Scalability of Gaussian Process

Zhenwen Dai

Spotify

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Outline

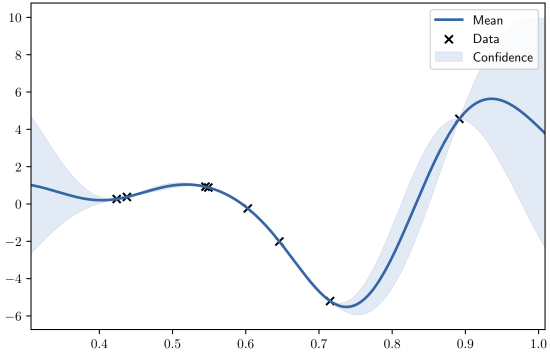
- What is the scalability issue of Gaussian Process?
- Numerical solution
- Model/Inference Approximation
- Mini-batch Training

Gaussian Process Regression

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:

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

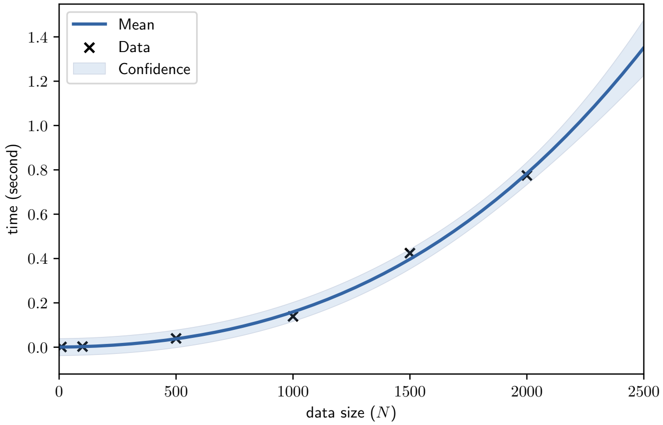
- Take a Cholesky decomposition: $\mathbf{L} = \texttt{chol}(\mathbf{K}+\sigma^2\mathbf{I})$, such that $\mathbf{K}+\sigma^2\mathbf{I} = \mathbf{L}\mathbf{L}^\top$.
- The computational complexity is $O(N^3 + N^2 + N)$. Therefore, the overall complexity including the computation of $\mathbf{K}$ is $O(N^3)$.

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

```
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
```

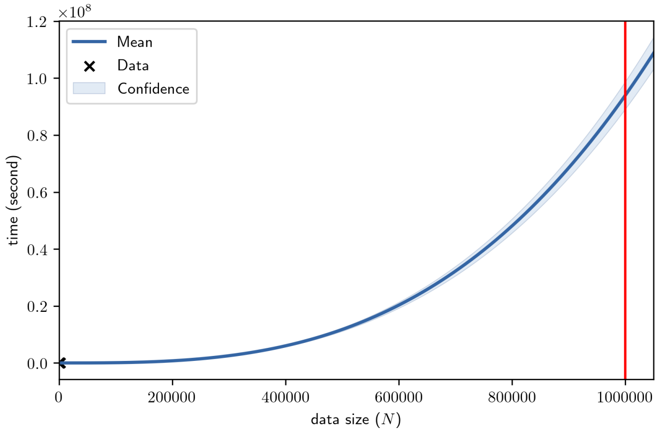
Empirical analysis of computational time

- 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.



Well, it is only a matrix inversion.

- The cubic complexity $O(N^3)$ mainly comes from $\mathbf{y}^\top(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\mathbf{y}$.
- There must be some *Numerical Linear Algebra* algorithms to speed it up!?

