Scalable Gaussian Processes

Zhenwen Dai

Amazon

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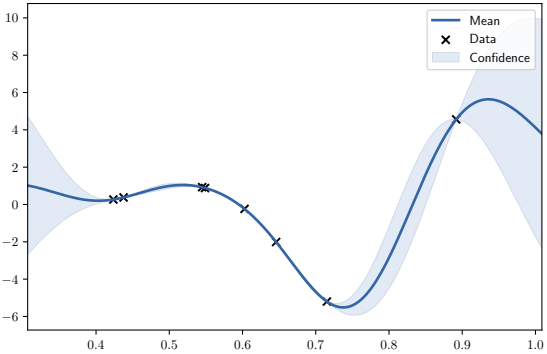
Gaussian process

Input and Output Data:

$$\mathbf{y} = (y_1, \ldots, y_N), \quad \mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)^\top$$

$$p(\mathbf{y}|\mathbf{f}) = \mathcal{N}\left(\mathbf{y}|\mathbf{f}, \sigma^2\mathbf{I}\right), \quad p(\mathbf{f}|\mathbf{X}) = \mathcal{N}\left(\mathbf{f}|0, \mathbf{K}(\mathbf{X}, \mathbf{X})\right)$$



Behind a Gaussian process fit

- Maximum likelihood estimate of the hyper-parameters.

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

- Prediction on a test point given the observed data and the optimized hyper-parameters.

$$p(\mathbf{f}_*|\mathbf{X}_*, \mathbf{y}, \mathbf{X}, \theta) = \mathcal{N}\left(\mathbf{f}_*|\mathbf{K}_*(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{y}, \mathbf{K}_{**} - \mathbf{K}_*(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{K}_*^\top\right)$$

How to implement the log-likelihood (1)

- Compute the covariance matrix $\mathbf{K}$:

$$\mathbf{K} = \begin{pmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \cdots & k(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & \ddots & \vdots \\ k(\mathbf{x}_N, \mathbf{x}_1) & \cdots & k(\mathbf{x}_N, \mathbf{x}_N) \end{pmatrix}$$

  where $k(\mathbf{x}_i, \mathbf{x}_j) = \gamma \exp\left(-\frac{1}{2l^2}(\mathbf{x}_i - \mathbf{x}_j)^\top (\mathbf{x}_i - \mathbf{x}_j)\right)$

- The complexity is $O(N^2 Q)$.

How to implement the log-likelihood (2)

- Plug in the log-pdf of multi-variate normal distribution:

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

- Take a Cholesky decomposition: $\mathbf{L} = \texttt{chol}(\mathbf{K}+\sigma^2\mathbf{I})$.
- The computational complexity is $O(N^3+N^2+N)$. Therefore, the overall complexity including the computation of $\mathbf{K}$ is $O(N^3)$.

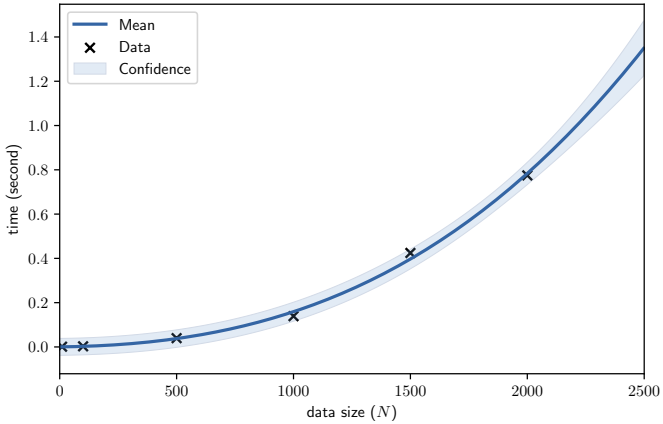
A quick profiling (N=1000, Q=10)

Time unit is microsecond.

```
Line #      Time    % 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
```

