CS-E4895 Gaussian Processes
Lecture 7: Large-scale Gaussian Processes

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based on slides by Zhenwen Dai, Michael Riis Andersen, Ti John, and Arno Solin

Roadmap for today

1. What is the computational issue?
2. Exploiting structure in data and/or GP prior
3. Solving the linear system approximately (with Conjugate Gradients)
4. Local approximations: Split problem into smaller chunks
5. Global approximations: Inducing points
6. Variational inference for sparse GPs
7. Recap

Section 1

What is the computational issue?

Gaussian process regression: Operations

Learning hyperparameters: Maximize (log) marginal likelihood:

$$\theta^* = \arg\max_\theta \log p(\boldsymbol{y} \mid X, \theta) = \arg\max_\theta \log \mathcal{N}(\boldsymbol{y} \,|\, \mathbf{0}, \mathbf{K} + \sigma^2 \mathbf{I})$$

Test point prediction (mean, variance):

$$\begin{aligned} p(f_* \mid \boldsymbol{y}) &= \mathcal{N}\left(f_* \mid \mu_*, \sigma_*^2\right) \\ \mu_* &= \boldsymbol{k}_{f_* f} \left(\boldsymbol{K}_{ff} + \sigma^2 \boldsymbol{I}\right)^{-1} \boldsymbol{y} \\ \sigma_*^2 &= k_{f_* f_*} - \boldsymbol{k}_{f_* f} \left(\boldsymbol{K}_{ff} + \sigma^2 \boldsymbol{I}\right)^{-1} \boldsymbol{k}_{f_* f}^\top \end{aligned}$$

Computational complexity of Gaussian process regression

Data set with N observations, computing posterior for 1 test point:

$$\mu_* = \boldsymbol{k}_{f_* f} \left(\boldsymbol{K}_{ff} + \sigma^2 \boldsymbol{I} \right)^{-1} \boldsymbol{y}$$
$$\sigma_*^2 = k_{f_* f_*} - \boldsymbol{k}_{f_* f} \left(\boldsymbol{K}_{ff} + \sigma^2 \boldsymbol{I} \right)^{-1} \boldsymbol{k}_{f_* f}^\top$$

What is computational complexity? What is the dominating operation?

- Matrix–vector multiplication (mvm):
  for $\boldsymbol{A} \in \mathbb{R}^{N \times M}$ and $\boldsymbol{b} \in \mathbb{R}^M$, computing $\boldsymbol{A}\boldsymbol{b}$ costs $\mathcal{O}(NM)$
- Matrix inverse: for $\boldsymbol{C} \in \mathbb{R}^{N \times N}$, computing $\boldsymbol{C}^{-1}$ costs $\mathcal{O}\left(N^3\right)$
- $\boldsymbol{\alpha} = \left(\boldsymbol{K}_{ff} + \sigma^2 \boldsymbol{I} \right)^{-1} \boldsymbol{y}$ scales as $\mathcal{O}\left(N^3\right)$, $\mu_* = \boldsymbol{k}_{f_* f} \boldsymbol{\alpha}$ scales as $\mathcal{O}(N)$

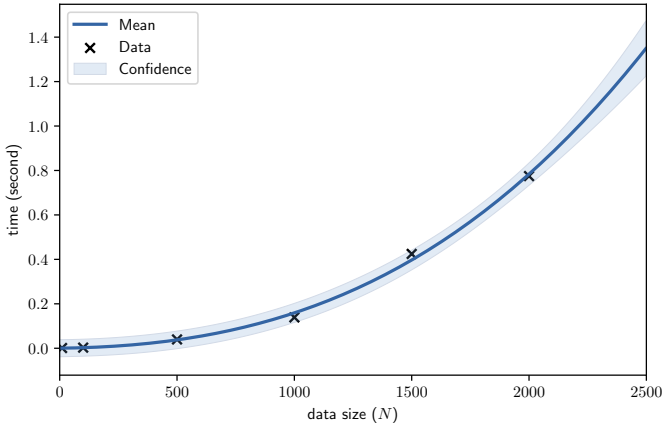
Log marginal likelihood

$$
\begin{aligned}
\log p(\mathbf{y} \mid \mathbf{X}) &= \log \mathcal{N}\left(\mathbf{y} \mid 0, \mathbf{K} + \sigma^2 \mathbf{I}\right) \\
&= -\frac{1}{2} \log |2\pi(\mathbf{K} + \sigma^2 \mathbf{I})| - \frac{1}{2} \mathbf{y}^\top (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{y} \\
&= -\frac{N}{2} N \log 2\pi - \sum_i \log \mathbf{L}_{ii} - \frac{1}{2} \|\mathbf{L}^{-1} \mathbf{y}\|^2
\end{aligned}
$$

- Cholesky decomposition: $\mathbf{L} = \texttt{chol}(\mathbf{K} + \sigma^2 \mathbf{I})$, such that $\mathbf{K} + \sigma^2 \mathbf{I} = \mathbf{L}\mathbf{L}^\top$.
- $\mathcal{O}(N^3)$ computational complexity

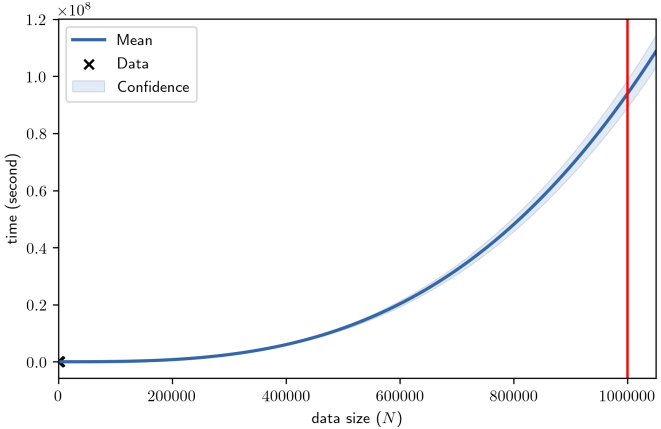
Empirical analysis of computational time

N	10	100	500	1000	1500	2000
time	1.3ms	8.5ms	28ms	0.12s	0.29s	0.76s



What if we have 1 million data points?

Predicted computational time: 9.4×10^7 seconds ≈ 2.98 years.



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

Biggest bottlenecks

```
Line #    Time(ms)   % Time      Line Contents
 2                            def log_likelihood(kern, X, Y, sigma2):
 3           6.0       0.0        N = X.shape[0]
 4       55595.0      58.7        K = kern.K(X)
 5        4369.0       4.6        Ky = K + np.eye(N)*sigma2
 6       30012.0      31.7        L = np.linalg.cholesky(Ky)
 7        4361.0       4.6        LinvY = dtrtrs(L, Y, lower=1)[0]
 8          49.0       0.1        logL = N*np.log(2*np.pi)/-2.
 9          82.0       0.1        logL += np.square(LinvY).sum()/-2.
10         208.0       0.2        logL += -np.log(np.diag(L)).sum()
11           2.0       0.0        return logL
```

- constructing $\mathbf{K}$
- computing Cholesky of $\mathbf{K}$

How can we address the bottleneck?