Quadratic Optimization Formulation

- Consider the problem:
$$\mathbf{v} = \hat{\mathbf{K}}^{-1}\mathbf{y}, \quad \hat{\mathbf{K}} = \mathbf{K} + \sigma^2\mathbf{I}$$
- Rewrite it as a linear system:
$$\hat{\mathbf{K}}\mathbf{v} - \mathbf{y} = 0$$
- This can be formulated as a quadratic optimization:
$$\mathbf{v}^* = \arg\min_{\mathbf{v}} \mathbf{v}^\top\hat{\mathbf{K}}\mathbf{v} - \mathbf{v}^\top\mathbf{y}$$

Conjugate Gradient Method (1)

- Conjugate Gradient (CG) method is an efficient solver for the quadratic problem:

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

- Solve it by finding n linearly independent vectors $\{\mathbf{d}_1, \mathbf{d}_N\}$ such that:

$$\mathbf{v}^* = \mathbf{v}_0 + \alpha_1 \mathbf{d}_1 + \ldots + \alpha_N \mathbf{d}_N$$

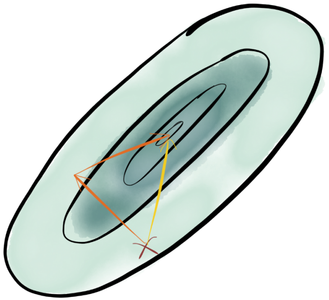

Conjugate Gradient (CG)

Figure taken from [Davies, 2015]

Conjugate Gradient Method (2)

- CG is an iterative algorithm.
- CG recovers the exact solution after N iterations.
- We get an approximate solution with $\#$iterations $<< N$.
- Each iteration is $O(N^2)$.

Conjugate Gradient:

$$\mathbf{d}_0 = \mathbf{u}_0 = \mathbf{y} - \hat{\mathbf{K}}\mathbf{v}_0$$
$$\alpha_i = \frac{\mathbf{u}_i^\top \mathbf{u}}{\mathbf{d}_i^\top \hat{\mathbf{K}} \mathbf{d}_i}$$
$$\mathbf{v}_{i+1} = \mathbf{v}_i + \alpha_i \mathbf{d}_i$$
$$\mathbf{u}_{i+1} = \mathbf{u}_i - \alpha_i \hat{\mathbf{K}} \mathbf{d}_i$$
$$\beta_{i+1} = \frac{\mathbf{u}_{i+1}^\top \mathbf{u}_{i+1}}{\mathbf{u}_i^\top \mathbf{u}_i}$$
$$\mathbf{d}_{i+1} = \mathbf{u}_{i+1} + \beta_{i+1} \mathbf{d}_i$$

Convergence and Preconditioning

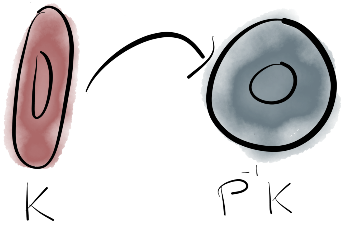
- Numerical stability and rate of convergence of CG are *sensitive* to the condition number:

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

- Improve the condition number by solving:

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

- Ideally $\mathbf{P}^{-1} = \hat{\mathbf{K}}^{-1}$ so that $\kappa(\mathbf{P}^{-1}\hat{\mathbf{K}}) = 1$.

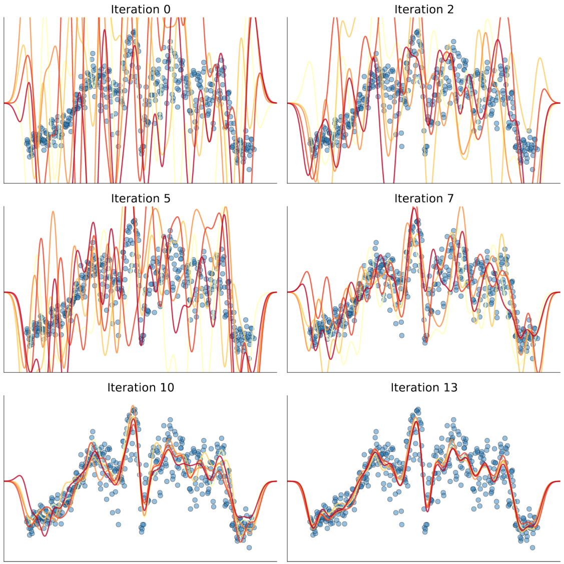


Preconditioning

Figure taken from [Davies, 2015]

Example of CG

- Example from [Davies, 2015].
- Estimate the posterior mean of GP.
- 5 separate runs $(N = 415)$
- CG is implemented in GPyTorch [Gardner et al., 2018].