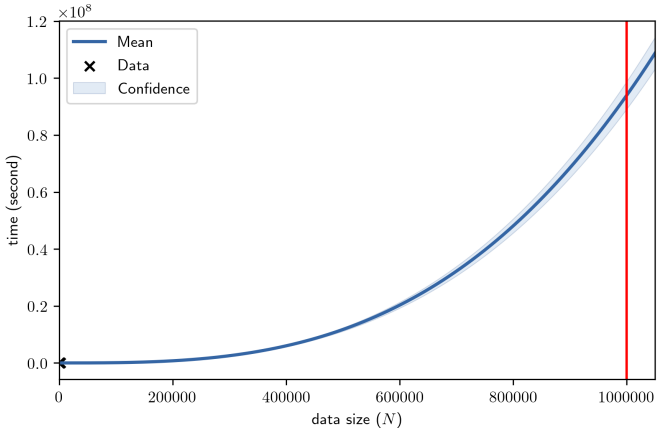
Empirical analysis of computational time

- I collect the run time for $N = \{10, 100, 500, 1000, 1500, 2000\}$.
- They take 1.3ms, 8.5ms, 28ms, 0.12s, 0.29s, 0.76s.



What if we have 1 million data points?

The mean of predicted computational time is 9.4×10^7 seconds ≈ 2.98 years.

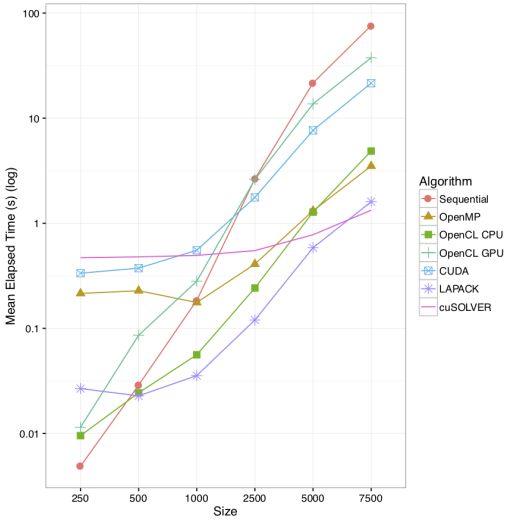


What about waiting for faster computers?

- Computational time $= \frac{\text{amount of work}}{\text{computer speed}}$
- If the computer speed increase at the pace of 20% year over year:
  - After 10 years, it will take about 176 days.
  - After 50 years, it will take about 2.9 hours.
- If we double the size of data, it takes 11.4 years to catch up.

What about parallel computing / GPU?

- Ongoing works about speeding up Cholesky decomposition with multi-core CPU or GPU.
- Main limitation: heavy communication and shared memory.

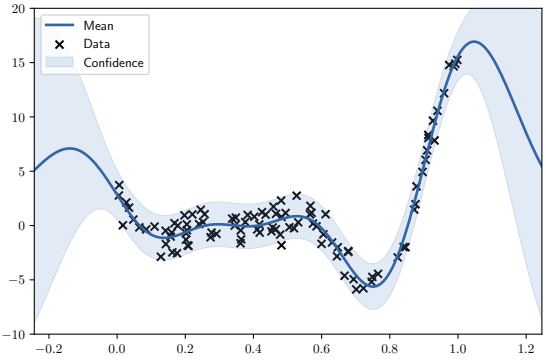


Other approaches

- Apart from speeding up the exact computation, there have been a lot of works on approximation of GP inference.
- These methods often target at some specific scenario and provide good approximation for the targeted scenarios.
- Provide an overview about common approximations.

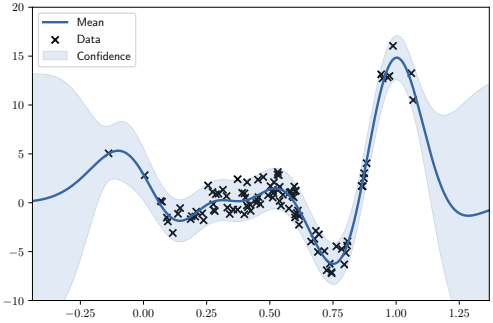
Big data (?)

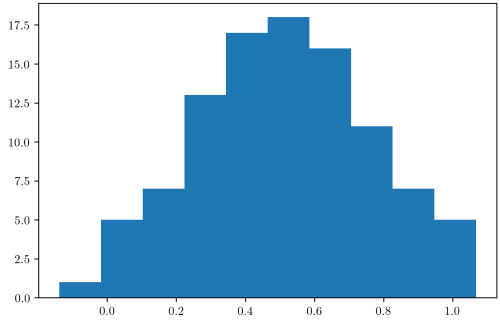
- lots of data $\neq$ complex function
- In real world problems, we often collect a lot of data for modeling relatively simple relations.



