood

$$\log p(\mathbf{y}) = \log \int p(\mathbf{y}|\mathbf{f}) p(\mathbf{f}|\mathbf{u}) p(\mathbf{u}) d\mathbf{f} d\mathbf{u}$$

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Maximize over $q(\mathbf{u})$:

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Variational learning of inducing variables

Theorem 1 (bound).

For arbitrary GP model:

$$p(\mathbf{y}) \geq \int G(\mathbf{y}, \mathbf{u}) p(\mathbf{u}) d\mathbf{u}, \quad G(\mathbf{y}, \mathbf{u}) = e^{\int p(\mathbf{f}|\mathbf{u}) \log p(\mathbf{y}|\mathbf{f}) d\mathbf{f}}$$

For GP regression:

$$\mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_{ff} + \sigma^2 I) \geq \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf} + \sigma^2 I) e^{-\frac{1}{2\sigma^2}\mathrm{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}\right)}$$

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Theorem 2 (monotonicity property). If we have inducing variables $\mathbf{u}$ and add an extra u_i the bound can only increase

$$\int G(\mathbf{y}, \mathbf{u}, u_i) p(\mathbf{u}, u_i) d\mathbf{u} \geq \int G(\mathbf{y}, \mathbf{u}) p(\mathbf{u}) d\mathbf{u}$$

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Computation of the bound and the approximate GP prediction scale as $O(nm^2)$ where m is the number of inducing variables

Variational learning of inducing variables

For GP regression the bound has an interesting form:

$$\mathcal{F}(Z, \theta) = \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf} + \sigma^2 I) - \frac{1}{2\sigma^2}\mathrm{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}\right)$$

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We maximize $\mathcal{F}(Z,\boldsymbol{\theta})$ over Z and kernel hyperparameters $\boldsymbol{\theta}$:

- Z is a variational parameter

Variational learning of inducing variables

The approximate posterior/predictive Gaussian process:

$$
\begin{aligned}
q(\mathbf{f}_*) &= \int p(\mathbf{f}_*|\mathbf{f},\mathbf{u}) q(\mathbf{f},\mathbf{u}) d\mathbf{f} d\mathbf{u} \\
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where we used the consistency $\int p(\mathbf{f}_*|\mathbf{f},\mathbf{u}) p(\mathbf{f}|\mathbf{u}) d\mathbf{f} = p(\mathbf{f}|\mathbf{u})$

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There is a very important thing to be said here:

- This is not a discretized, truncated or low rank approximation (it is full rank **and NOT low rank as many people believe**)
- This is because the conditional GP $p(\mathbf{f}_*|\mathbf{u})$ is an infinite object