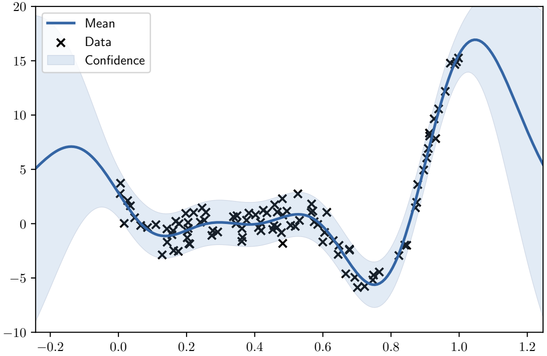


$O(N^2)$ is still slow!

Gaussian Process Model/Inference Approximation

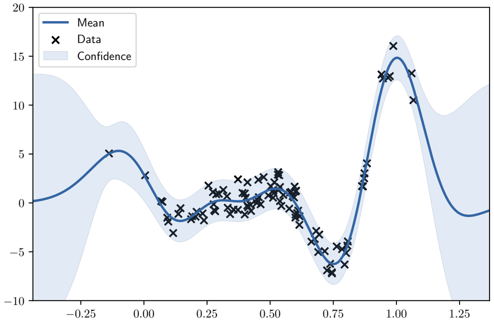
Big data (?)

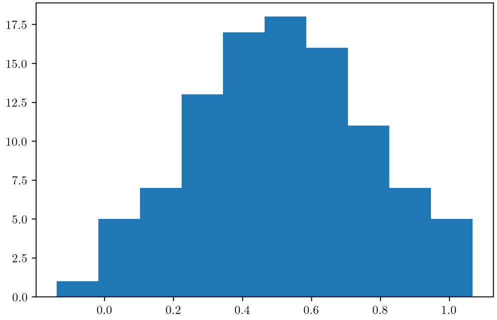
- lots of data $\neq$ complex function
- In real world problems, we often collect a lot of data for modeling relatively simple relations.



Data subsampling?

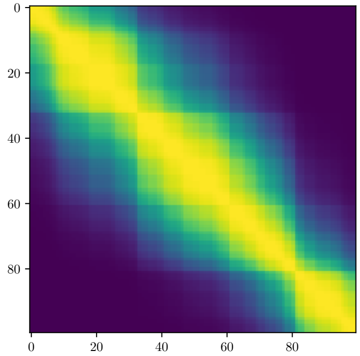
- Real data often do not evenly distributed.
- We tend to get a lot of data on common cases and very few data on rare cases.

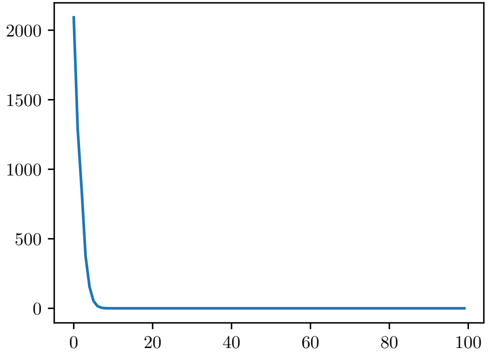




Covariance matrix of redundant data

- 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 $\tilde{\mathbf{K}}$.

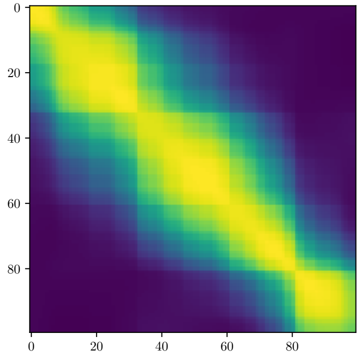
$\tilde{\mathbf{K}} = \mathbf{K}_z \mathbf{K}_{zz}^{-1} \mathbf{K}_z^\top$, where $\mathbf{K}_z = \mathbf{K}(\mathbf{X}, \mathbf{Z})$ and $\mathbf{K}_{zz} = \mathbf{K}(\mathbf{Z}, \mathbf{Z})$.