Data subsampling?

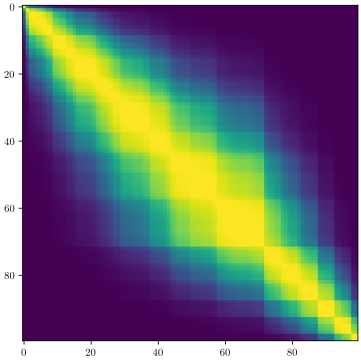
- Real data often do not evenly distributed.
- We tend to get a lot of data on common cases and very few data on rare cases.

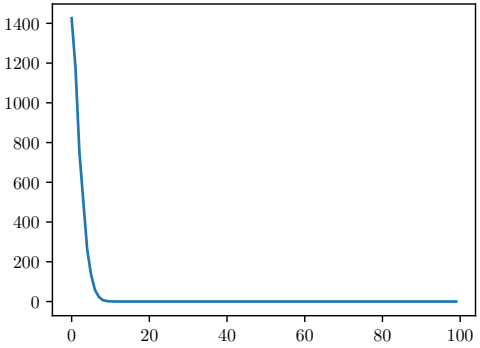




Covariance matrix of redundant data

- With redundant data, the covariance matrix becomes low rank.
- What about low rank approximation?





Low-rank approximation

- Let's recall the log-likelihood of GP:

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

  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 Nyström approximation by Williams and Seeger [Williams and Seeger, 2001].

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

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

Efficient computation using Woodbury formula

- The naive formulation does not bring any computational benefits.

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

- Apply the Woodbury formula:

$$(\mathbf{K}_z\mathbf{K}_{zz}^{-1}\mathbf{K}_z^\top + \sigma^2\mathbf{I})^{-1} = \sigma^{-2}\mathbf{I} - \sigma^{-4}\mathbf{K}_z(\mathbf{K}_{zz} + \sigma^{-2}\mathbf{K}_z^\top\mathbf{K}_z)^{-1}\mathbf{K}_z^\top$$

- 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

- The above approach is called Nyström approximation by Williams and Seeger [2001].
- The approximation is directly done on the covariance matrix without the concept of pseudo data.
- The approximation becomes exact if the whole data set is taken, *i.e.*, $\mathbf{K}\mathbf{K}^{-1}\mathbf{K}^{\top} = \mathbf{K}$.
- The subset selection is done randomly.

Gaussian process with Pseudo Data (1)

- Snelson and Ghahramani [2006] proposes the idea of having pseudo data, which is later referred to as Fully independent training conditional (FITC).
- Augment the training data $(\mathbf{X}, \mathbf{y})$ with pseudo data $\mathbf{u}$ at location $\mathbf{Z}$.

$$p\left(\begin{bmatrix}\mathbf{y}\\ \mathbf{u}\end{bmatrix} \mid \begin{bmatrix}\mathbf{X}\\ \mathbf{Z}\end{bmatrix}\right) = \mathcal{N}\left(\begin{bmatrix}\mathbf{y}\\ \mathbf{u}\end{bmatrix} | 0, \begin{bmatrix}\mathbf{K}_{ff} + \sigma^2\mathbf{I} & \mathbf{K}_{fu}\\ \mathbf{K}_{fu}^\top & \mathbf{K}_{uu}\end{bmatrix}\right)$$

where $\mathbf{K}_{ff} = \mathbf{K}(\mathbf{X}, \mathbf{X})$, $\mathbf{K}_{fu} = \mathbf{K}(\mathbf{X}, \mathbf{Z})$ and $\mathbf{K}_{uu} = \mathbf{K}(\mathbf{Z}, \mathbf{Z})$.

Gaussian process with Pseudo Data (2)

- Thanks to the marginalization property of Gaussian distribution,

$$p(\mathbf{y}|\mathbf{X}) = \int_{\mathbf{u}} p(\mathbf{y}, \mathbf{u}|\mathbf{X}, \mathbf{Z}).$$

- Further re-arrange the notation:

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

where $p(\mathbf{u}|\mathbf{Z}) = \mathcal{N}(\mathbf{u}|0, \mathbf{K}_{uu})$,
$p(\mathbf{y}|\mathbf{u}, \mathbf{X}, \mathbf{Z}) = \mathcal{N}\left(\mathbf{y}|\mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{u}, \mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^{\top} + \sigma^2\mathbf{I}\right)$.

