Sparse Gaussian Process Toolbox

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Toolbox Overview

Uses:

- Gaussian process ($\mathcal{GP}$) latent model
- Sequential approximation to the posterior
- Sparsification of the resulting process
- *MATLAB* programming language
- *NETLAB* toolbox

Provides:

- GUI demos for teaching $\mathcal{GP}$s
- Variety of error or likelihood functions
- Bayesian hyperparameter selection

Freely available from:

- `http://www.tuebingen.mpg.de/~csatol`
- `http://www.ncrg.aston.ac.uk/Projects/SSGP`

Gaussian Process Inference

Gaussian process ($\mathcal{GP}$) models are *probabilistic* kernel methods. $\mathcal{GP}$s specify priors over a function space. Any finite sample from the random function has joint Gaussian distribution with covariance given by a kernel function. The *prior* is thus

$$p_0(\boldsymbol{f}) = \frac{1}{(2\pi)^{N/2}|\boldsymbol{K}_N|^{1/2}} \exp\left(-\frac{1}{2}\boldsymbol{f}^T\boldsymbol{K}_N^{-1}\boldsymbol{f}\right) \qquad (1)$$

where

$$\boldsymbol{f} = [f(\boldsymbol{x}_1), \ldots, f(\boldsymbol{x}_N)]^T \quad \text{are samples from the function}$$

$$\boldsymbol{K}_N = \{K_0(\boldsymbol{x}_i, \boldsymbol{x}_j|\theta)\}_{i,j=1}^N \quad \text{is the sample covariance matrix}$$

where $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ are the inputs and θ is the set of parameters of K_0. For common $\mathcal{GP}$ models the likelihoods factorise:

$$P(\mathcal{D}) = \prod_{n=1}^N t(y_n|\boldsymbol{f}) \doteq \prod_{n=1}^N t_n(\boldsymbol{f})$$

The posterior *process* is

$$p_{\text{post}}(\boldsymbol{f}) = \frac{1}{Z} p_0(\boldsymbol{f}) P(\mathcal{D}|\boldsymbol{f})$$

For non-Gaussian likelihoods the posterior is not a $\mathcal{GP}$, thus it is analytically intractable.

There are **problems of:** *(solved by)*

- tractability for non-Gaussian likelihoods: *variational appr.*
- representation for large datasets: *sparse appr.*

Approximations to the Posterior

Representation of the posterior moments

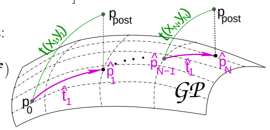
Using $\mathcal{GP}$ priors, the moments of the posterior process are:

$$\begin{aligned} \langle f_{\boldsymbol{x}} \rangle_{\text{post}} &= \langle f_{\boldsymbol{x}} \rangle_0 + \sum_{i=1}^N K_0(\boldsymbol{x}, \boldsymbol{x}_i)\alpha(i) \\ K(\boldsymbol{x}, \boldsymbol{x}')_{\text{post}} &= K_0(\boldsymbol{x}, \boldsymbol{x}') + \sum_{i,j=1}^N K_0(\boldsymbol{x}, \boldsymbol{x}_i) C(ij) K_0(\boldsymbol{x}_j, \boldsymbol{x}') \end{aligned} \qquad (2)$$

where $\alpha(i)$ and $C(ij)$ are parameters driven by the likelihood function.
The representation suggests an approximation: the posterior is approximated by the closest $\mathcal{GP}$ in a KL-sense. The process approximation is reduced to finding the parameters $\boldsymbol{\alpha} = [\alpha(1), \ldots, \alpha(N)]^T$ and $\boldsymbol{C} = \{C(i,j)\}_{i,j=1}^N$.

Approximation to the posterior process

The approximations are sequential, including a single case at each step. We use the *expectation-propagation (or TAP) algorithm* where the posterior is constructed from local Gaussian approximation $\hat{t}_i(\boldsymbol{f})$ to each factor in the likelihood [Minka 2000; Opper and Winther 2001].