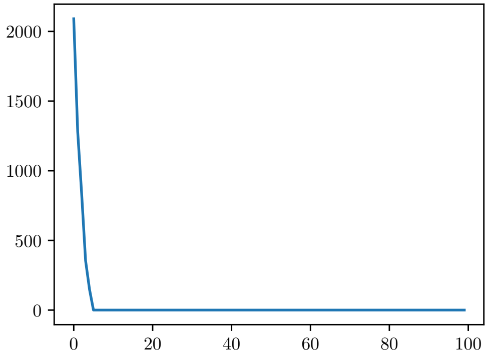
- Note that $\tilde{\mathbf{K}} \in \mathbb{R}^{N \times N}$, $\mathbf{K}_z \in \mathbb{R}^{N \times M}$ and $\mathbf{K}_{zz} \in \mathbb{R}^{M \times M}$.
- The log-likelihood is approximated by

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

Nyström approximation example

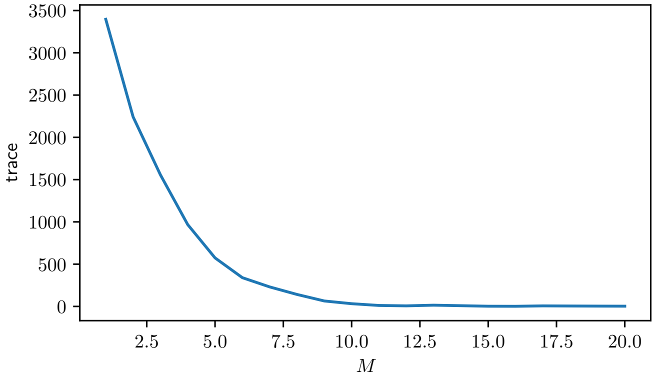
The covariance matrix with Nyström approximation using 5 random data points:





Nyström approximation example

Compute tr $\left(\mathbf{K} - \tilde{\mathbf{K}}\right)$ with different M.



Nyström approximation implementation

- The naïve formulation does **not** bring any computational benefits.

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

- $\tilde{\mathbf{K}} + \sigma^2\mathbf{I}$ is a $N \times N$ matrix!

Efficient computation using Woodbury formula

- Rewrite the log-likelihood

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

- by applying the Woodbury formula:

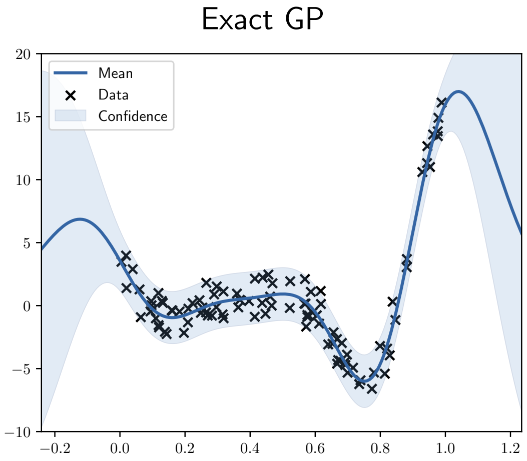
$$(\mathbf{K}_z\mathbf{K}_{zz}^{-1}\mathbf{K}_z^\top + \sigma^2\mathbf{I})^{-1} = \sigma^{-2}\mathbf{I} - \sigma^{-4}\mathbf{K}_z(\mathbf{K}_{zz} + \sigma^{-2}\mathbf{K}_z^\top\mathbf{K}_z)^{-1}\mathbf{K}_z^\top$$

