Gaussian Processes for Big Data

James Hensman

joint work with

Nicoló Fusi, Neil D. Lawrence

Overview

Motivation

Sparse Gaussian Processes

Stochastic Variational Inference

Examples

Overview

Motivation

Sparse Gaussian Processes

Stochastic Variational Inference

Examples

Motivation

Inference in a GP has the following demands:

$$\begin{aligned} \text{Complexity:} \quad & \mathcal{O}(n^3) \\ \text{Storage:} \quad & \mathcal{O}(n^2) \end{aligned}$$

Inference in a *sparse* GP has the following demands:

$$\begin{aligned} \text{Complexity:} \quad & \mathcal{O}(nm^2) \\ \text{Storage:} \quad & \mathcal{O}(nm) \end{aligned}$$

where we get to pick m!

Still not good enough!

Big Data

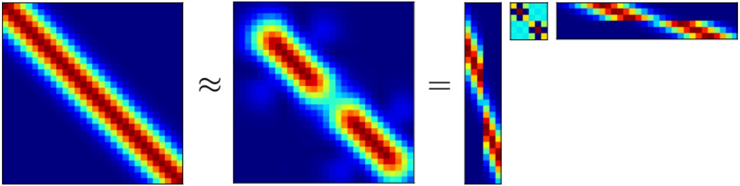
- In parametric models, stochastic optimisation is used.
- This allows for application to Big Data.

This work

- Show how to use Stochastic Variational Inference in GPs
- Stochastic optimisation scheme: each step requires $\mathcal{O}(m^3)$

Overview

Computational savings



$$\mathbf{K}_{nn} \approx \mathbf{Q}_{nn} = \mathbf{K}_{nm}\mathbf{K}_{mm}^{-1}\mathbf{K}_{mn}$$

Instead of inverting $\mathbf{K}_{nn}$, we make a low rank (or Nyström) approximation, and invert $\mathbf{K}_{mm}$ instead.

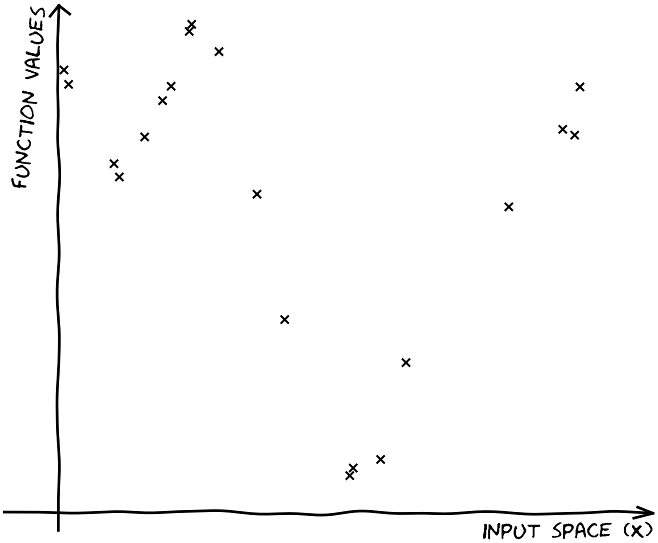
Information capture

Everything we want to do with a GP involves marginalising $\mathbf{f}$

- Predictions
- Marginal likelihood
- Estimating covariance parameters

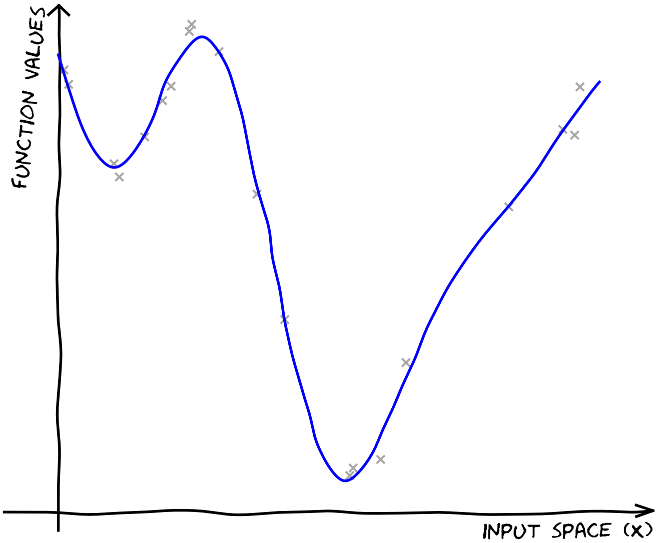
The posterior of $\mathbf{f}$ is the central object. This means inverting $\mathbf{K}_{nn}$.