FITC approximation (1)

- So far, $p(\mathbf{y}|\mathbf{X})$ has not been changed, but there is no speed-up, $\mathbf{K}_{ff} \in \mathbb{R}^{N \times N}$ in $\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^{\top} + \sigma^2\mathbf{I}$.
- The FITC approximation assumes

$$\tilde{p}(\mathbf{y}|\mathbf{u}, \mathbf{X}, \mathbf{Z}) = \mathcal{N}\left(\mathbf{y}|\mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{u}, \mathbf{\Lambda} + \sigma^2\mathbf{I}\right),$$

  where $\mathbf{\Lambda} = (\mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^{\top}) \circ \mathbf{I}$.

FITC approximation (2)

- Marginalize $\mathbf{u}$ from the model definition:

$$\tilde{p}(\mathbf{y}|\mathbf{X},\mathbf{Z}) = \mathcal{N}\left(\mathbf{y}|0, \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^{\top} + \mathbf{\Lambda} + \sigma^2\mathbf{I}\right)$$

- Woodbury formula can be applied in the sam way as in Nyström approximation:

$$(\mathbf{K}_z\mathbf{K}_{zz}^{-1}\mathbf{K}_z^{\top} + \mathbf{\Lambda} + \sigma^2\mathbf{I})^{-1} = \mathbf{A} - \mathbf{A}\mathbf{K}_z(\mathbf{K}_{zz} + \mathbf{K}_z^{\top}\mathbf{A}\mathbf{K}_z)^{-1}\mathbf{K}_z^{\top}\mathbf{A},$$

where $\mathbf{A} = (\mathbf{\Lambda} + \sigma^2\mathbf{I})^{-1}$.

FITC approximation (3)

- FITC allows the pseudo data not being a subset of training data.
- The inducing inputs $\mathbf{Z}$ can be optimized via gradient optimization.
- Like Nyström approximation, when taking all the training data as inducing inputs, the FITC approximation is equivalent to the original GP:

$$\tilde{p}(\mathbf{y}|\mathbf{X}, \mathbf{Z} = \mathbf{X}) = \mathcal{N}\left(\mathbf{y}|0, \mathbf{K}_{ff} + \sigma^2\mathbf{I}\right)$$

- FITC can be combined easily with expectation propagation (EP). Bui et al. [2017] provides an overview and a nice connection with variational sparse GP.

Model Approximation vs. Approximate Inference

When the exact model/inference is intractable, typically there are two types of approaches:

- Approximate the original model with a simpler one such that inference becomes tractable, like Nyström approximation, FITC.
- Keep the original model but derive an approximate inference method which is often *not* able to return the true answer, like variational inference.

Model Approximation vs. Approximate Inference

A problem with model approximation is that

- when an approximated model requires some tuning, e.g., for hyper-parameters, it is unclear how to improve it based on training data.
- In the case of FITC, we know the model is correct if $\mathbf{Z} = \mathbf{X}$, however, optimizing $\mathbf{Z}$ will not necessarily lead to a better location.
- In fact, optimizing $\mathbf{Z}$ can lead to overfitting. [Quiñonero-Candela and Rasmussen, 2005]

Variational Sparse Gaussian Process (1)

- Titsias [2009] introduces a variational approach for sparse GP.
- It follows the same concept of pseudo data:

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

where $p(\mathbf{u}|\mathbf{Z}) = \mathcal{N}(\mathbf{u}|0,\mathbf{K}_{uu})$,
$p(\mathbf{y}|\mathbf{u},\mathbf{X},\mathbf{Z}) = \mathcal{N}\left(\mathbf{y}|\mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{u}, \mathbf{K}_{ff} - \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^{\top} + \sigma^2\mathbf{I}\right)$.