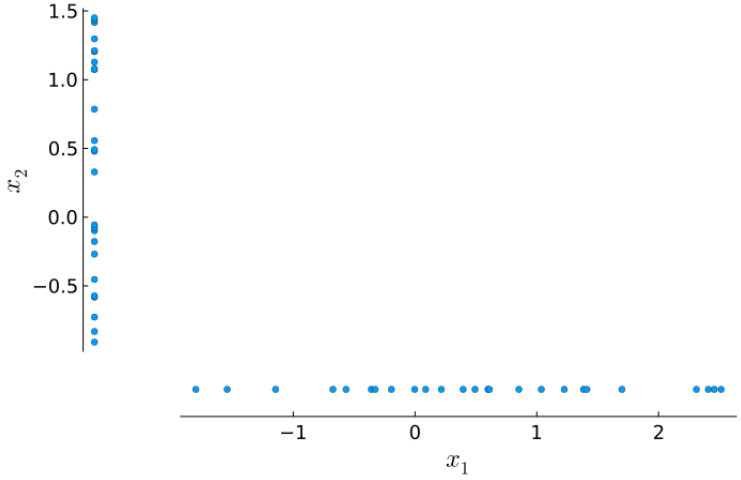
The naïve $\mathcal{O}(n^3)$ computational bottleneck ($\mathcal{O}(n^2)$ memory) can be tackled by

- **Exploiting structure in the data**
  (data on grid, inputs are in 1D, ...)
- **Exploiting structure in the GP prior**
  (GP prior is stationary, separable over input dimensions, ...)
- Solving the linear system approximately
  (conjugate-gradient solvers)
- Split problem into smaller chunks
  (local experts, subset of data, divide & conquer, ...)
- Approximate the problem
  (Nyström, low-rank, inducing points, ...)
- Approximate the problem solution
  (SVGP = sparse (and stochastic) variational methods)

Section 2

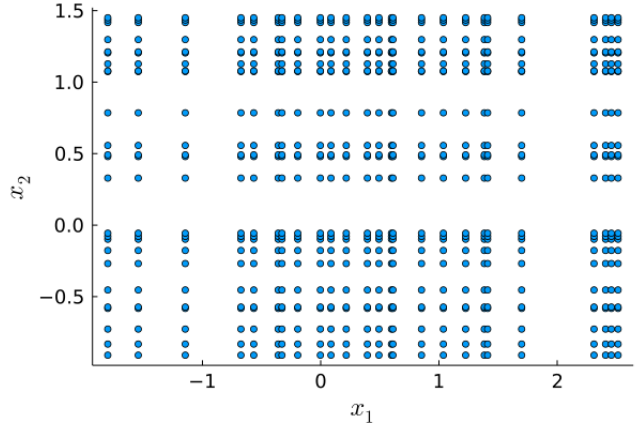
Exploiting structure in data and/or GP prior

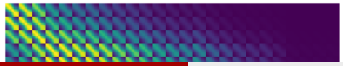
Exploiting structure: Inputs on grid



Exploiting structure: Inputs on grid

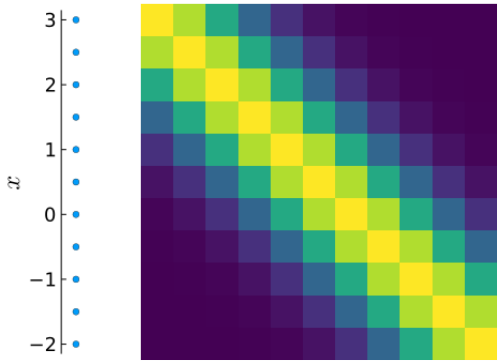
and *separable* kernel: $k(\boldsymbol{x}, \boldsymbol{x}') = \prod_{d=1}^{D} k_d(x_d, x'_d)$





Exploiting structure: Inputs on *regular* grid

and *stationary* kernel: $k(x, x') = k(x - x')$



Toeplitz structure: $K_{i,j} = K_{i+1,j+1} = k(x_i - x_j)$

efficient mvm via FFT: computation $\mathcal{O}(N + M \log M)$, storage $\mathcal{O}(N + M)$.

What if inputs are not exactly on grid?

Interpolate (e.g., cubically) kernel matrix between grid points: "KISS-GP"

- Can use very fine grids: very accurate
- Works well in small dimensions (up to 4)

What about higher dimensions?

More structure:

- Additive kernel
- Product kernel

Time series, graphs: sparse precision matrix, state space formulation

What about arbitrary kernels?

Section 3

Solving the linear system approximately (with Conjugate Gradients)

Matrix inverse as quadratic optimization

Rewrite matrix inverse

$$\boldsymbol{v} = \hat{K}^{-1}\boldsymbol{y}, \qquad \hat{K} = \mathbf{K} + \sigma^2\mathbf{I}$$

as linear system:

$$\hat{K}\boldsymbol{v} - \boldsymbol{y} = 0$$

Solve as quadratic optimization problem:

$$\boldsymbol{v}^* = \arg\min_{\boldsymbol{v}} \boldsymbol{v}^\top \hat{K}\boldsymbol{v} - \boldsymbol{v}^\top \boldsymbol{y}$$

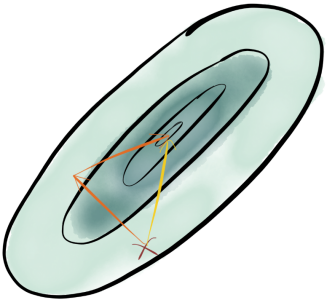
Conjugate Gradients

Efficiently solve

$$\boldsymbol{v}^* = \arg\min_{\boldsymbol{v}} \boldsymbol{v}^\top \hat{K} \boldsymbol{v} - \boldsymbol{v}^\top \boldsymbol{y}$$

using Conjugate Gradients (CG)

- Iterative method
- Each step is $\mathcal{O}(N^2)$
- Recovers exact solution after N steps $\rightarrow \mathcal{O}(N^3)$
- *Approximate* solution in much fewer steps! ("easier" problems: less steps)



Conjugate Gradient (CG)

Figure taken from Davies (2015)

Convergence and preconditioning

Condition number: ratio of largest to smallest eigenvalue,

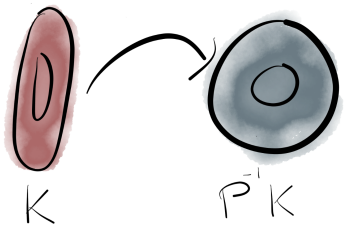
$$\kappa(\hat{K}) = \frac{\lambda_{\text{max}}(\hat{K})}{\lambda_{\text{min}}(\hat{K})}$$

High condition numbers: numerically unstable, slow convergence

Improve by preconditioning: Instead of $\hat{K}\boldsymbol{v} - \boldsymbol{y} = 0$, solve

$$P^{-1}\hat{K}\boldsymbol{v} - P^{-1}\boldsymbol{y} = 0$$

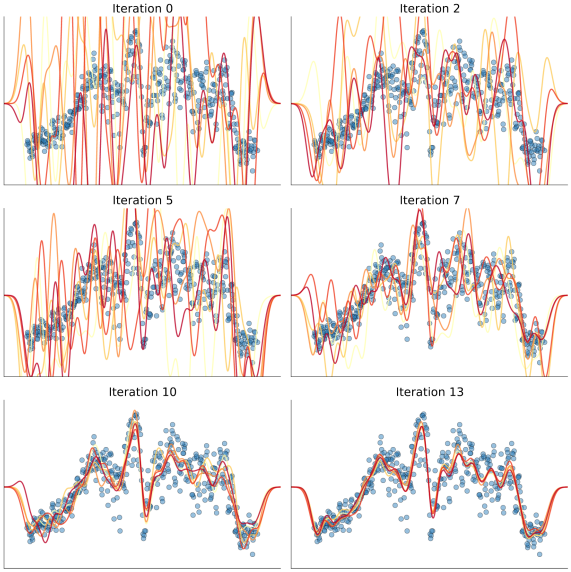
If $P^{-1} = \hat{K}^{-1}$, then $\kappa(P^{-1}\hat{K}) = 1$ and we solve in one step.