We define the approximating process:

$$p_{\text{post}}(\boldsymbol{f}) \approx \hat{p}(\boldsymbol{f}) \propto p_0(\boldsymbol{f}) \prod_{n=1}^N \hat{t}_n(\boldsymbol{f})$$

and compute it using the algorithm:

- Initialise $\hat{t}_n(\boldsymbol{f}) = 1$ $i = 1, \ldots, N$.
- For each input n compute: $\quad p_0^{\setminus n}(\boldsymbol{f}) \propto \dfrac{\hat{p}(\boldsymbol{f})}{\hat{t}_n(\boldsymbol{f})}$
- Approximate the *local* posterior and substitute back $\hat{t}_n(\boldsymbol{f})$ based on:

$$\frac{1}{Z_n} p_0^{\setminus n}(\boldsymbol{f}) t_n(\boldsymbol{f}) \approx p_{\text{post}}^n(\boldsymbol{f}) = \frac{1}{\hat{Z}_n} p_0^{\setminus i}(\boldsymbol{f}) \hat{t}_n(\boldsymbol{f}) \quad \Rightarrow \quad t_n(\boldsymbol{f}) \approx \frac{Z_n}{\hat{Z}_n} \hat{t}_n(\boldsymbol{f}) \qquad (3)$$

At the equilibrium point we have an approximation to the *marginal likelihood* (or evidence) as:

$$Z = \int d\boldsymbol{f}\; p_0(\boldsymbol{f}) \prod_{n=1}^N t_n(\boldsymbol{f}) \approx \prod_{n=1}^N \frac{Z_n}{\hat{Z}_n} \int d\boldsymbol{f}\; p_0(\boldsymbol{f}) \hat{t}_n(\boldsymbol{f}) \qquad (4)$$

Sparsification

If $t_n(\boldsymbol{f})$ depends only on f_n, then $\boldsymbol{f}$ reduces to f_n. The random variable f_n can further be eliminated by

$$f_n \to \hat{f}_n = \pi_n \boldsymbol{f}_{\text{B}} \quad \text{, where B is a predefined set of inputs}$$

(B can be from the training/test data) The approximated posterior $\mathcal{GP}$ has the mean function and covariance kernel defined as:

$$\begin{aligned} \langle f_{\boldsymbol{x}} \rangle_{\text{post}} &= \langle f_{\boldsymbol{x}} \rangle_0 + \sum_{i \in \text{B}} K_0(\boldsymbol{x}, \boldsymbol{x}_i) \hat{\alpha}(i) \\ K(\boldsymbol{x}, \boldsymbol{x}')_{\text{post}} &= K_0(\boldsymbol{x}, \boldsymbol{x}') + \sum_{i,j \in \text{B}} K_0(\boldsymbol{x}, \boldsymbol{x}_i) \hat{C}(ij) K_0(\boldsymbol{x}_j, \boldsymbol{x}') \end{aligned}$$

Important: user control over the size of B. $\Rightarrow$ possible to use large datasets.

Matlab Implementation

Uses a *matlab structure* `net`. The initialisation of the structure with the default values for the fields is done using:

`net = ogp(` i_{dim}`,`o_{dim}`,covarfn,covpar);`

where i_{dim} is the dimension of inputs, o_{dim} is the dimension of outputs – one can define pairs of $\mathcal{GP}$s for more than a single latent variable in the likelihood. Associated to each input dimension there is an ARD [MacKay 1992] parameter:

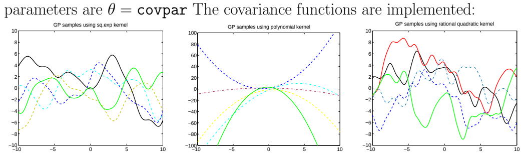
$\log(\nu)$`=net.inweights`

and the kernel functions depend on the weighted product:

$$\langle \boldsymbol{x}, \boldsymbol{x}' \rangle = \sum_i \gamma_i x_i x_i' \quad \text{which is used in the kernels below}$$

Kernel functions for the prior process

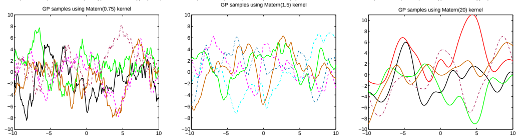
`covarfn,covpar` define the covariance function for the $\mathcal{GP}$. The kernel hyperparameters are θ = `covpar` The covariance functions are implemented:



`sqexp`: $K(\boldsymbol{x},\boldsymbol{x}') = \exp(-\|\boldsymbol{x}-\boldsymbol{x}'\|^2/2)$

`poly`: $K(\boldsymbol{x},\boldsymbol{x}') = (1+\langle \boldsymbol{x},\boldsymbol{x}' \rangle)^d$

`ratquad`: $K(\boldsymbol{x},\boldsymbol{x}') = (1+\|\boldsymbol{x}-\boldsymbol{x}'\|^2)^{-d}$



`user` - extensibility of the toolbox with user–defined covariance function **(example: Matèrn kernel)** [Stein 1999]:

$$K(\boldsymbol{x}, \boldsymbol{x}') = \frac{A}{\Gamma(\nu) 2^{(\nu-1)}} \left(\sqrt{2\nu}d\right) K_\nu \left(\sqrt{2\nu}d\right)$$

where K_ν is the modified Bessel function of the second kind. Allows transition from rough covariances to squared exponentials by $\nu \to \infty$.

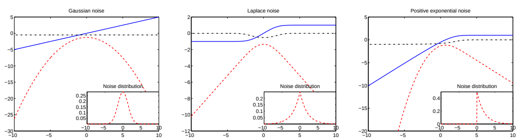
Likelihood models

The toolbox requires a function which returns the local update coefficients from eq. (3). It is specified by

`net = ogpinit(net,@likfn,likpar)`

For Gaussian noise model (`c_reg_gauss`) no approximation is needed.

Implemented likelihood models

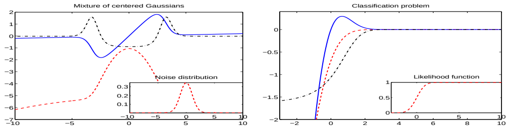


GAUSSIAN: $t_n(f_n) \propto e^{-\frac{\lambda(y_n - f_n)^2}{2}}$

LAPLACE: $t_n(f_n) \propto e^{-\lambda|y_n - f_n|}$

POS. EXP: Laplace + $y_n > f_n$

Obs: Nonstandard likelihood models are difficult to deal with using conventional kernel methods.



MIXTURES: $t_n(f_n) = \sum_i \pi_i N_i(y_n - f_n, \sigma_i^2)$

CLASSIFICATION: $t_n(f_n) \propto \int_{-\infty}^{y_n f_n} dz\; e^{-z^2/2}$

Inference and prediction

Iterating the following two-steps (EM algorithm):

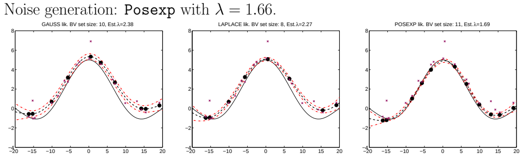
- Given the set of kernel-, and likelihood parameters, find $\mathcal{GP}_{opt}$ using the *EP* algorithm.
  `net = ogptrain(net,xTrain,yTrain,foptions);`
- Fixing the $\mathcal{GP}$, optimising the *evidence from eq.* (4) with respect to hyperparameters. For any kernel parameter θ

$$\frac{\partial \ln Z}{\partial \theta} = \text{tr}\left[\frac{\partial \ln Z}{\partial \boldsymbol{K}_B} \frac{\partial \boldsymbol{K}_B}{\partial \theta}\right]$$

`net = ogphyplearn(net,its)`

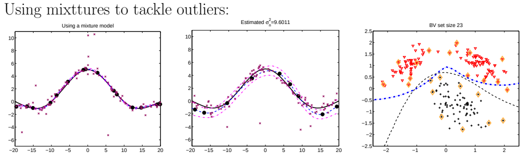
Examples

Noise generation: **Posexp** with $\lambda = 1.66$.



GAUSSIAN — LAPLACE — POS. EXP

Using mixttures to tackle outliers:



MIXTURE — GAUSSIAN LIKELIHOOD — CLASSIFICATION

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