$\mathbf{X}, \mathbf{y}$



$\mathbf{X}, \mathbf{y}$

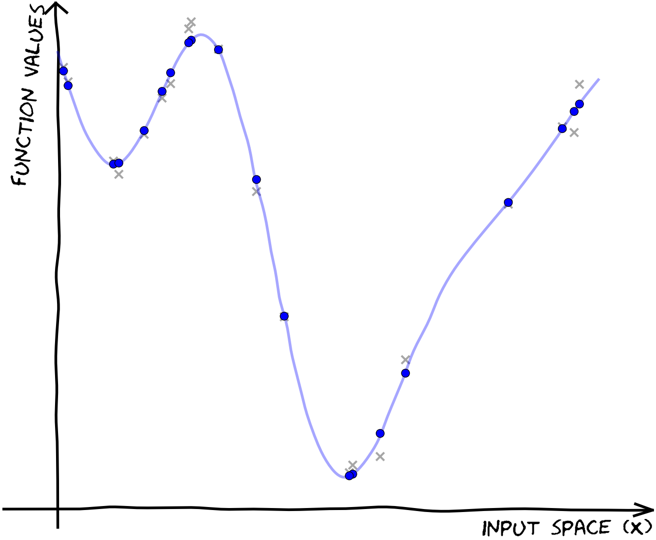
$f(\mathbf{x}) \sim \mathcal{GP}$



$\mathbf{X}, \mathbf{y}$

$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{nn})$

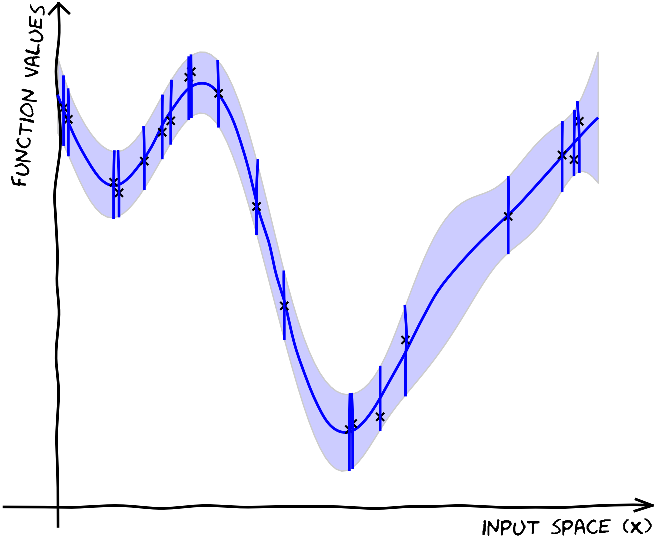


$\mathbf{X}, \mathbf{y}$

$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{nn})$

$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$

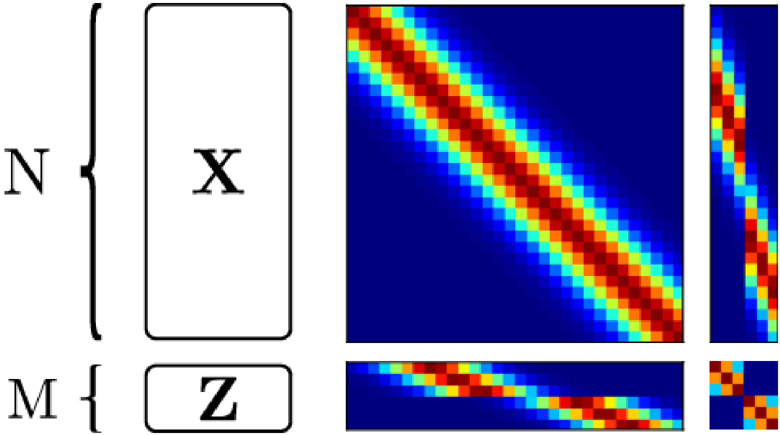


Introducing $\mathbf{u}$

Take and extra M points on the function, $\mathbf{u} = f(\mathbf{Z})$.