Preconditioning

Figure taken from Davies (2015)

CG example


Iteration 0
Iteration 2
Iteration 5
Iteration 7
Iteration 10
Iteration 13

Section 4

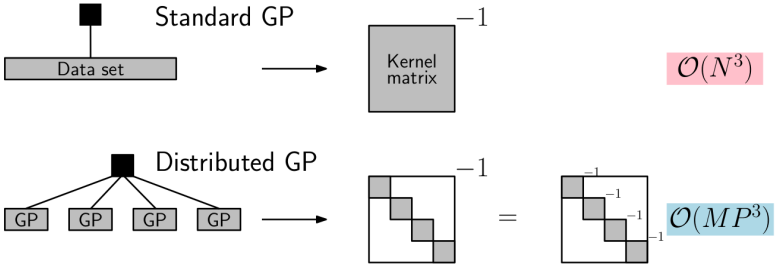
Local approximations: Split problem into smaller chunks

1. What is the computational issue?
2. Exploiting structure in data and/or GP prior
3. Solving the linear system approximately (with Conjugate Gradients)
4. Local approximations: Split problem into smaller chunks
5. Global approximations: Inducing points
6. Variational inference for sparse GPs
7. Recap

Combining "local experts"

- Split input domain/dataset (size N) into M subsets (size $P \approx N/M$)
- Fit M independent GP models (shared kernel hyperparameters): $\mathcal{O}(P^3)$ each
- Aggregate predictions
  - $+$ Mixture of experts
  - $\times$ product of experts, e.g.

$$p(f_* \,|\, \boldsymbol{x}_*, \mathcal{D}) \propto \prod_{k=1}^{M} p_k(f_* \,|\, \boldsymbol{x}_*, \mathcal{D}^{(k)})$$



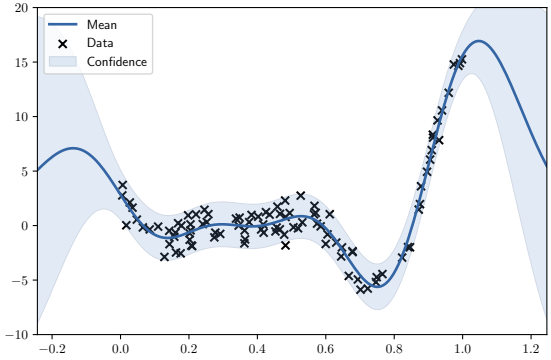
Section 5

Global approximations: Inducing points

1. What is the computational issue?
2. Exploiting structure in data and/or GP prior
3. Solving the linear system approximately (with Conjugate Gradients)
4. Local approximations: Split problem into smaller chunks
5. Global approximations: Inducing points
   - Data redundancy
   - Nyström approximation
   - Pseudo data / inducing points
6. Variational inference for sparse GPs
7. Recap

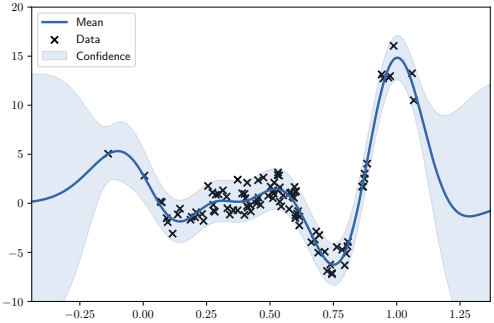
Big data (?)

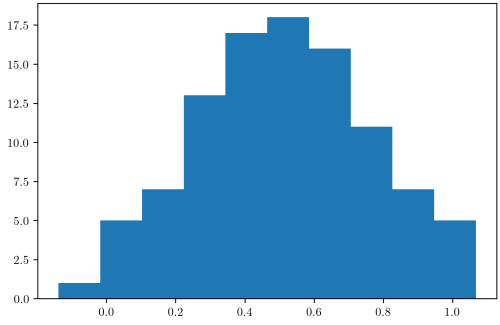
- Lots of data $\neq$ complex function
- In real world problems, we often collect a lot of data for modeling relatively simple relations.



Data subsampling?

- Real data generally not evenly distributed.
- Typically a lot of data on common cases, very few data on rare cases.





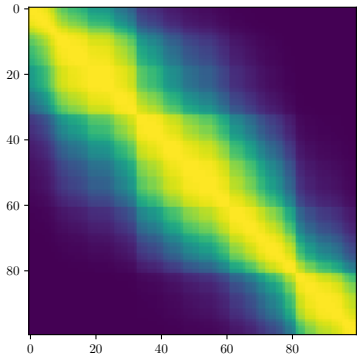
Sparse Gaussian processes

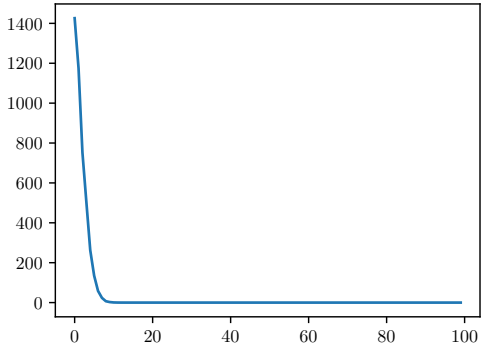
"Sparse GP" refers to various different approximations:

- Nyström approximation
- Fully independent training conditional (FITC)
- Variational sparse Gaussian process

Covariance matrix of redundant data

- With redundant data, the covariance matrix becomes low rank.





- What about low rank approximation?

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Low-rank approximation

- Recall GP marginal log-likelihood:

$$\log p(\mathbf{y} \mid \mathbf{X}) = \log \mathcal{N}\left(\mathbf{y} \mid \mathbf{0}, \mathbf{K} + \sigma^2 \mathbf{I}\right),$$

  where $\mathbf{K}$ is the covariance matrix computed from $\mathbf{X}$ according to the kernel function $k(\cdot, \cdot)$ and σ^2 is the variance of the Gaussian noise distribution.
- Assume $\mathbf{K}$ to be low rank.
- This leads to the Nyström approximation by Williams and Seeger

Approximation by subset

- Let's randomly pick a subset from the training data: $\mathbf{Z} \in \mathbb{R}^{M \times Q}$.
- Approximate the covariance matrix $\mathbf{K}$ by $\tilde{\mathbf{K}}$.