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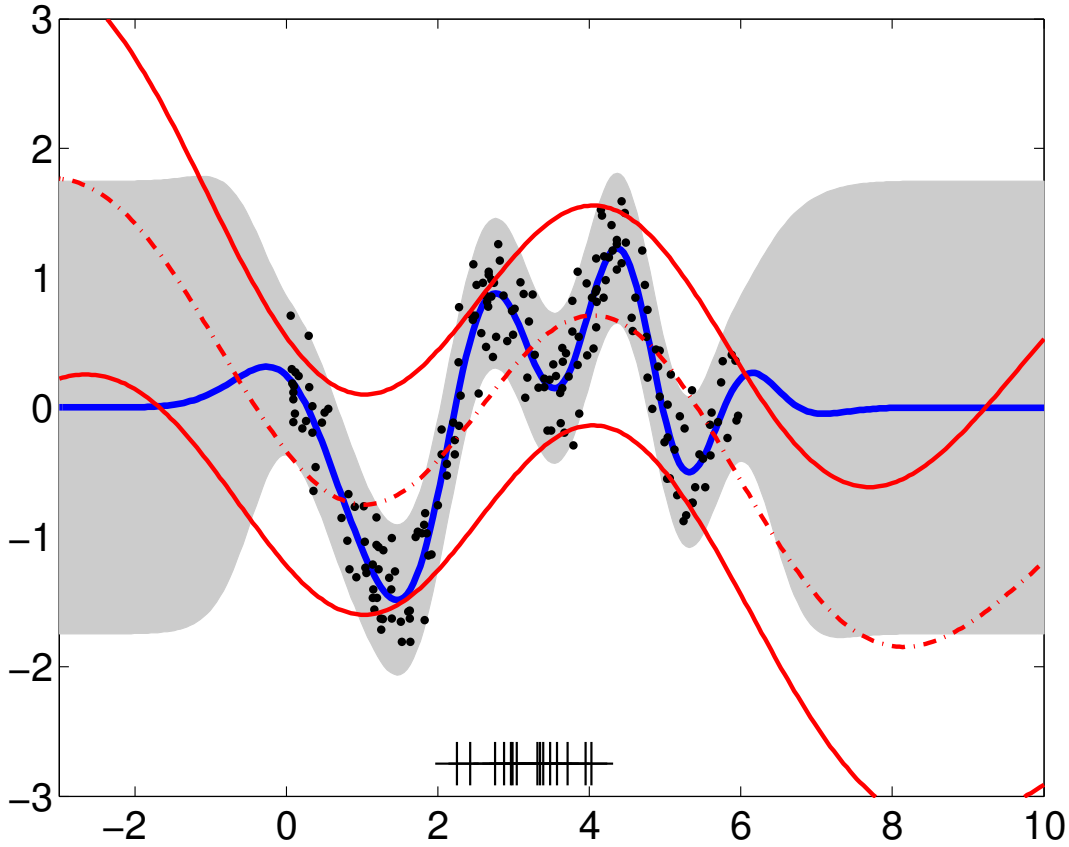
The approximation can be thought of been **restricted not to explore freely the information in the training data**. But it maintains fully the non-parametric nature of the model

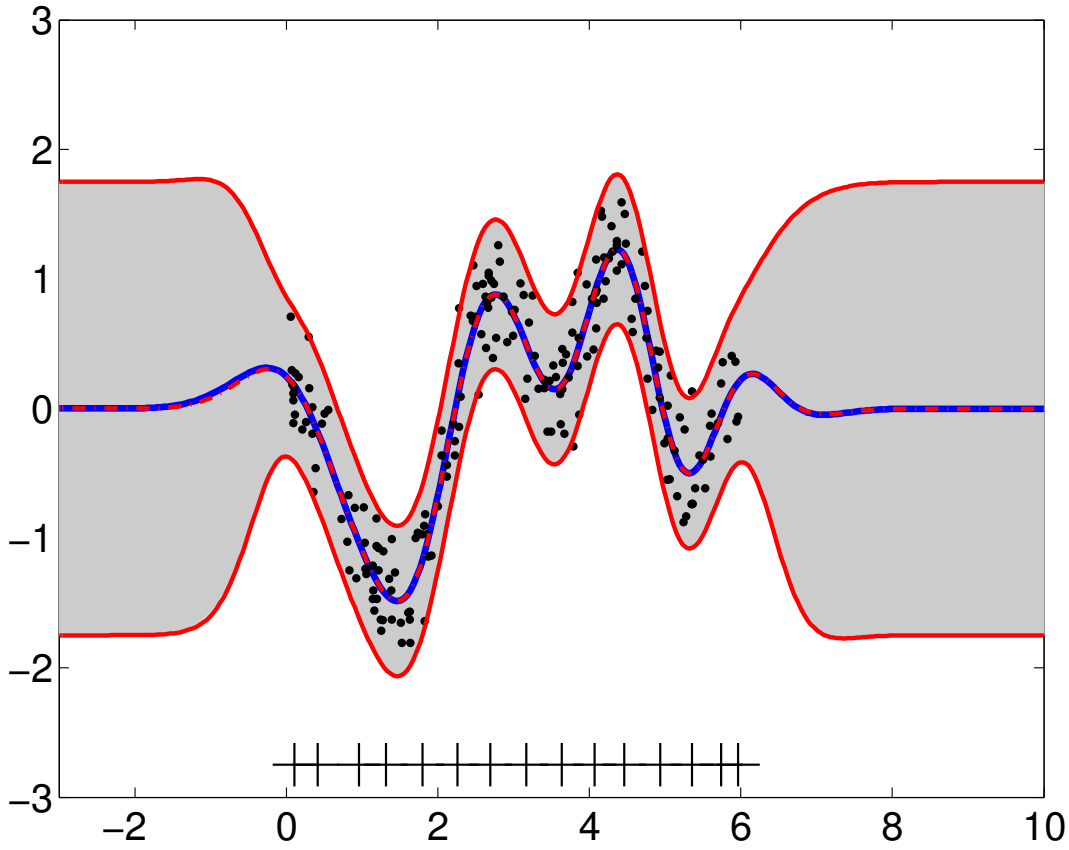
Variational learning of inducing variables