Variational Sparse Gaussian Process (2)

- Instead of approximate the model, Titsias [2009] derives a variational lower bound.
- Normally, a variational lower bound of a marginal likelihood, also known as evidence lower bound (ELBO), looks like

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

Special Variational Posterior

- Titsias [2009] defines an unusual variational posterior:

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

- Plug it into the lower bound:

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

Special Variational Posterior

- 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 $q(\mathbf{u})$:

$$\mu^*, \Sigma^* = \arg\max_{\mu,\Sigma} \mathcal{L}(\mu, \Sigma).$$

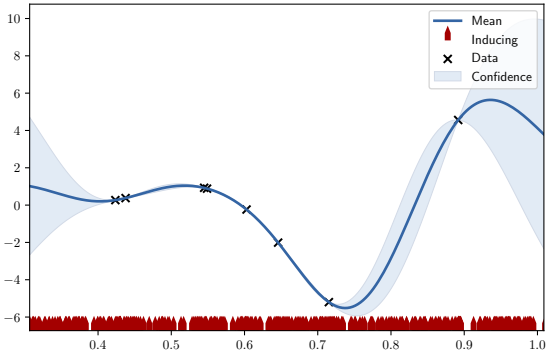
- Make the bound as tight as possible by plugging in μ^* and Σ^*:

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

- 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.



Are big covariance matrices always (almost) low-rank?

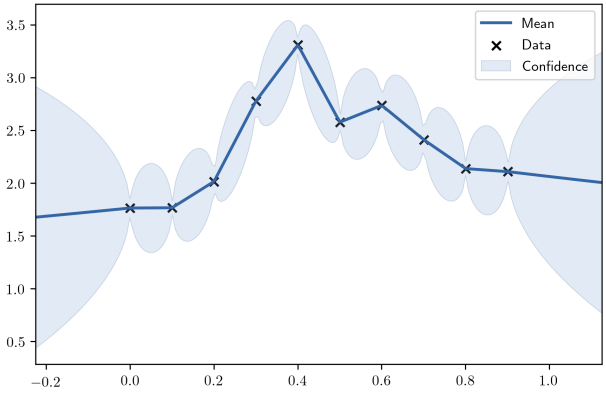
- Of course, not.
- A time series example

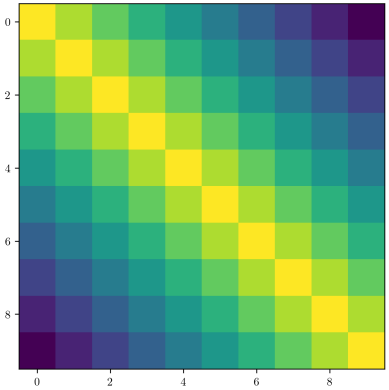
$$y = f(t) + \epsilon$$

- The data are collected with even time interval continuously.

A time series example: 10 data points

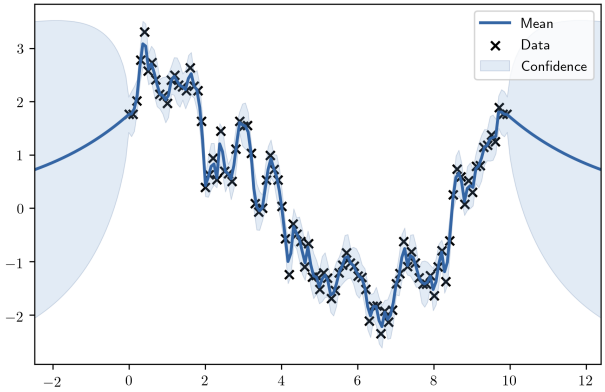
When we observe until $t = 1.0$:

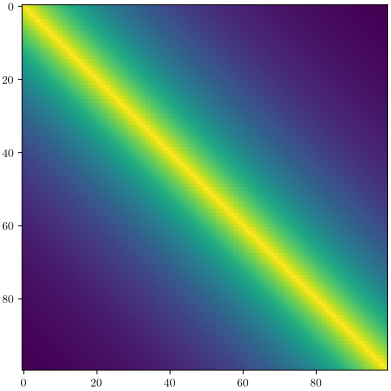




A time series example: 100 data points

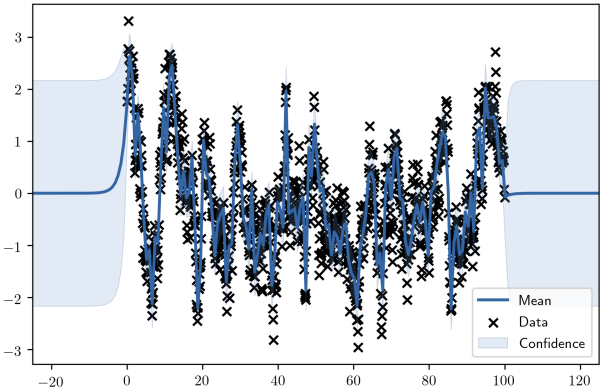
When we observe until $t = 10.0$:

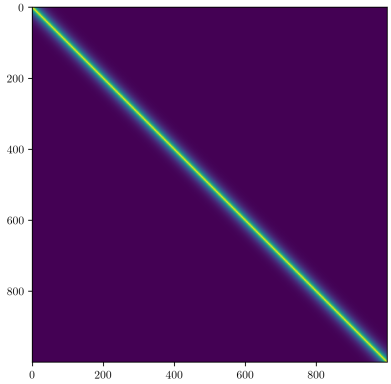




A time series example: 1000 data points

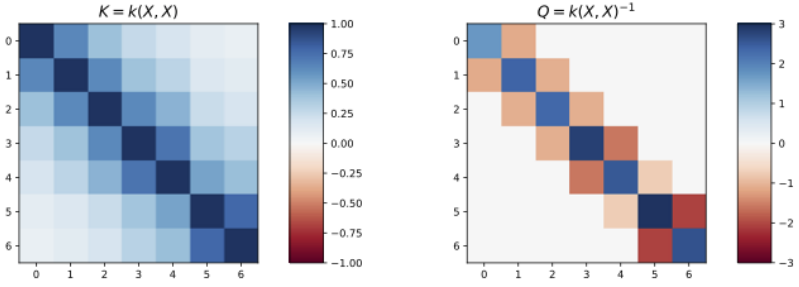
When we observe until $t = 100.0$:





Banded precision matrix

- For the kernels like the Matern family, the precision matrix is banded.
- For example, given a Matern $\frac{1}{2}$ or known as exponential kernel: $k(x, x') = \sigma^2 \exp(-\frac{|x-x'|}{l^2})$.



This slide is taken from Nicolas Durrande [**?**].

Closed form precision matrix

- The precision matrix of Matern kernels can be computed in closed form.
- The lower triangular matrix from the Cholesky decomposition of the precision matrix is banded as well.

$$\log(\mathbf{y}|\mathbf{X}) = -\frac{1}{2}\log|2\pi(LL^\top)^{-1}| - \frac{1}{2}\mathsf{tr}\left(\mathbf{y}\mathbf{y}^\top LL^\top\right)$$

  where L is the lower triangular matrix from the Cholesky decomposition of the precision matrix Q, $Q = LL^\top$.
- The computational complexity becomes $O(N)$.

Other approximations

- deterministic/stochastic frequency approximation
- distributed approximation
- conjugate gradient methods for covariance matrix inversion

Q & A!

Parallel Sparse Gaussian Process

- Beyond Approximate the inference method, maybe we could exploit parallelization.
- For Gaussian process, it turns out to be very hard, because parallel Cholesky decomposition is very difficult.
- Dai et al. [2014] and Gal et al. [2014] proposes a parallel inference method for sparse GP.

Data Parallelism

- Consider a training set: $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$.
- Assume there are C computational cores/machines.
- A data parallelism algorithm divides the data set into C partitions as evenly as possible: $\mathcal{D} = \bigcup_{c=1}^{C} \mathcal{D}_c$.
- The parallelism happens in the way that the function running on each core only requiring the data from the local partition.

A simple example: neural network regression

$$l = \sum_{n=1}^{N} ||y_n - f_\theta(\mathbf{x}_n)||^2 = \sum_{c=1}^{C} \sum_{n_c \in \mathcal{D}_c} ||y_{n_c} - f_\theta(\mathbf{x}_{n_c})||^2$$

1. Each core computes its local objective $l_c = \sum_{n_c \in \mathcal{D}_c} ||y_{n_c} - f_\theta(\mathbf{x}_{n_c})||^2$.
2. Each core computes the gradient of its local object $\partial l_c / \partial \theta$.
3. Aggregate all the local objectives and gradients $l = \sum_{c=1}^{C} l_c$ and $\partial l / \partial \theta = \sum_{c=1}^{C} \partial l_c / \partial \theta$.
4. Take a step along the gradient following a gradient descent algorithm.
5. Repeat Step 1 until converge.