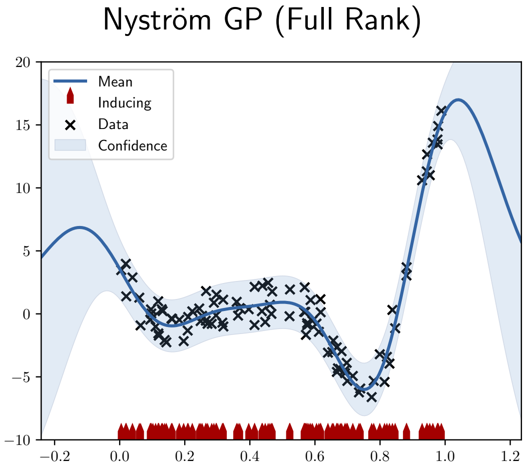
- Note that $(\mathbf{K}_{zz} + \sigma^{-2}\mathbf{K}_z^\top\mathbf{K}_z) \in \mathbb{R}^{M\times M}$.
- The computational complexity reduces to $O(NM^2)$.

Nyström approximation summary

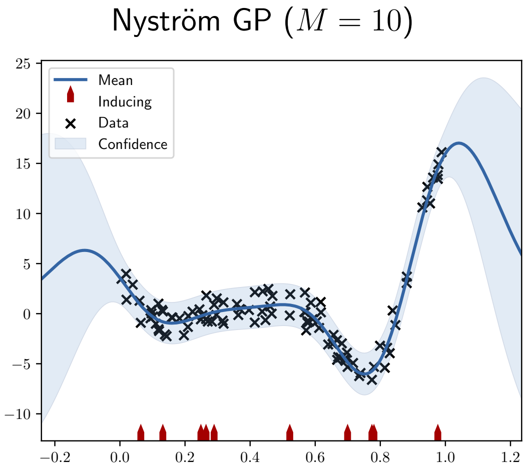
- The approximation is directly done on the covariance matrix without the concept of pseudo data.
- The approximation becomes exact if the whole data set is taken, *i.e.*, $\mathbf{K}\mathbf{K}^{-1}\mathbf{K}^\top = \mathbf{K}$.
- The subset selection is done randomly.

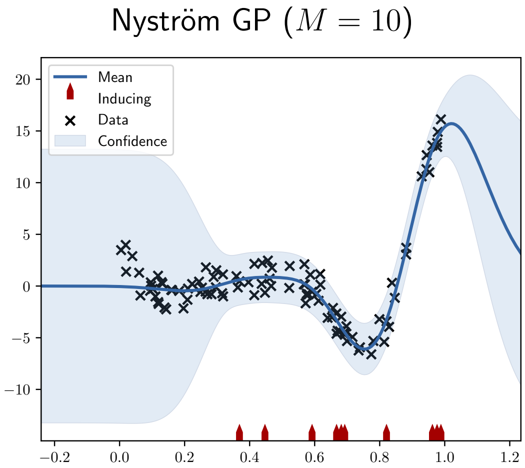
Examples of Nyström approximation (1)





Examples of Nyström approximation (2)





$N = 100$

Issues with random sampling

- Performance can be bad if unlucky.
- Areas with lots of data get more samples.
- *Can we do better?*

Take a step back

- In the log-likelihood of GP

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

- the covariance $\mathbf{K}$ is **computed** using the kernel function $k(\cdot, \cdot)$ on the inputs $\mathbf{X}$.
- Let's construct the Nyström approximation differently.

Pseudo data

- Imagine that there are a set of additional data points $\mathbf{Z} = (\mathbf{z}_1, \ldots, \mathbf{z}_M)^\top$.
- $\mathbf{z}$ lies in the **same** space as $\mathbf{x}$ does.
- The corresponding outputs $\mathbf{u} = (u_1, \ldots, u_M)$ are unknown.
- $\mathbf{Z}$ and $\mathbf{u}$ are referred to as **pseudo data**.
- $\mathbf{Z}$ are referred to as **inducing inputs**.
- $\mathbf{u}$ are referred to as **inducing variables**.