Full GP that scales as $O(n^3) = O(200^3)$
Variational approximation that scales as $O(nm^2) = O(200 \times 15^2)$ **at initialization**

- The crosses $(+)$ are the initial values of the inducing inputs Z

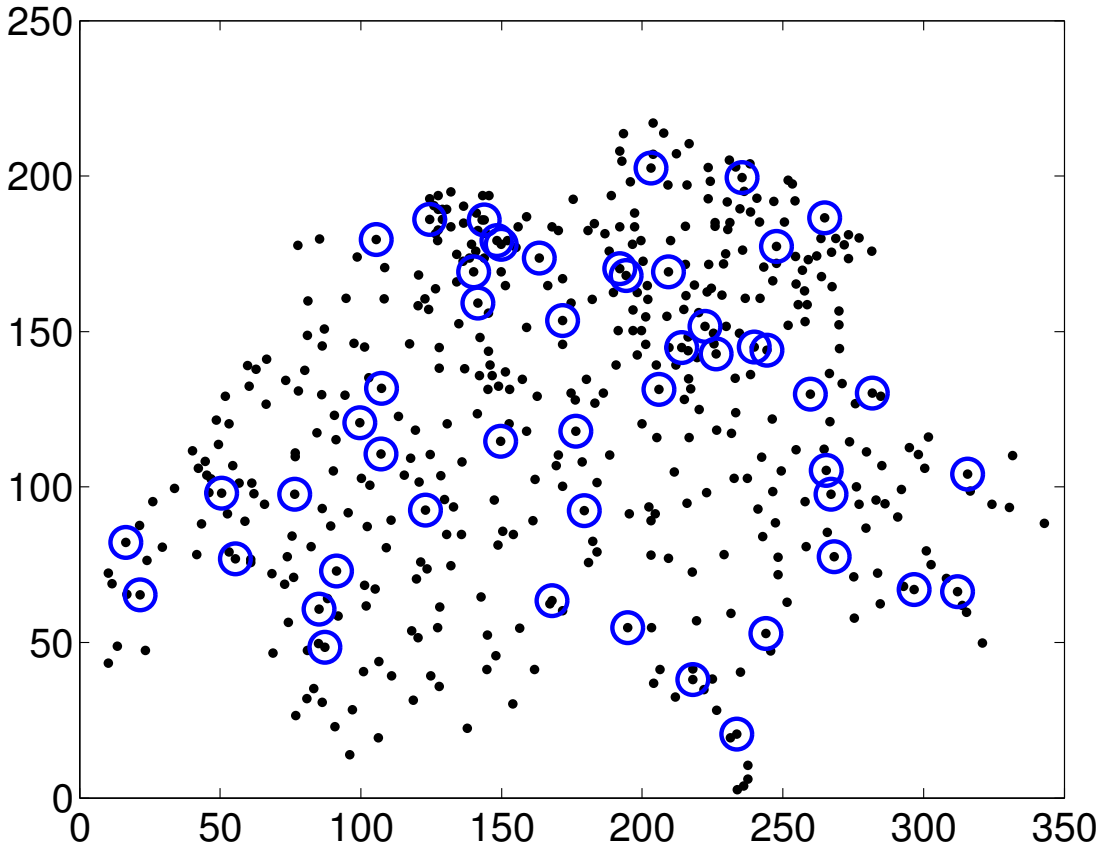
Variational learning of inducing variables