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

Introducing **u**



Introducing $\mathbf{u}$

Take and extra M points on the function, $\mathbf{u} = f(\mathbf{Z})$.

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

$$\begin{aligned} p(\mathbf{y} \mid \mathbf{f}) &= \mathcal{N}\left(\mathbf{y}|\mathbf{f}, \sigma^2 \mathbf{I}\right) \\ p(\mathbf{f} \mid \mathbf{u}) &= \mathcal{N}\left(\mathbf{f}|\mathbf{K}_{nm}\mathbf{K}_{mm}1\mathbf{u}, \widetilde{\mathbf{K}}\right) \\ p(\mathbf{u}) &= \mathcal{N}\left(\mathbf{u}|\mathbf{0}, \mathbf{K}_{mm}\right) \end{aligned}$$

$\mathbf{X}, \mathbf{y}$

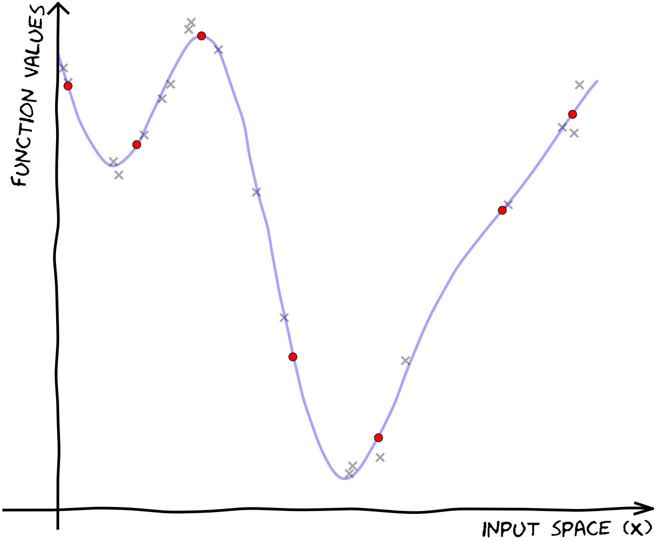
$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{nn})$

$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$

$\mathbf{Z}, \mathbf{u}$

$p(\mathbf{u}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{mm}$



$\mathbf{X}, \mathbf{y}$

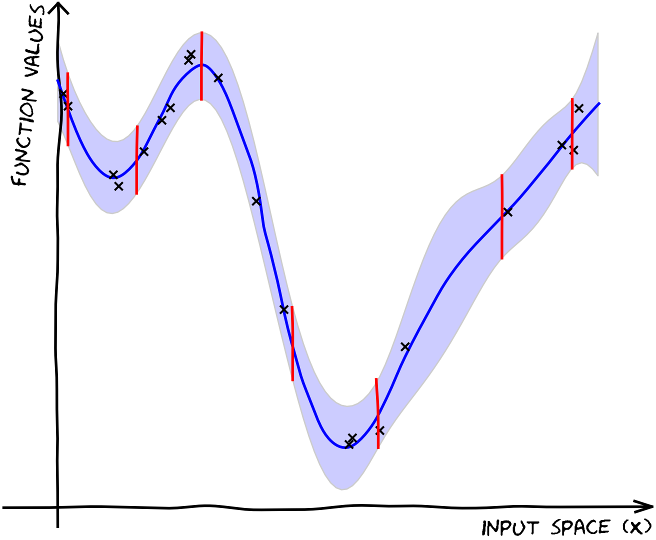
$f(\mathbf{x}) \sim \mathcal{GP}$

$p(\mathbf{f}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{nn})$

$p(\mathbf{f} \mid \mathbf{y}, \mathbf{X})$

$p(\mathbf{u}) = \mathcal{N}(\mathbf{0}, \mathbf{K}_{mm}$

$\widetilde{p}(\mathbf{u} \mid \mathbf{y}, \mathbf{X})$



The alternative posterior

Instead of doing

$$p(\mathbf{f}\,|\,\mathbf{y}, \mathbf{X}) = \frac{p(\mathbf{y}\,|\,\mathbf{f})p(\mathbf{f}\,|\,\mathbf{X})}{\int p(\mathbf{y}\,|\,\mathbf{f})p(\mathbf{f}\,|\,\mathbf{X})\mathrm{d}\mathbf{f}}$$