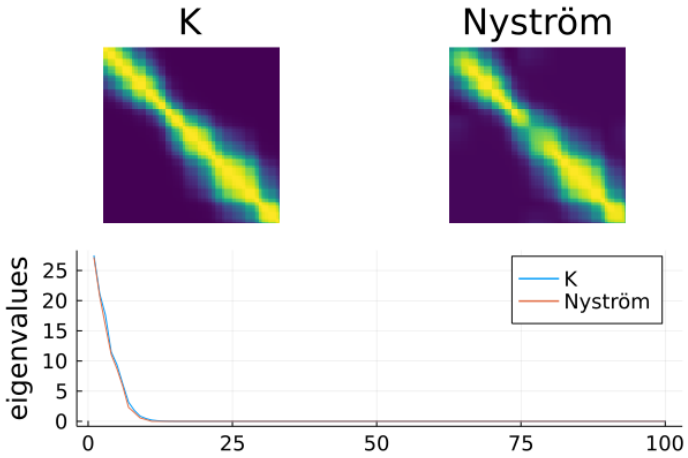
$$\tilde{\mathbf{K}} = \mathbf{K}_z \mathbf{K}_{zz}^{-1} \mathbf{K}_z^\top, \text{ where } \mathbf{K}_z = \mathbf{K}(\mathbf{X}, \mathbf{Z}) \text{ and } \mathbf{K}_{zz} = \mathbf{K}(\mathbf{Z}, \mathbf{Z}).$$

- Note that $\tilde{\mathbf{K}} \in \mathbb{R}^{N \times N}$, $\mathbf{K}_z \in \mathbb{R}^{N \times M}$ and $\mathbf{K}_{zz} \in \mathbb{R}^{M \times M}$.
- The log-likelihood is approximated by

$$\log p(\mathbf{y} \mid \mathbf{X}, \theta) \approx \log \mathcal{N}\left(\mathbf{y} \mid \mathbf{0}, \mathbf{K}_z \mathbf{K}_{zz}^{-1} \mathbf{K}_z^\top + \sigma^2 \mathbf{I}\right).$$

Nyström approximation example

Nyström approximation using 10 random data points:



Efficient computation using Woodbury formula

Naive formulation: still $\mathcal{O}(N^3)$!

$$\tilde{\mathcal{L}} = -\frac{1}{2}\log|2\pi(\tilde{\mathbf{K}} + \sigma^2\mathbf{I})| - \frac{1}{2}\mathbf{y}^\top(\tilde{\mathbf{K}} + \sigma^2\mathbf{I})^{-1}\mathbf{y}$$

Apply the Woodbury matrix identity:

$$\begin{aligned}(UC \quad V \quad +A)^{-1} \quad &= A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1} \\ (\mathbf{K}_z\mathbf{K}_{zz}^{-1}\mathbf{K}_z^\top + \sigma^2\mathbf{I})^{-1} &= \sigma^{-2}\mathbf{I} - \sigma^{-4}\mathbf{K}_z(\mathbf{K}_{zz} + \sigma^{-2}\mathbf{K}_z^\top\mathbf{K}_z)^{-1}\mathbf{K}_z^\top\end{aligned}$$

- Note that $(\mathbf{K}_{zz} + \sigma^{-2}\mathbf{K}_z^\top\mathbf{K}_z) \in \mathbb{R}^{M\times M}$.
- The computational complexity reduces to $O(NM^2)$.

Nyström approximation

- Approximation directly on the covariance matrix
- Randomly selected subset of data points
- Approximation becomes exact if the whole data set is taken, *i.e.*, $\mathbf{K}\mathbf{K}^{-1}\mathbf{K}^{\top} = \mathbf{K}$.

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Inducing point methods

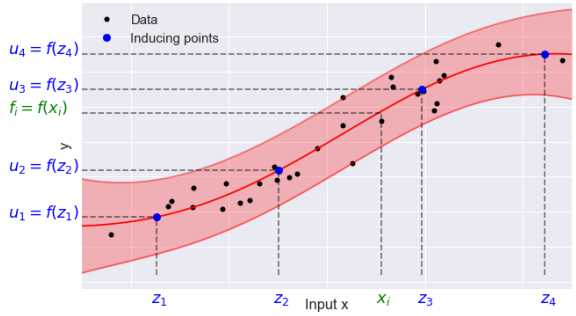
Main idea: "represent" the information from the full dataset using a smaller "virtual" dataset

- Recall our GP model:

$$p(\boldsymbol{y}, \boldsymbol{f}) = p(\boldsymbol{y} \mid \boldsymbol{f})p(\boldsymbol{f}), \quad \text{where} \quad \boldsymbol{f} = [f(\boldsymbol{x}_1), f(\boldsymbol{x}_2), \ldots, f(\boldsymbol{x}_N)]$$

- We will now introduce a set of *inducing points* $\{\boldsymbol{z}_m\}_{m=1}^M$
- They live in the same space as the input points, i.e. $\boldsymbol{x}_i, \boldsymbol{z}_j \in \mathbb{R}^D$
- 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



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

Section 6

Variational inference for sparse GPs

1. What is the computational issue?
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4. Local approximations: Split problem into smaller chunks
5. Global approximations: Inducing points
6. Variational inference for sparse GPs
   - Recap: Variational inference
   - Variational inference for inducing variables
   - Collapsed bound for Gaussian likelihood
   - Mini-batch learning
   - Mini-batch learning for GPs
   - Numerical considerations

Variational inference: The big picture

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

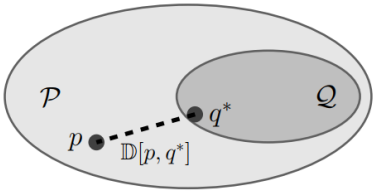
1. Define some "simple" family of distributions $\mathcal{Q}$.
2. Define some way to compute a "distance" $\mathbb{D}[p, q]$ between intractable distribution p and each distribution $q \in \mathcal{Q}$

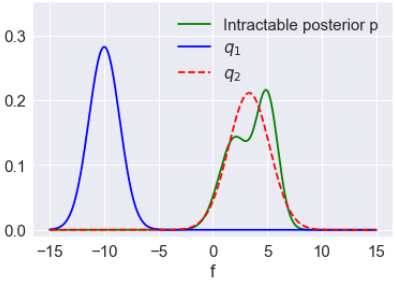
$$\mathbb{D}[p, q_1] > \mathbb{D}[p, q_2]$$

3. Search for $q \in \mathcal{Q}$ such that $\mathbb{D}[p, q]$ is minimized

$$q^* = \arg\min_{q \in \mathcal{Q}} \mathbb{D}[p, q]$$

4. Use q^* as an approximation of p





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

How to "measure distances" between distributions?

Here: *Kullback-Leibler divergence*

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

Important properties:

1. Non-symmetric: $\mathrm{KL}[q \,\|\, p] \neq \mathrm{KL}[p \,\|\, q]$
2. Positive: $\mathrm{KL} \geq 0$ (Gibbs' inequality)
3. Minimum: $\mathrm{KL}[q \,\|\, p] = 0 \iff q \equiv p$.