Full GP that scales as $O(n^3) = O(200^3)$

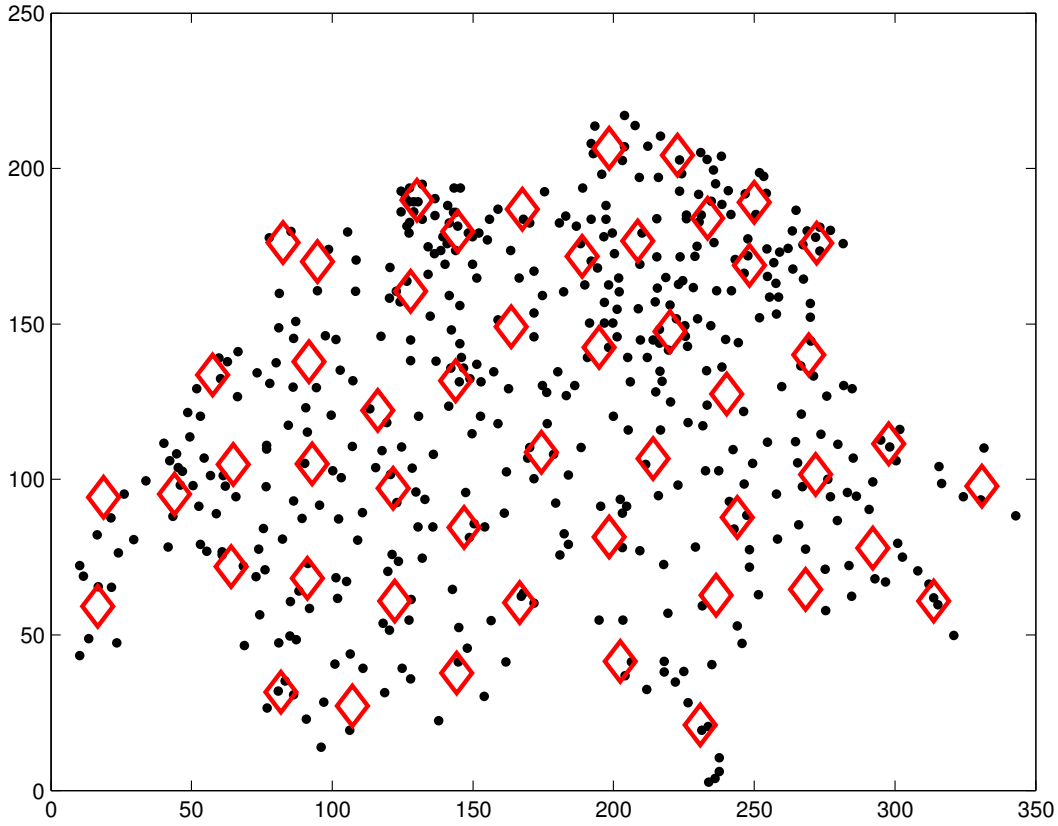
Variational approximation that scales as $O(nm^2) = O(200 \times 15^2)$ **after having maximized the bound**