We'll do

$$p(\mathbf{u}\,|\,\mathbf{y}, \mathbf{Z}) = \frac{p(\mathbf{y}\,|\,\mathbf{u})p(\mathbf{u}\,|\,\mathbf{Z})}{\int p(\mathbf{y}\,|\,\mathbf{u})p(\mathbf{u}\,|\,\mathbf{Z})\mathrm{d}\mathbf{u}}$$

The alternative posterior

Instead of doing

$$p(\mathbf{f}\,|\,\mathbf{y},\mathbf{X}) = \frac{p(\mathbf{y}\,|\,\mathbf{f})p(\mathbf{f}\,|\,\mathbf{X})}{\int p(\mathbf{y}\,|\,\mathbf{f})p(\mathbf{f}\,|\,\mathbf{X})\mathrm{d}\mathbf{f}}$$

We'll do

$$p(\mathbf{u}\,|\,\mathbf{y},\mathbf{Z}) = \frac{p(\mathbf{y}\,|\,\mathbf{u})p(\mathbf{u}\,|\,\mathbf{Z})}{\int p(\mathbf{y}\,|\,\mathbf{u})p(\mathbf{u}\,|\,\mathbf{Z})\mathrm{d}\mathbf{u}}$$

but $p(\mathbf{y}\,|\,\mathbf{u})$ involves inverting $\mathbf{K}_{nn}$

Variational marginalisation of $\mathbf{f}$

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

Variational marginalisation of $\mathbf{f}$

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

$$\ln p(\mathbf{y}|\mathbf{u}) = \ln \mathbb{E}_{p(\mathbf{f}|\mathbf{u},\mathbf{X})} \left[p(\mathbf{y}|\mathbf{f}) \right]$$

Variational marginalisation of $\mathbf{f}$

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

$$\ln p(\mathbf{y}|\mathbf{u}) = \ln \mathbb{E}_{p(\mathbf{f}|\mathbf{u},\mathbf{X})} \left[p(\mathbf{y}|\mathbf{f}) \right]$$

$$\ln p(\mathbf{y}|\mathbf{u}) \geq \mathbb{E}_{p(\mathbf{f}|\mathbf{u},\mathbf{X})} \left[\ln p(\mathbf{y}|\mathbf{f}) \right] \triangleq \ln \widetilde{p}(\mathbf{y}|\mathbf{u})$$

Variational marginalisation of $\mathbf{f}$

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

$$\ln p(\mathbf{y}|\mathbf{u}) = \ln \mathbb{E}_{p(\mathbf{f}|\mathbf{u},\mathbf{X})} \left[p(\mathbf{y}|\mathbf{f}) \right]$$

$$\ln p(\mathbf{y}|\mathbf{u}) \geq \mathbb{E}_{p(\mathbf{f}|\mathbf{u},\mathbf{X})} \left[\ln p(\mathbf{y}|\mathbf{f}) \right] \triangleq \ln \widetilde{p}(\mathbf{y}|\mathbf{u})$$

No inversion of $\mathbf{K}_{nn}$ required

An approximate likelihood

$$\widetilde{p}(\mathbf{y} \mid \mathbf{u}) = \prod_{i=1}^{n} \mathcal{N}\left(\mathbf{y}_i | \mathbf{k}_{mn}^{\top} \mathbf{K}_{mm}^{-1} \mathbf{u}, \sigma^2\right) \exp\left\{-\frac{1}{2\sigma^2}\left(k_{nn} - \mathbf{k}_{mn}^{\top} \mathbf{K}_{mm}^{-1} \mathbf{k}_{mn}\right)\right\}$$

A straightforward likelihood approximation, and a penalty term

Overview

$$\log p(\mathbf{y} \,|\, \mathbf{X}) \geq \left\langle \mathcal{L}_1 + \log p(\mathbf{u}) - \log q(\mathbf{u}) \right\rangle_{q(\mathbf{u})} \triangleq \mathcal{L}_3. \tag{1}$$

$$\begin{aligned} \mathcal{L}_3 = \sum_{i=1}^{n} \Bigg\{ & \log \mathcal{N}\left(y_i | \mathbf{k}_{mn}^{\top} \mathbf{K}_{mm}^{-1} \mathbf{m}, \beta^{-1} \right) \\ & - \frac{1}{2} \beta \widetilde{k}_{i,i} - \frac{1}{2} \operatorname{tr}\left(\mathbf{S} \boldsymbol{\Lambda}_i \right) \Bigg\} \\ & - \mathrm{KL}\left(q(\mathbf{u}) \,\|\, p(\mathbf{u}) \right) \end{aligned} \tag{2}$$

Optimisation

The variational objective $\mathcal{L}_3$ is a function of

- the parameters of the covariance function
- the parameters of $q(\mathbf{u})$
- the inducing inputs, $\mathbf{Z}$

Strategy: set $\mathbf{Z}$. Take the data in small minibatches, take stochastic gradient steps in the covariance function parameters, stochastic *natural* gradient steps in the parameters of $q(\mathbf{u})$.