Variational inference: Minimizing $\mathrm{KL}[q(\boldsymbol{f}) \,\|\, p(\boldsymbol{f} \mid \boldsymbol{y})]$ by bounding

$$\mathrm{KL}[q(\boldsymbol{f}) \,\|\, p(\boldsymbol{f} \mid \boldsymbol{y})] = \mathrm{KL}[q(\boldsymbol{f}) \,\|\, p(\boldsymbol{f})] - \int q(\boldsymbol{f}) \big[\log p(\boldsymbol{y} \mid \boldsymbol{f})\big] \mathrm{d}\boldsymbol{f} + \log p(\boldsymbol{y})$$

$$\log p(\boldsymbol{y}) = \underbrace{\int q(\boldsymbol{f}) \big[\log p(\boldsymbol{y} \mid \boldsymbol{f})\big] \mathrm{d}\boldsymbol{f} - \mathrm{KL}[q(\boldsymbol{f}) \,\|\, p(\boldsymbol{f})]}_{\mathcal{L}[q]} + \underbrace{\mathrm{KL}[q(\boldsymbol{f}) \,\|\, p(\boldsymbol{f} \mid \boldsymbol{y})]}_{\geq 0}$$

$$\geq \int q(\boldsymbol{f}) \big[\log p(\boldsymbol{y} \mid \boldsymbol{f})\big] \mathrm{d}\boldsymbol{f} - \mathrm{KL}[q(\boldsymbol{f}) \,\|\, p(\boldsymbol{f})] = \mathcal{L}[q]$$

- $\log p(\boldsymbol{y})$ is a constant
- $\mathcal{L}[q]$ does not depend on $p(\boldsymbol{f} \mid \boldsymbol{y})$
- $\mathcal{L}[q] \leq \log p(\boldsymbol{y})$, so $\mathcal{L}[q]$ is a *lower bound* on the marginal log likelihood
- Maximizing $\mathcal{L}[q]$ is equivalent to minimizing $\mathrm{KL}[q(\boldsymbol{f}) \,\|\, p(\boldsymbol{f} \mid \boldsymbol{y})]$

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

Variational inference: ELBO

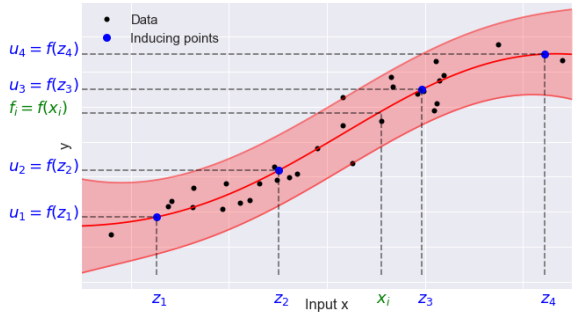
$$\log p(\boldsymbol{y}) \geq \mathcal{L}[q] = \underbrace{\int q(\boldsymbol{f}) \big[\log p(\boldsymbol{y} \mid \boldsymbol{f})\big] \mathrm{d}\boldsymbol{f}}_{\text{data fit}} - \underbrace{\mathrm{KL}[q(\boldsymbol{f}) \,\|\, p(\boldsymbol{f})]}_{\text{regularization}}$$

$\mathcal{L}[q]$ often called the *Evidence Lower Bound* (ELBO)

- To approximate $p(\boldsymbol{f} \mid \boldsymbol{y})$, use $q(\boldsymbol{f}) = \mathcal{N}(\boldsymbol{f} \mid \boldsymbol{m}, \boldsymbol{S})$
- Define $\boldsymbol{\lambda} = \{\boldsymbol{m}, \boldsymbol{S}\}$, then we can write $\mathcal{L}[q] = \mathcal{L}[\boldsymbol{\lambda}]$
- In practice, we optimize $\mathcal{L}[\boldsymbol{\lambda}]$ using gradient-based methods

1. What is the computational issue?
2. Exploiting structure in data and/or GP prior
3. Solving the linear system approximately (with Conjugate Gradients)
4. Local approximations: Split problem into smaller chunks
5. Global approximations: Inducing points
6. Variational inference for sparse GPs
   - Recap: Variational inference
   - Variational inference for inducing variables
   - Collapsed bound for Gaussian likelihood
   - Mini-batch learning
   - Mini-batch learning for GPs
   - Numerical considerations

Joint model over function values and inducing variables



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

Inducing point methods: the joint model

- The augmented model

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

- We recover the original model by marginalizing over $\boldsymbol{u}$:

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

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

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

Inducing point methods: the joint model II

- The joint model

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

- Using Gaussian conditional densities (lecture #1):

$$\begin{aligned} p(\boldsymbol{y} \mid \boldsymbol{f}) &= \mathcal{N}\left(\boldsymbol{y} \mid \boldsymbol{f}, \sigma^2 \boldsymbol{I}\right) \\ p(\boldsymbol{f} \mid \boldsymbol{u}) &= \mathcal{N}\left(\boldsymbol{f} \mid \boldsymbol{K}_{nm} \boldsymbol{K}_{mm}^{-1} \boldsymbol{u}, \tilde{\boldsymbol{K}}\right), \quad \tilde{\boldsymbol{K}} = \boldsymbol{K}_{nn} - \boldsymbol{K}_{nm} \boldsymbol{K}_{mm}^{-1} \boldsymbol{K}_{mn} \\ p(\boldsymbol{u}) &= \mathcal{N}\left(\boldsymbol{u} \mid \boldsymbol{0}, \boldsymbol{K}_{mm}\right) \end{aligned}$$

- Covariance of inducing points: $[\boldsymbol{K}_{mm}]_{ij} = k(\boldsymbol{z}_i, \boldsymbol{z}_j)$
- Cross-covariance between inducing points and training: $[\boldsymbol{K}_{mn}]_{ij} = k(\boldsymbol{z}_i, \boldsymbol{x}_j)$
- Covariance of training points: $[\boldsymbol{K}_{nn}]_{ij} = k(\boldsymbol{z}_i, \boldsymbol{x}_j)$

Variational Sparse Gaussian Process

- Typical variational lower bound of a marginal likelihood:

$$\begin{aligned}\log p(\mathbf{y} \mid \mathbf{X}) &= \log \int_{\mathbf{f},\mathbf{u}} p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z}) p(\mathbf{u} \mid \mathbf{Z}) \\ &\geq \int_{\mathbf{f},\mathbf{u}} q(\mathbf{f}, \mathbf{u}) \log \frac{p(\mathbf{y} \mid \mathbf{f}) p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z}) p(\mathbf{u} \mid \mathbf{Z})}{q(\mathbf{f}, \mathbf{u})} \equiv \mathcal{L}\end{aligned}$$

- Let's define a *special* variational posterior (make use of structure in our problem):

$$q(\mathbf{f}, \mathbf{u}) = p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}), \quad \text{where } q(\mathbf{u}) = \mathcal{N}(\mathbf{u} \mid \mu, \Sigma).$$

- Plug it into the lower bound:

$$\begin{aligned}\mathcal{L} &= \int_{\mathbf{f},\mathbf{u}} p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}) \log \frac{p(\mathbf{y} \mid \mathbf{f}) \cancel{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z})} p(\mathbf{u} \mid \mathbf{Z})}{\cancel{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z})} q(\mathbf{u})} \\ &= \langle \log p(\mathbf{y} \mid \mathbf{f}) \rangle_{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u})} - \mathrm{KL}[q(\mathbf{u}) \,\|\, p(\mathbf{u} \mid \mathbf{Z})]\end{aligned}$$

Likelihood term

- Remember: $p(\boldsymbol{y} \mid \boldsymbol{f}) = \prod_{i=1}^{N} p(y_i \mid f_i)$
- Let's have a closer look at the first term

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

Decomposing the likelihood term

- Let's define the univariate distribution

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

- Variational expectations term:

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

- As in the previous lecture:
  - Decomposes into a sum over 1D integrals
  - Solved analytically for some likelihoods
  - Fast to approximate using numerical integration for others

Sparse variational posterior for **Gaussian** likelihood

- Variational posterior:

$$q(\mathbf{f}, \mathbf{u}) = p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}), \quad \text{where } q(\mathbf{u}) = \mathcal{N}(\mathbf{u} \mid \mu, \Sigma).$$