Variational learning of inducing variables



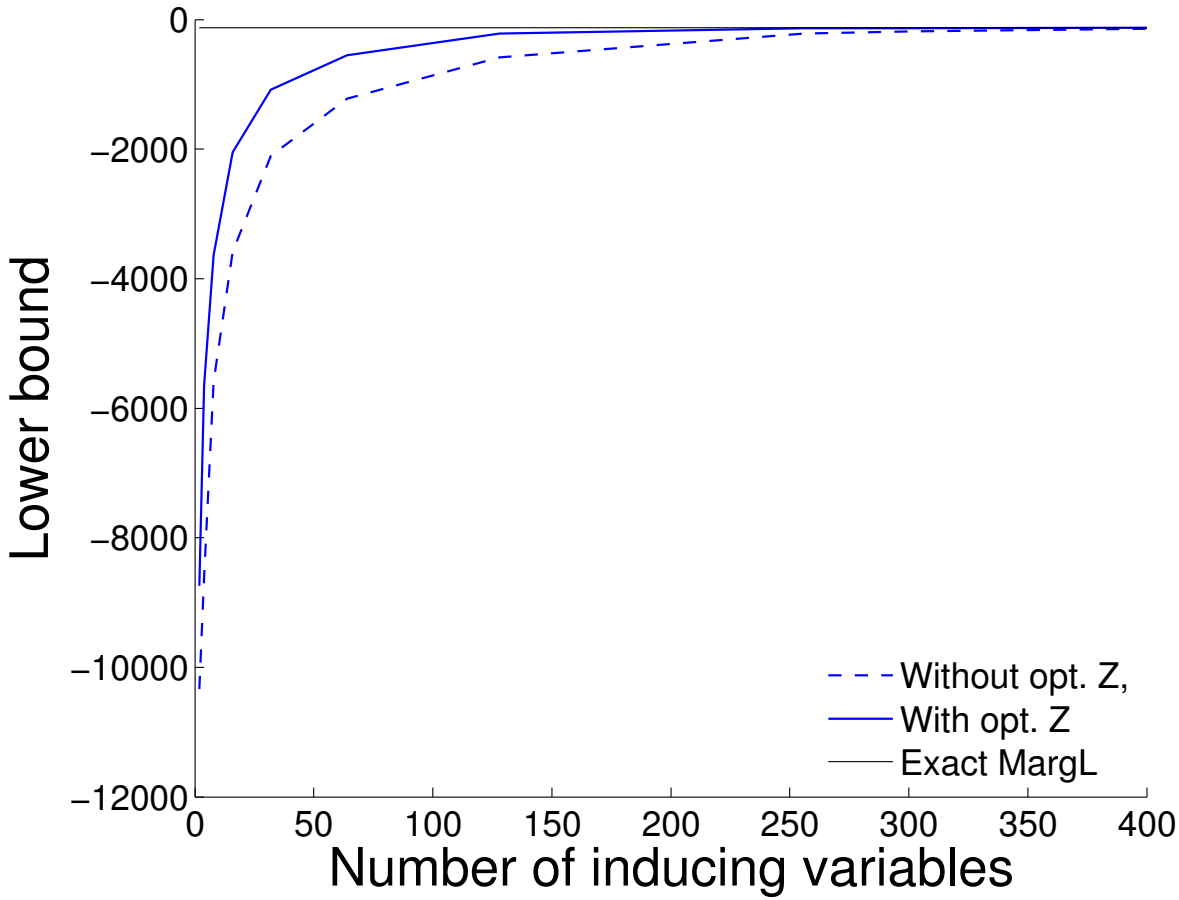
Initial locations of the inducing inputs Z

Variational learning of inducing variables



Locations of the inducing inputs after having maximized the bound

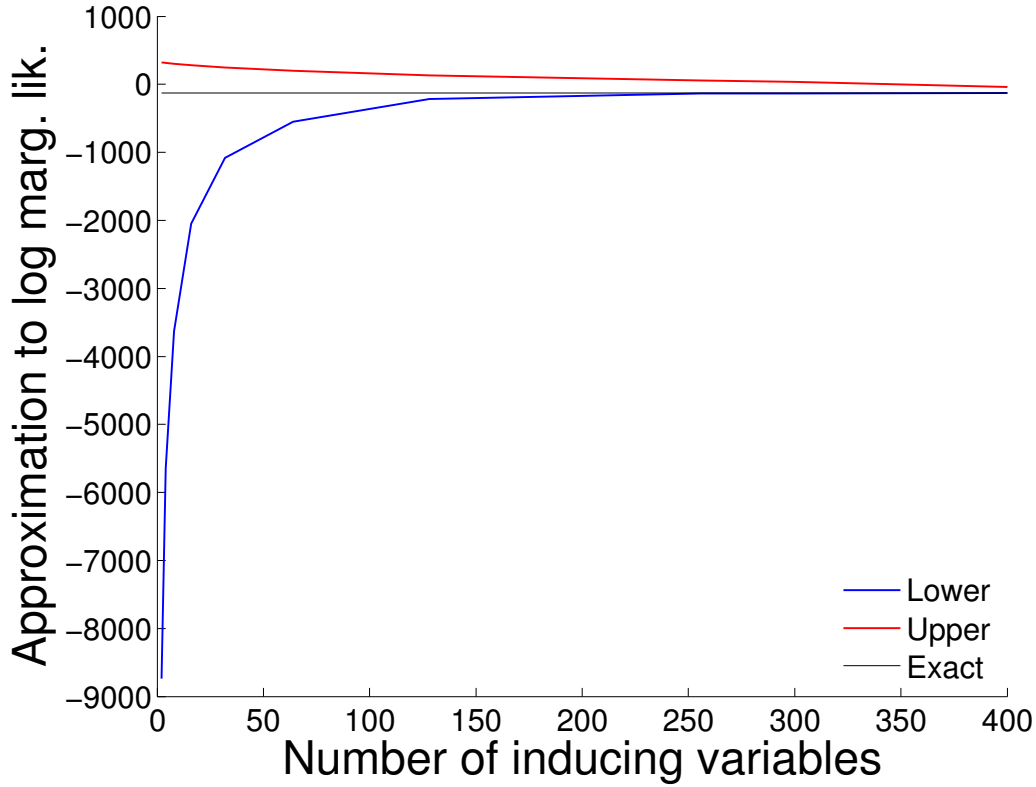
Variational learning of inducing variables