Pseudo data approximation

- With pseudo data $\mathbf{Z}$ and $\mathbf{u}$,
- the covariance of $\mathbf{u}$, $\mathbf{K}_{uu}$, can be computed $k(\cdot, \cdot)$ on the inputs $\mathbf{Z}$.
- The cross covariance between $\mathbf{f}$ and $\mathbf{u}$, $\mathbf{K}_{ff}$, can be computed as well.
- We can construct a similar approximation: $\tilde{\mathbf{K}} = \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^{\top}$.

Optimizing the pseudo data locations

- How does it differ from Nyström approximation?
- The inducing inputs are explicitly parameterized by $\mathbf{Z}$.
- Search for the optimal $\mathbf{Z}$ via optimization:

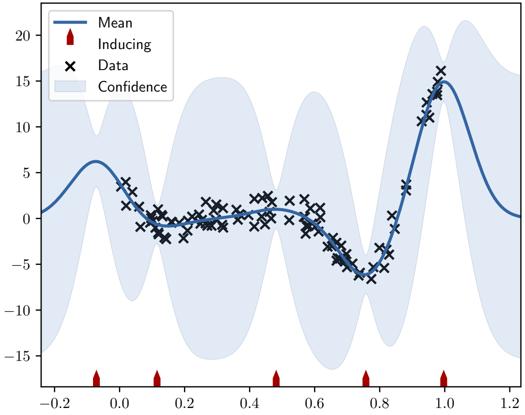
$$\mathbf{Z}^* = \arg\max_{\mathbf{Z}} \log \mathcal{N}\left(\mathbf{y}|0, \mathbf{K}_{fu}\mathbf{K}_{uu}^{-1}\mathbf{K}_{fu}^\top + \sigma^2\mathbf{I}\right).$$

- Does it work? Not really.

Deterministic Training Conditional (DTC)

- This formulation is known as Deterministic Training Conditional (DTC).
- Five inducing points moves out of scope.
- Overfits: Its logL is -156.73, while the logL of exact GP is -167.36.

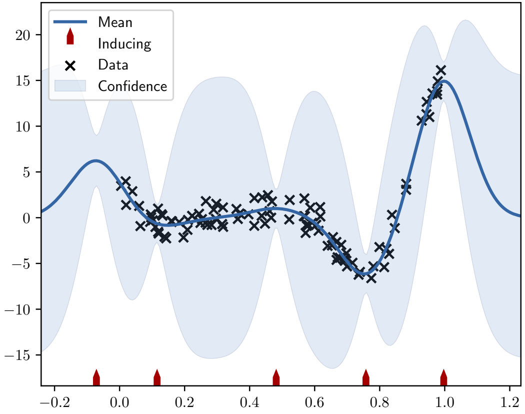
GP-DTC ($M = 10$)



Deterministic Training Conditional (DTC) (2)

- The inducing inputs adds a lot of parameters to the model.
- This model behaves much more like parametric model.
- The original DTC method [Seeger et al., 2003] greedily selects a subset of training data as the inducing points.

GP-DTC ($M = 10$)



Take a different approach

- Assume the pseudo data follow the same distribution as the observed data.
- In other words, $\mathbf{f}$ and $\mathbf{u}$ jointly follows the same GP:

$$p(\mathbf{f}, \mathbf{u}|\mathbf{X}, \mathbf{Z}).$$

- Compared to the original GP, the prior distribution is **not** changed because

$$p(\mathbf{f}|\mathbf{X}) = \int p(\mathbf{f}, \mathbf{u}|\mathbf{X}, \mathbf{Z})\mathrm{d}\mathbf{u}.$$

- Alternatively, the prior distribution can be written as

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

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

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 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:

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

- Plug it into the lower bound:

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

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 $q(\mathbf{u})$:

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

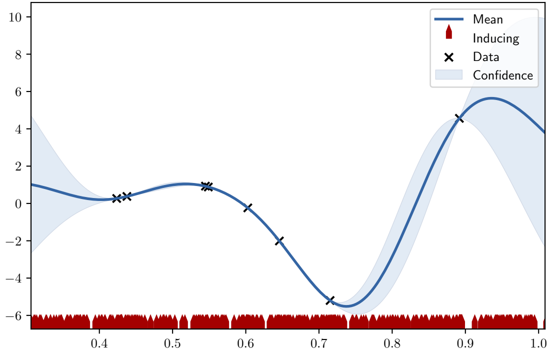
- Make the bound as tight as possible by plugging in μ^* and Σ^*:

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

- 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.