- Lower bound:

$$\begin{aligned}
\mathcal{L} &= \int_{\mathbf{f},\mathbf{u}} p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}) \log \frac{p(\mathbf{y} \mid \mathbf{f}) \cancel{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z})} p(\mathbf{u} \mid \mathbf{Z})}{\cancel{p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z})} q(\mathbf{u})} \\
&= \langle \log p(\mathbf{y} \mid \mathbf{f}) \rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X},\mathbf{Z}) q(\mathbf{u})} - \mathrm{KL}[q(\mathbf{u}) \,\|\, p(\mathbf{u} \mid \mathbf{Z})] \\
&= \left\langle \log \mathcal{N}\left(\mathbf{y} \mid \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{u}, \sigma^2\mathbf{I}\right) \right\rangle_{q(\mathbf{u})} - \mathrm{KL}[q(\mathbf{u}) \,\|\, p(\mathbf{u} \mid \mathbf{Z})]
\end{aligned}$$

- There is no inversion of any big covariance matrices in the first term:

$$-\frac{N}{2} \log 2\pi\sigma^2 - \frac{1}{2\sigma^2} \left\langle (\mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{u} - \mathbf{y})^\top (\mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{u} - \mathbf{y}) \right\rangle_{q(\mathbf{u})}$$

- The overall complexity of the lower bound is $O(NM^2)$.

Tighten the Bound

- Find the optimal parameters of $q(\mathbf{u})$:

$$(\boldsymbol{m}^*, \mathbf{S}^*) = \arg\max_{\boldsymbol{m},\mathbf{S}} \mathcal{L}(\boldsymbol{m}, \mathbf{S}).$$

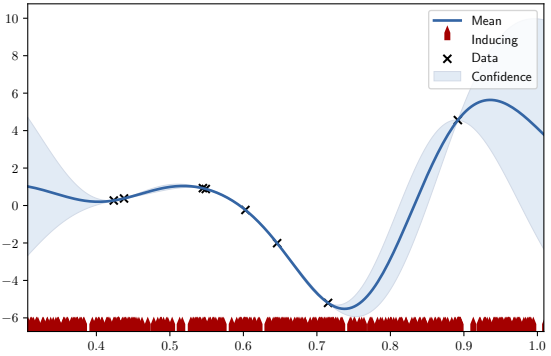
- Make the bound as tight as possible by plugging in $\boldsymbol{m}^*$ and $\mathbf{S}^*$:

$$\mathcal{L} = \log \mathcal{N}\left(\mathbf{y} \mid \mathbf{0}, \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^\top + \sigma^2\mathbf{I}\right) - \frac{1}{2\sigma^2}\text{tr}\left(\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^\top\right).$$

- The 1st term is the same as in the Nyström approximation.
- The overall complexity of the lower bound remains $O(NM^2)$.

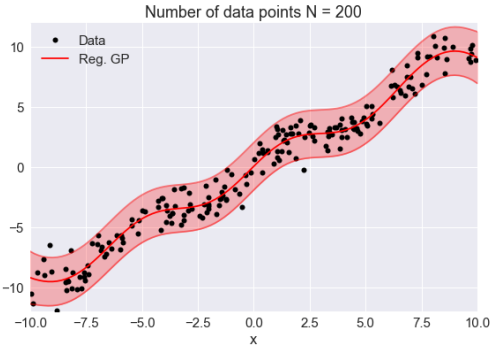
Variational sparse GP

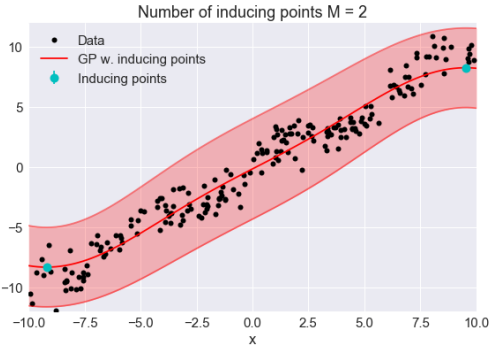
- Note that $\mathcal{L}$ is not a valid log-pdf, $\int_{\mathbf{y}} \exp(\mathcal{L}(\mathbf{y})) \leq 1$, due to the trace term.
- As inducing points are variational parameters, optimizing the inducing inputs $\mathbf{Z}$ always leads to a better bound.
- The model does not "overfit" with too many inducing points.



Example: Number of inducing points

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





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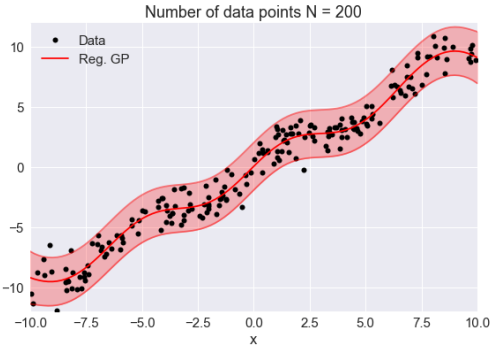

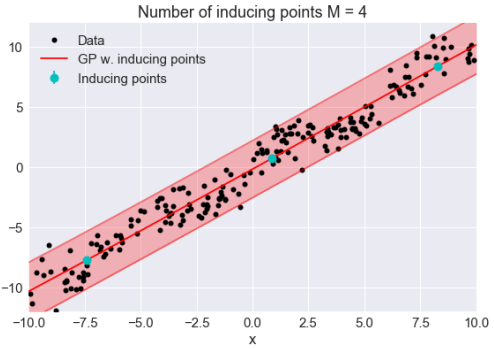

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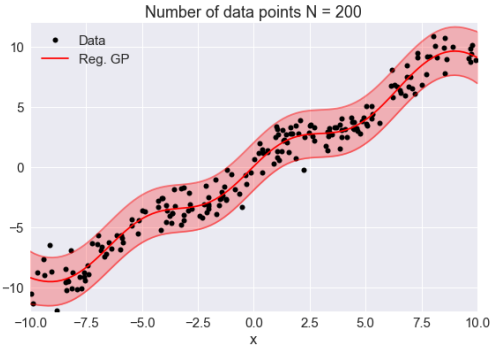

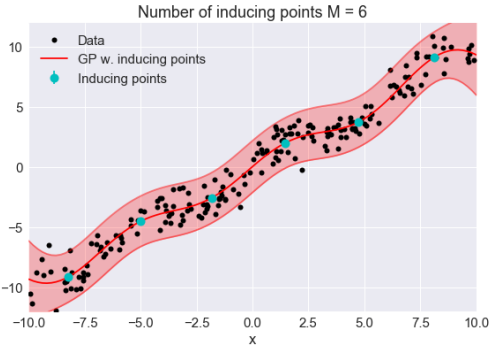

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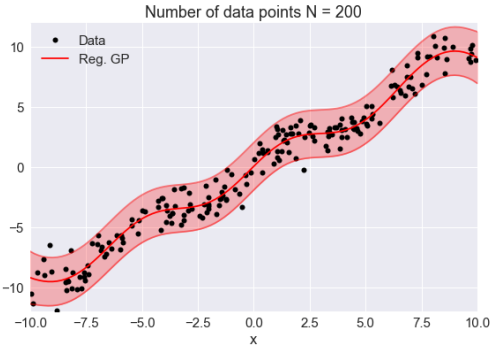