Maximization wrt the inducing inputs Z improves the approximation

(The example is based on the Boston housing data and Z is initialized to a random subset of training inputs)

Variational learning of inducing variables



If the bound flattens as we add more inducing variables we typically have reached full GP

To further assess the approximation we can consult an upper bound

$$p(\mathbf{y}) \leq \frac{1}{(2\pi)^{\frac{n}{2}} \left|\mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf} + \sigma^2 I\right|^{\frac{1}{2}}} e^{-\frac{1}{2}\mathbf{y}^T\left(\mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf} + c + \sigma^2 I\right)^{-1}\mathbf{y}}$$

where $c = \mathrm{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}\right)$

Variational learning of inducing variables

When the bound becomes tight?

$$\mathcal{F}(Z,\theta) = \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf} + \sigma^2 I) - \frac{1}{2\sigma^2}\mathrm{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}\right)$$

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When the trace term is zero the bound becomes tight, i.e.

$$\text{If } \text{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}\right) = 0 \Rightarrow \mathbf{K}_{ff} = \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}, \ \mathcal{F} = \log p(\mathbf{y})$$

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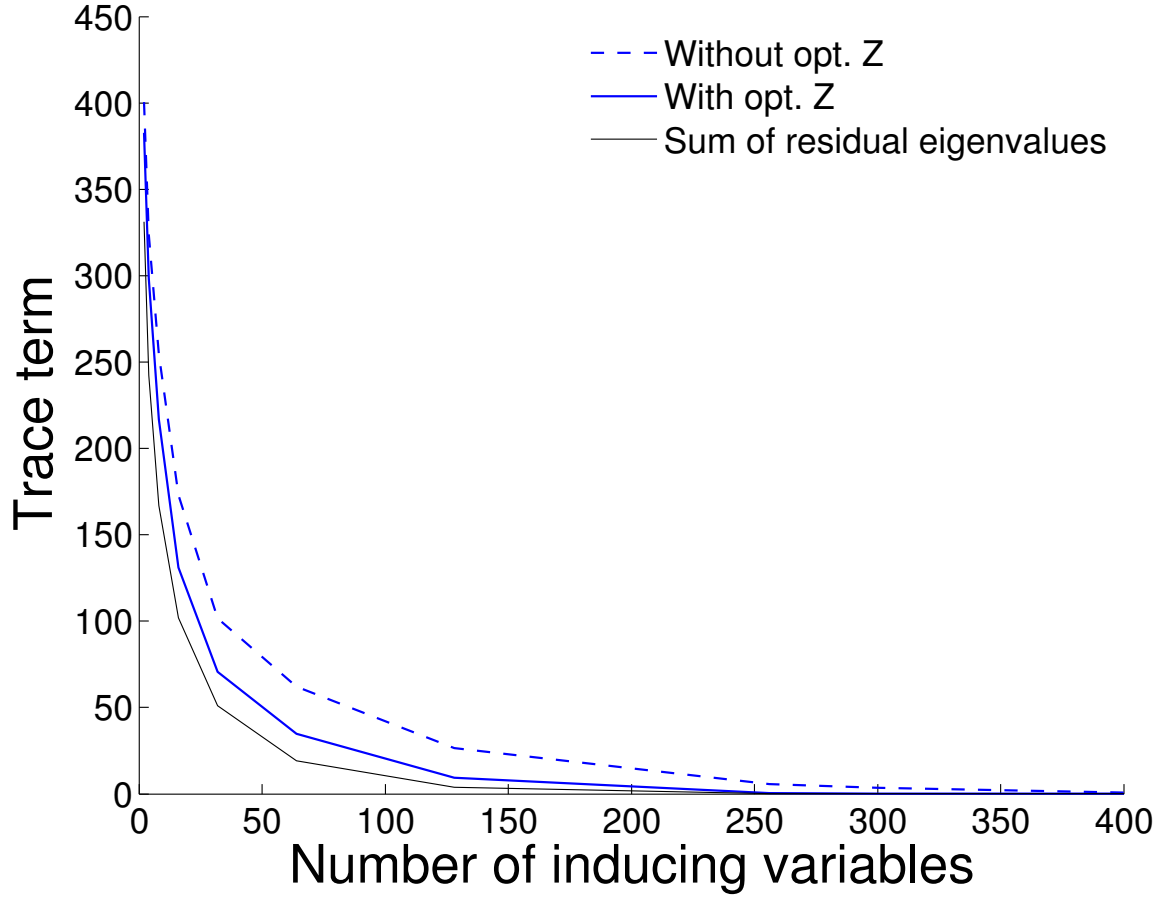
Question: what is the best we can do if we use $m < n$ inducing variables?