Limitations of Sparse GP

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.

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,

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

- Stochastic gradient descent (SGD) updates the parameters by

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

- 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:

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

- The variational lower bound of sparse GP:

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

“Uncollapsed” Lower Bound

- Hensman et al. [2013] discovers that the “uncollapsed” variational lower bound of sparse GP can be used for mini-batch learning.
- The “uncollapsed” variational lower bound of sparse GP:

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

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

“Uncollapsed” Lower Bound

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

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

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

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

Stochastic Variational GP (SVGP)

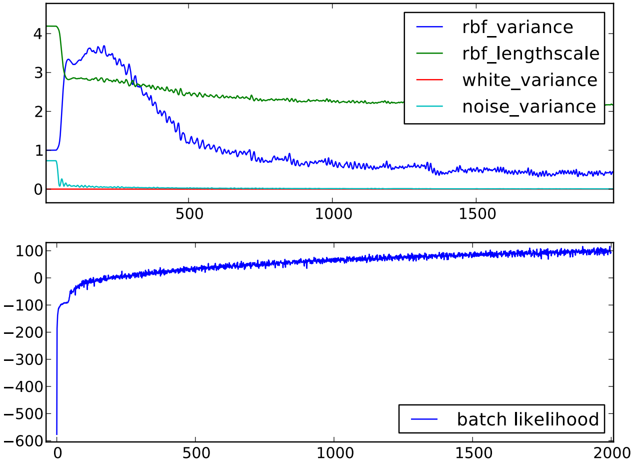
- The resulting lower bound can be written as the sum over the data,

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

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

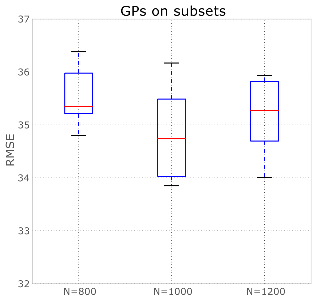
$$\theta_{t+1} = \theta_t - \eta \frac{\mathrm{d}\mathcal{L}_{\mathsf{MB}}}{\mathrm{d}\theta}.$$

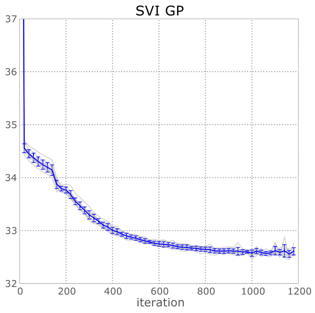
2D Synthetic Data

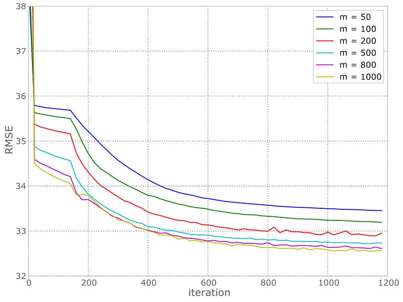


Airline Delay Data

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







The pros and cons of SVGP

Pros

- With mini-batch learning, the computational complexity reduces from $O(NM^2)$ to $O(M^3)$.

Cons

- The variational distribution $q(\mathbf{u})$ needs to be explicitly optimized.
- The number of variational parameters increase from MQ to $(2M + M^2)Q$.
- Optimization relies on SGD methods and the methods like L-BFGS are no longer applicable.
- It can be challenging to initialize $q(\mathbf{u})$.

Questions?

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