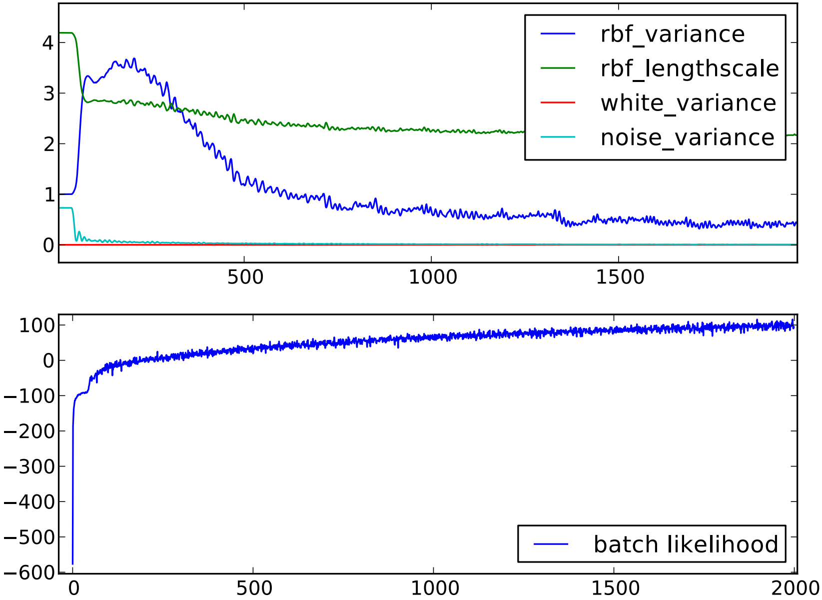
Overview

Motivation

Sparse Gaussian Processes

Stochastic Variational Inference

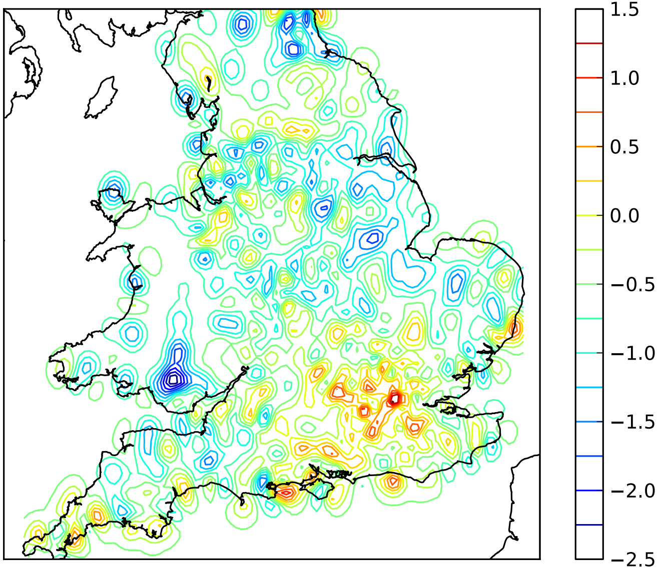
Examples

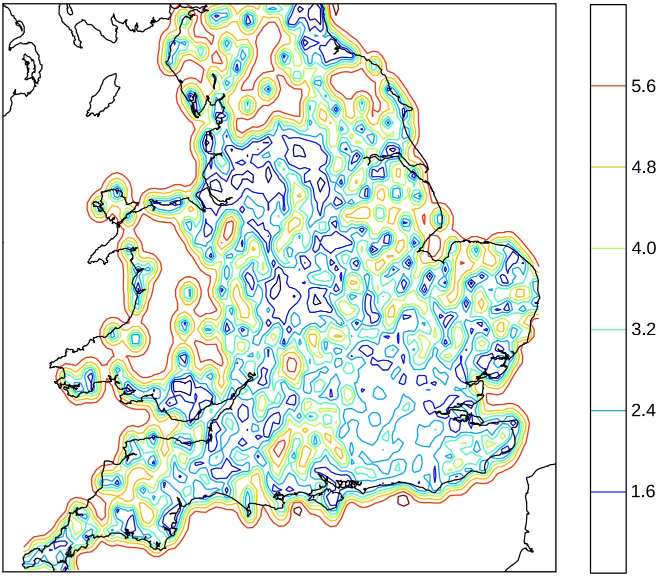


rbf_variance
rbf_lengthscale
white_variance
noise_variance
4
3
2
1
0
500
1000
1500
100
0
−100
−200
−300
−400
−500
−600
batch likelihood
0
500
1000
1500
2000

UK apartment prices

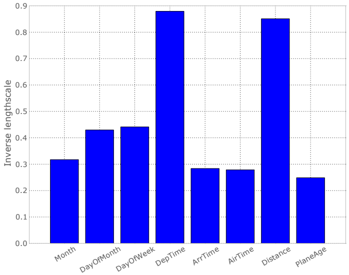
- Monthly price paid data for February to October 2012 (England and Wales)
- from `http://data.gov.uk/dataset/land-registry-monthly-price-paid-data/`
- 75,000 entries
- Cross referenced against a postcode database to get lattitude and longitude
- Regressed the normalised logarithm of the apartment prices