Variational learning of inducing variables



It holds that $\text{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{uf}\right) \geq \sum_{i=m+1}^{n} \lambda_i$

where $\lambda_1 \geq \lambda_2 \geq .... \geq \lambda_n$ are the eigenvalues of $\mathbf{K}_{ff}$

Some history

Early work (that set the foundation of these approximations) is: Csato and Opper (2002); Seeger (2003); Seeger, Williams and Lawrence (2003)

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Hensman, Fusi and Lawrence (2013) (combined the framework with stochastic data sub-sampling variational inference)

Determinantal point processes

Lets now discuss how we can extend this approximation to determinantal point processes

Determinantal point processes

Given a discrete set of items $\mathcal{Y} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ a DPP defines a distribution over all 2^n possible subsets via a $n \times n$ kernel matrix $L_{\mathcal{Y}}$ such that $[L_{\mathcal{Y}}]_{ij} = L(\mathbf{x}_i, \mathbf{x}_j)$:

$$\Pr(\mathbf{Y} = Y) = \frac{\det(L_Y)}{\det(L_{\mathcal{Y}} + I)}$$

where L_Y is the kernel sub-matrix indexed by the elements of $Y \subseteq \mathcal{Y}$

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A DPP is a point process that favors repulsion, i.e. items with very similar descriptors (**x**s) are unlikely to appear in the same realization

- for full details see e.g. Kulesza and Taskar, Foundations and Trends in Machine Learning (2012)

Determinantal point processes

Given a set of observed subsets of items $(Y_1, \ldots, Y_T)$ we can fit the model by ML:

$$\mathcal{L}(\boldsymbol{\theta}) = \log \prod_{t=1}^{T} \frac{\det(L_{Y_t})}{\det(L_{\mathcal{Y}} + I)}$$

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To apply variational inference we need to compute an upper bound on $\det(L_{\mathcal{Y}} + I)$ or equivalently a lower bound on

$$\frac{1}{\det(L_{\mathcal{Y}} + I)}$$

Determinantal point processes

We assume an inducing subset $Z \subseteq \mathcal{Y}$. From the bound in GP regression we know that:

$$\mathcal{N}(\mathbf{y}|\mathbf{0}, L_{\mathcal{Y}}+\sigma^2 I) \geq \mathcal{N}(\mathbf{y}|\mathbf{0}, L_{\mathcal{Y}Z}L_Z^{-1}L_{Z\mathcal{Y}}+\sigma^2 I)e^{-\frac{1}{2\sigma^2}\mathrm{tr}\left(L_{\mathcal{Y}}-L_{\mathcal{Y}Z}L_Z^{-1}L_{Z\mathcal{Y}}\right)}$$