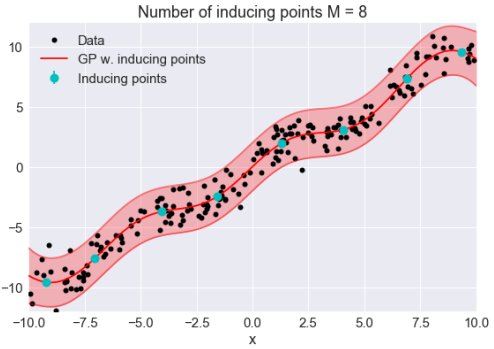

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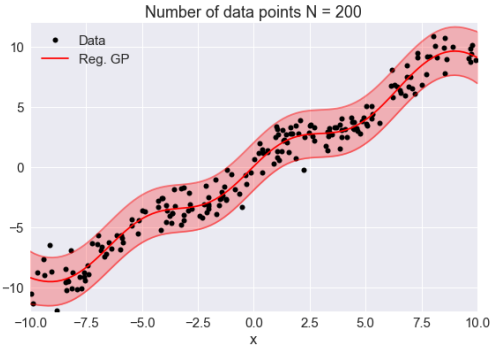

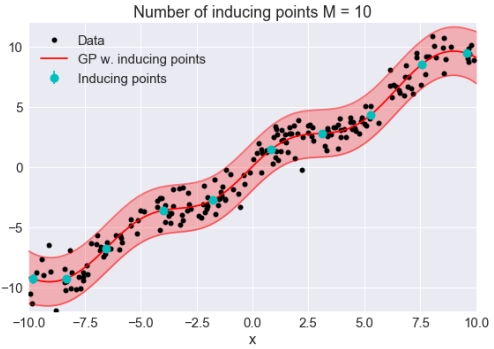

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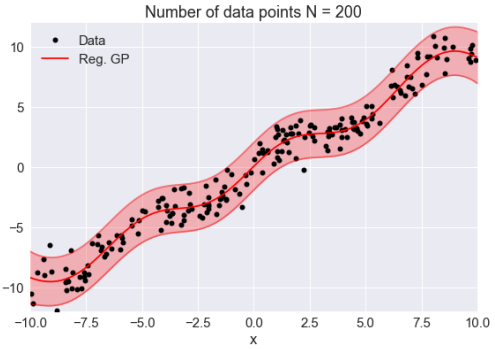

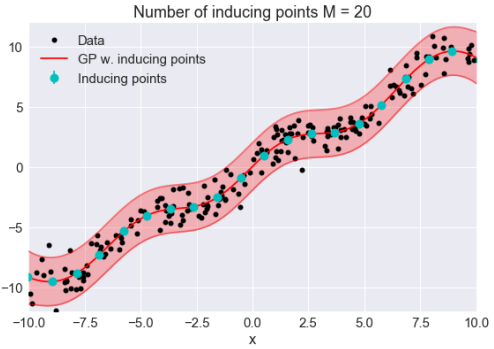

Limitations of sparse GPs

Variational sparse GP has computational complexity $O(NM^2)$.

The computation becomes infeasible under two scenarios:

- The number of data points N is very high, e.g., millions of data points.
- The function is very complex, which requires tens of thousands of inducing points.

1. What is the computational issue?
2. Exploiting structure in data and/or GP prior
3. Solving the linear system approximately (with Conjugate Gradients)
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Mini-batch learning (1)

- Mini-batch learning allows DNNs to be trained on millions of data points.
- Given a set of inputs and labels, $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^N$, $(\mathbf{x}_i, y_i) \sim p(\mathbf{x}, y)$, the true loss function is defined as

$$c_{\text{true}} = \int l(f_\theta(\mathbf{x}), y) p(\mathbf{x}, y) \, \mathrm{d}\mathbf{x} \, \mathrm{d}y \approx \frac{1}{N} \sum_{i=1}^{N} l(f_\theta(\mathbf{x}), y) = c,$$

  where $f_\theta(\cdot)$ is DNN and $l(\cdot, \cdot)$ is the loss function.
- Gradient descent (GD) updates the parameters by

$$\theta_{t+1} = \theta_t - \eta \frac{\mathrm{d}c}{\mathrm{d}\theta}.$$

Mini-batch learning (2)

- Mini-batch learning approximates the loss by subsampling the data,

$$c_{\text{MB}} = \frac{1}{B} \sum_{\mathbf{x}_i, y_i \sim \tilde{p}(\mathbf{x}, y)} l(f_\theta(\mathbf{x}_i), y_i).$$

- Stochastic gradient descent (SGD) updates the parameters by

$$\theta_{t+1} = \theta_t - \eta \frac{\mathrm{d}c_{\text{MB}}}{\mathrm{d}\theta}.$$

- Can mini-batch learning be applied to GPs as well?

Mini-batch Learning for GPs

- Mini-batch learning relies on the objective being an expectation w.r.t. the data, i.e., $\langle l(f_\theta(\mathbf{x}), y) \rangle_{p(\mathbf{x},y)}$.
- The log-marginal likelihood of GP:

$$\log \mathcal{N}\left(\mathbf{y} \mid \mathbf{0}, \mathbf{K} + \sigma^2 \mathbf{I}\right)$$

- The variational lower bound of sparse GP:

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

- Not an expectation w.r.t. the data!

"Uncollapsed" lower bound

- Let's revisit original ("uncollapsed") variational lower bound of sparse GP:

$$\mathcal{L} = \langle \log p(\mathbf{y} \mid \mathbf{f}) \rangle_{p(\mathbf{f}|\mathbf{u},\mathbf{X},\mathbf{Z})q(\mathbf{u})} - \mathrm{KL}[q(\mathbf{u}) \,\|\, p(\mathbf{u})]$$

- The 2nd term, $\mathrm{KL}[q(\mathbf{u}) \,\|\, p(\mathbf{u})]$, does not depend on the data.

"Uncollapsed" lower bound

- In the 1st term, as $p(\mathbf{y} \mid \mathbf{f}) = \mathcal{N}\left(\mathbf{y} \mid \mathbf{f}, \sigma^2\mathbf{I}\right)$,

$$\log p(\mathbf{y} \mid \mathbf{f}) = \sum_{n=1}^{N} \log \mathcal{N}\left(y_n \mid f_n, \sigma^2\right)$$

- Denote $q(\mathbf{f} \mid \mathbf{X}, \mathbf{Z}) = \int p(\mathbf{f} \mid \mathbf{u}, \mathbf{X}, \mathbf{Z}) q(\mathbf{u}) \, \mathrm{d}\mathbf{u}$.

$$\begin{aligned}
\left\langle \log p(\mathbf{y} \mid \mathbf{f}) \right\rangle_{q(\mathbf{f}|\mathbf{X},\mathbf{Z})} &= \left\langle \sum_{n=1}^{N} \log \mathcal{N}\left(y_n \mid f_n, \sigma^2\right) \right\rangle_{q(\mathbf{f}|\mathbf{X},\mathbf{Z})} \\
&= \sum_{n=1}^{N} \left\langle \log \mathcal{N}\left(y_n \mid f_n, \sigma^2\right) \right\rangle_{q(f_n|\mathbf{x}_n,\mathbf{Z})}
\end{aligned}$$

Stochastic Variational GP (SVGP)