Data Parallelism for Sparse GP

The variational lower bound (after applying Woodbury formula) is

$$\mathcal{L} = -\frac{N}{2}\log 2\pi\sigma^2 + \frac{1}{2}\log\frac{|\mathbf{K}_{uu}|}{|\mathbf{K}_{uu}+\sigma^{-2}\mathbf{\Phi}|} - \frac{1}{2\sigma^2}\mathbf{y}^\top\mathbf{y} + \frac{1}{2\sigma^4}\mathbf{y}^\top\mathbf{K}_{fu}(\mathbf{K}_{uu}+\mathbf{\Phi})^{-1}\mathbf{K}_{fu}^\top\mathbf{y} - \frac{1}{2\sigma^2}\phi + \frac{1}{2\sigma^2}\mathsf{tr}\left(\mathbf{K}_{uu}^{-1}\mathbf{\Phi}\right)$$

where $\mathbf{\Phi} = \mathbf{K}_{fu}^\top\mathbf{K}_{fu}$ and $\phi = \mathsf{tr}\left(\mathbf{K}_{ff}\right)$.

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- The lower bound is not fully distributable like in the simple example.
- All the terms involving data can be written as a sum across data points:

$$\mathbf{y}^\top \mathbf{y} = \sum_{n=1}^{N} y_n^2, \quad \mathbf{y}^\top \mathbf{K}_{fu} = \sum_{n=1}^{N} y_n \mathbf{K}_{f_n u}, \quad \mathbf{\Phi} = \sum_{n=1}^{N} \mathbf{K}_{f_n u}^\top \mathbf{K}_{f_n u}$$

$$\phi = \sum_{n=1}^{N} \mathbf{K}_{f_n f_n}, \text{where } \mathbf{K}_{f_n u} = \mathbf{K}(\mathbf{x}_n, \mathbf{Z}), \quad \mathbf{K}_{f_n f_n} = \mathbf{K}(\mathbf{x}_n, \mathbf{x}_n).$$

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1. **[local]** Compute all the data related terms locally: $\mathbf{y}_c^\top \mathbf{y}_c$, $\mathbf{y}_c^\top \mathbf{K}_{f_c u}$, $\mathbf{\Phi}_c$ and ϕ_c.
2. **[global]** Aggregate all the local terms and compute the lower bound $\mathcal{L}$ on one node.
3. **[global]** Compute the gradient of the bound w.r.t. the model parameters.
4. **[global]** Compute the gradient w.r.t. the local terms $\partial \mathcal{L}/\partial \mathbf{K}_{f_c u}$, $\partial \mathcal{L}/\partial \mathbf{\Phi}_c$ and $\partial \mathcal{L}/\partial \phi_c$ and broadcast to individual nodes.
5. **[local]** Compute the gradient contribution of the local terms and aggregate the local gradients into the final gradient.
6. **[global]** Take a gradient step and repeat Step 1.

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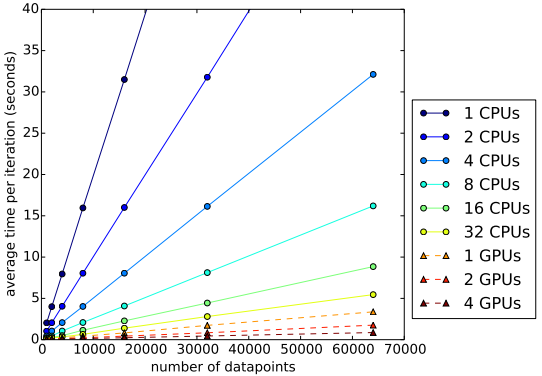

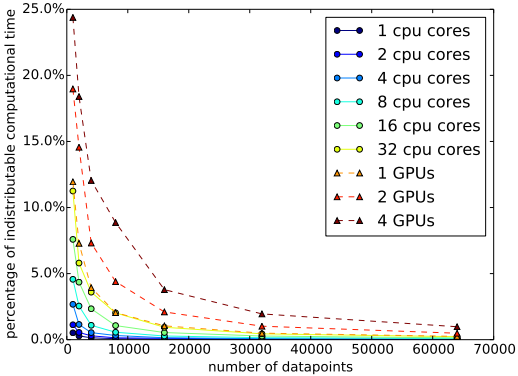

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