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By setting $\mathbf{y} = \mathbf{0}$ and $\sigma^2 = 1$:

$$\frac{1}{\det(L_{\mathcal{Y}} + I)^{\frac{1}{2}}} \geq \frac{1}{\det(L_{\mathcal{Y}Z}L_Z^{-1}L_{Z\mathcal{Y}} + I)^{\frac{1}{2}}} e^{-\frac{1}{2}\mathrm{tr}\left(L_{\mathcal{Y}}-L_{\mathcal{Y}Z}L_Z^{-1}L_{Z\mathcal{Y}}\right)}$$

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By taking the square:

$$\frac{1}{\det(L_{\mathcal{Y}}+I)} \geq \frac{1}{\det(L_{\mathcal{Y}Z}L_Z^{-1}L_{Z\mathcal{Y}}+I)} e^{-\mathrm{tr}\left(L_{\mathcal{Y}}-L_{\mathcal{Y}Z}L_Z^{-1}L_{Z\mathcal{Y}}\right)}$$

Determinantal point processes

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By applying the matrix determinant lemma and rearranging

$$\frac{1}{\det(L_{\mathcal{Y}} + I)} \geq \frac{\det(L_Z)}{\det(L_Z + L_{Z\mathcal{Y}} L_{\mathcal{Y}Z})} e^{-\mathrm{tr}(L_{\mathcal{Y}}) + \mathrm{tr}\left(L_Z^{-1} L_{Z\mathcal{Y}} L_{\mathcal{Y}Z}\right)}$$

which is computed in $O(nm^2)$ where m is the size of Z

Determinantal point processes

$$\frac{1}{\det(L_Y + I)} \geq \frac{1}{\det(L_{YZ} L_Z^{-1} L_{ZY} + I)} e^{-\mathrm{tr}\left(L_Y - L_{YZ} L_Z^{-1} L_{ZY}\right)}$$

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which is computed in $O(nm^2)$ where m is the size of Z

We can now substitute the bound on the likelihood and maximize the overall lower bound. Z is a variational parameter exactly as in the GP case

Determinantal point processes

If the space of items is continuous, i.e. $\mathcal{Y} = \mathbb{R}^D$, and assuming $\int L(\mathbf{x}, \mathbf{x}) d\mathbf{x} < \infty$ a DPP has density

$$\mathrm{P}(\mathbf{Y} = Y) = \frac{\det(L_Y)}{\prod_{i=1}^{\infty}(\lambda_i + 1)}$$

where λ_is are the eigenvalues of the kernel function. The model now is doubly intractable as typically we don't know the eigenvalues of the kernel

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However, we can compute a lower bound:

$$\frac{1}{\prod_{i=1}^{\infty}(\lambda_i + 1)} \geq \frac{\det(L_Z)}{\det(L_Z + \Psi)} e^{-\int L(\mathbf{x},\mathbf{x}) d\mathbf{x} + \mathrm{tr}(L_Z^{-1}\Psi)}$$

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$$[\Psi]_{ij} = \int L(\mathbf{z}_i, \mathbf{x}) L(\mathbf{x}, \mathbf{z}_j) d\mathbf{x}$$

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Z are again variational parameters and can be taken to be pseudo-inputs

Determinantal point processes

Discrete case:

$$\frac{1}{\det(L_{\mathcal{Y}} + I)} \geq \frac{\det(L_Z)}{\det(L_Z + L_{Z\mathcal{Y}} L_{\mathcal{Y}Z})} e^{-\mathrm{tr}(L_{\mathcal{Y}}) + \mathrm{tr}\left(L_Z^{-1} L_{Z\mathcal{Y}} L_{\mathcal{Y}Z}\right)}$$

Continuous case:

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These bounds have similar structure with the ones of Affandi, Fox, Adams and Taskar, ICML (2014)

- The important difference is that the new bounds do not depend on the difficult to compute eigenvalues of the kernel matrix or the unknown eigenvalues of the full kernel operator
- So the current variational framework should be applicable to a wider class of DPPs

Discussion

Summary: Variational inference based on inducing variables provides a rigorous mechanism to approximate GPs and DPPs

Some challenges:

- Can we further reduce the computational complexity of these methods?
- Can we use similar ideas in other Bayesian non-parametric models such as those based on Dirichlet processes?