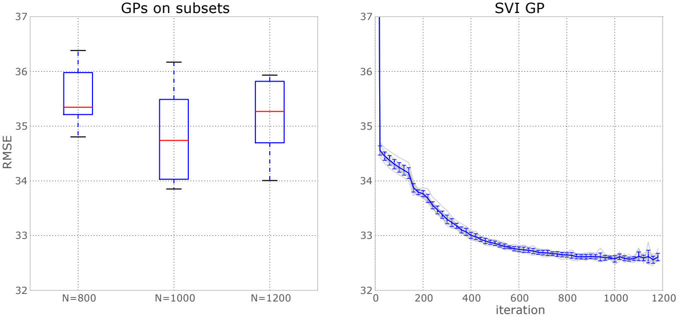

1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
−2.5


5.6
4.8
4.0
3.2
2.4
1.6

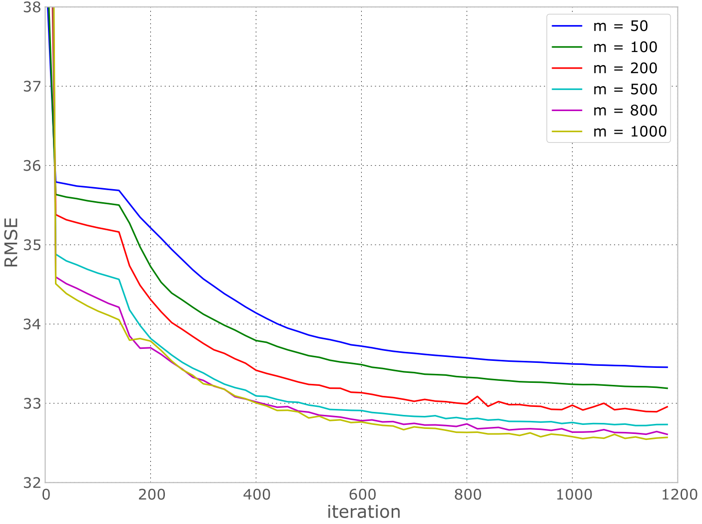
Airline data

- Flight delays for every commercial flight in the USA from January to April 2008.
- Average delay was 30 minutes.
- We randomly selected 800,000 datapoints (we have limited memory!)
- 700,000 train, 100,000 test





GPs on subsets
RMSE
37
36
35
34
33
32
N=800
N=1000
N=1200
SVI GP
0
200
400
600
800
1000
1200
iteration



RMSE
iteration
32
33
34
35
36
37
38
0
200
400
600
800
1000
1200
m = 50
m = 100
m = 200
m = 500
m = 800
m = 1000

Download the code!

`github.com/SheffieldML/GPy`

Cite our paper!

Hensman, Fusi and Lawrence,
Gaussian Processes for Big Data
Proceedings of UAI 2013