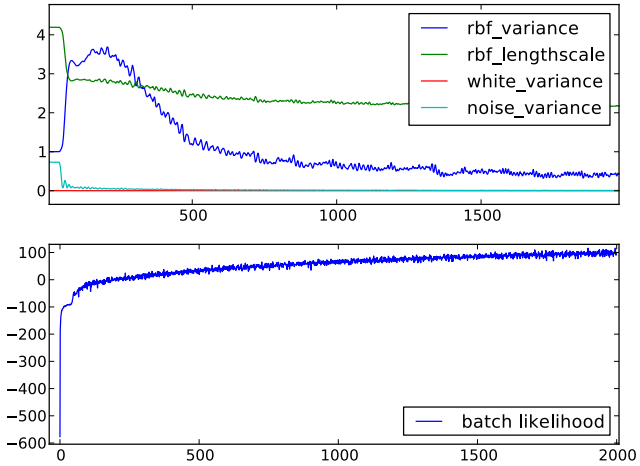
- The resulting lower bound can be written as the sum over the data,

$$\begin{aligned}\mathcal{L} &= \sum_{n=1}^{N} \left\langle \log \mathcal{N}\left(y_n \mid f_n, \sigma^2\right) \right\rangle_{q(f_n|\mathbf{x}_n,\mathbf{Z})} - \mathrm{KL}[q(\mathbf{u}) \,\|\, p(\mathbf{u})] \\ &\approx \frac{N}{B} \sum_{\mathbf{x}_i, y_i \sim \tilde{p}(\mathbf{x},y)} \left\langle \log \mathcal{N}\left(y_i \mid f_i, \sigma^2\right) \right\rangle_{q(f_i|\mathbf{x}_i,\mathbf{Z})} - \mathrm{KL}[q(\mathbf{u}) \,\|\, p(\mathbf{u})] = \mathcal{L}_{\mathsf{MB}}\end{aligned}$$

- This allows us to do mini-batch learning with SGD,

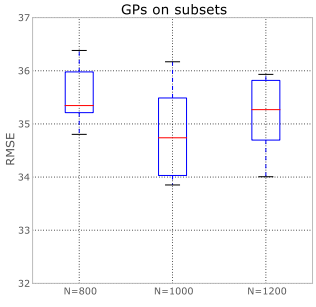
$$\theta_{t+1} = \theta_t - \eta \frac{\mathrm{d}\mathcal{L}_{\mathsf{MB}}}{\mathrm{d}\theta}.$$

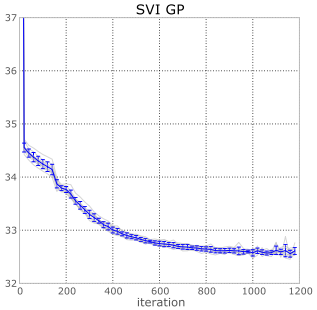
Example: 2D synthetic data

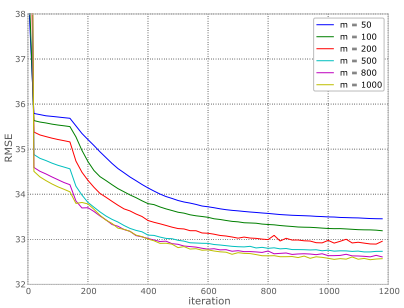


Example: Airline delay data

Flight delays for every commercial flight in the USA from January to April 2008. 700,000 train, 100,000 test







Example from the paper

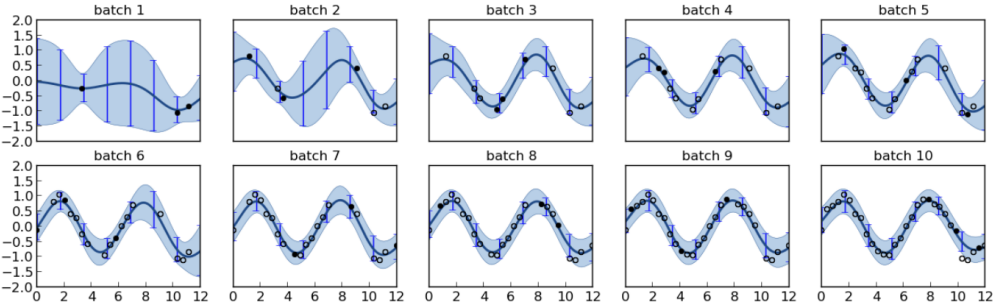


Figure 2: Stochastic variational inference on a trivial GP regression problem. Each pane shows the posterior of the GP after a batch of data, marked as solid points. Previoulsy seen (and discarded) data are marked as empty points, the distribution $q(\mathbf{u})$ is represented by vertical errorbars.

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

Avoid direct inverses

- Kernel matrix may have high condition number (particularly under squared exponential kernel)

$\rightarrow$ direct inverse numerically unstable

- Instead: Cholesky and (triangular) solve
- Sparse inducing points help

Jitter

- Kernel matrix is positive definite . . . or is it?
- Might not be *numerically* positive definite (near-zero but negative eigenvalues)

→ Cholesky failures. . .

- Solution: add small diagonal *jitter* (or *nugget*) to kernel matrix (e.g., $10^{-6}\mathbf{I}$)
- Corresponds to "observing" function values under (very small) noise to make up for finite machine precision

Whitening

- Prior $p(\boldsymbol{u})$ strongly correlates the elements of $q(\boldsymbol{u}) = \mathcal{N}(\boldsymbol{m}, \mathbf{S})$
  $\rightarrow$ Optimization over $\boldsymbol{m}$ and $\mathbf{S}$ is challenging

- **Whitening**: reparameterization
  - Define $\boldsymbol{u} = \mathbf{L}\boldsymbol{v}$(+prior mean)
    where $\mathbf{L} = \texttt{chol}(\mathbf{K})$ or $\mathbf{K} = \mathbf{L}\mathbf{L}^\top$
  - Prior $p(\boldsymbol{v}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$, completely uncorrelated
  - Optimize over $q(\boldsymbol{v}) = \mathcal{N}(\boldsymbol{m}', \mathbf{S}')$ instead
  - Approximate posterior $q(\boldsymbol{u}) = \mathcal{N}(\mathbf{L}\boldsymbol{m}', \mathbf{L}\mathbf{S}'\mathbf{L}^\top)$

- (similar idea to preconditioning in CG)

How do we initialize all these parameters?

- Kernel hyperparameters: as for exact GP regression
  see `https://tinyurl.com/guide2gp` (scale your data!)
- Approximate posterior $q(\boldsymbol{u})$: at the prior $\mathcal{N}(\mathbf{0}, \mathbf{K})$
  whitening: initialize $q(\boldsymbol{v}) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
- Inducing point locations Z:
  - Low dimensions: grid
  - (Randomly shuffled!) subset of data
  - Cluster centers (e.g., k-means)
  - Determinantal point process
- Random restarts

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)

Section 7

Recap

Recap on scaling to large data

The naïve $\mathcal{O}(n^3)$ computational bottleneck ($\mathcal{O}(n^2)$ memory) can be tackled by

- Exploiting structure in the data
  (data on grid, inputs are in 1D, ...)
- Exploiting structure in the GP prior
  (GP prior is stationary, separable over input dimensions, ...)
- Solving the linear system approximately
  (conjugate-gradient solvers)
- Split problem into smaller chunks
  (local experts, subset of data, divide & conquer, ...)
- Approximate the problem
  (Nyström, low-rank, inducing points, ...)
- Approximate the problem solution
  (SVGP = sparse (and stochastic) variational methods)

End of today's lecture

- Computational bottlenecks in exact GP regression (most methods typically apply to general likelihoods)
- The limitations we discussed on the first lecture are actually not that severe
- We will look at one more approach for speeding up GPs later in the course