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GPstuff: Bayesian Modeling with Gaussian Processes

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Abstract

The GPstuff toolbox is a versatile collection of Gaussian process models and computational tools required for Bayesian inference. The tools include, among others, various inference methods, sparse approximations and model assessment methods.

Keywords: Gaussian process, Bayesian hierarchical model, nonparametric Bayes

1. Introduction

Gaussian process (GP) prior provides a flexible building block for many hierarchical Bayesian models (Rasmussen and Williams, 2006). GPstuff (v4.1) is a versatile collection of computational tools for GP models and it has already been used in several published projects, for example, in epidemiology, species distribution modeling and building energy usage modeling (see Vanhatalo et al., 2013, and project web pages for references). GPstuff combines models and inference tools in a modular format. It also provides various sparse GP models and methods for model assessment. The toolbox is compatible with Unix and Windows Matlab (at least r2009b or later). Most features work also with Octave (tested with 3.6.4). The toolbox is available from `http://becs.aalto.fi/en/research/bayes/gpstuff/` and also `http://mloss.org/software/view/451/`.

2. Implementation

In many practical GP models, the observations $\mathbf{y} = [y_1, ..., y_n]^{\mathrm{T}}$ related to inputs (covariates) $\mathbf{X} = \{\mathbf{x}_i = [x_{i,1}, ...x_{i,d}]^{\mathrm{T}}\}_{i=1}^n$ are assumed to be conditionally independent given a latent function (or predictor) $f(\mathbf{x})$ so that the likelihood $p(\mathbf{y}|\mathbf{f}, \gamma) = \prod_{i=1}^n p(y_i|f_i, \gamma)$, where $\mathbf{f} = [f(\mathbf{x}_1), ..., f(\mathbf{x}_n)]^{\mathrm{T}}$, fac-

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torizes over cases. The latent function is given a GP prior, $f \sim GP(m(\mathbf{x}|\phi), k(\mathbf{x},\mathbf{x}'|\theta))$ which is defined by the mean and covariance function, $m(\mathbf{x}|\phi)$ and $k(\mathbf{x},\mathbf{x}'|\theta)$ respectively. The parameters, $\vartheta = \{\gamma, \phi, \theta\}$, are given a hyperprior after which the posterior $p(\mathbf{f}|\mathbf{y},\mathbf{X})$ is approximated and used for prediction. Most of the models in GPstuff follow the above single latent dependency, but there are also models where each factor depends on multiple latent values.

We illustrate the construction and inference of a GP model with a regression example. First, we assume $y_i = f(\mathbf{x}_i) + \varepsilon_i$, $\varepsilon_i \sim N(0, \sigma^2)$, and give $f(\mathbf{x})$ a GP prior with a squared exponential covariance function, $k(\mathbf{x},\mathbf{x}') = \sigma^2_{\text{se}} \exp(||\mathbf{x}-\mathbf{x}'||^2/2l^2)$.

```
lik = lik_gaussian('sigma2', 0.2^2);                     % init. the likelihood
gpcf = gpcf_sexp('lengthScale', 1, 'magnSigma2', 0.2^2) % init. the cov. function
gp = gp_set('lik', lik, 'cf', gpcf);                     % init. the model struct
% Find MAP estimate of the parameters and predict to new inputs
opt=optimset('TolFun',1e-3,'TolX',1e-3,'Display','iter');  % optimization settings
gp=gp_optim(gp,x,y,'optimf',@fminscg,'opt',opt);         % x,y = training data
[Ef, Varf] = gp_pred(gp, x, y, xt);                      % xt = test inputs
```

The model is constructed modularly so that each mathematical function or distribution is represented by an "object" style structure. The structures `lik` and `gpcf` contain all the essential information about the likelihood and covariance function such as parameter values and function handles to construct a covariance matrix and its gradient with respect to the parameters. All the model blocks are collected into a GP structure constructed by `gp_set`.

There are two lines of approach for the inference. The first assumes a Gaussian observation model which enables an analytic solution for the marginal likelihood $p(\mathbf{y}|\mathbf{X},\vartheta)$ and the conditional posterior $p(\mathbf{f}|\mathbf{X},\mathbf{y},\vartheta)$. Using the relation $p(\vartheta|\mathbf{y},\mathbf{X}) \propto p(\mathbf{y}|\mathbf{X},\vartheta)p(\vartheta)$ the parameters, ϑ, can be optimized to the maximum a posterior (MAP) estimate or marginalized over with grid, central composite design (CCD), importance sampling (IS) or Markov chain Monte Carlo (MCMC) integration (Vanhatalo et al., 2010). With other observation models the marginal likelihood and the conditional posterior have to be approximated either with Laplace's method (LA) or expectation propagation (EP) (Rasmussen and Williams, 2006). An alternative approach is to sample from the joint posterior $p(\mathbf{f},\vartheta|\mathbf{X},\mathbf{y})$ with MCMC by alternating sampling from $p(\mathbf{f}|\mathbf{X},\mathbf{y},\vartheta)$ and $p(\vartheta|\mathbf{X},\mathbf{y},\mathbf{f})$.

Above, `gp_optim` returns a redefined model structure with parameter values optimized to their MAP estimate. Any optimizer with similar arguments to Matlab's optimizers can be used. `gp_pred` returns the conditional posterior predictive mean, $\mathrm{E}[f|\mathbf{y},\mathbf{X},\vartheta]$ and variance $\mathrm{Var}[f|\mathbf{y},\mathbf{X},\vartheta]$ at the test inputs.

Many sparse GPs have been proposed to speed up the computations with large data sets. GPstuff includes FI(T)C, PIC, SOR, DTC (Quiñonero-Candela and Rasmussen, 2005), VAR (Titsias, 2009), CS+FIC (Vanhatalo and Vehtari, 2008) sparse approximations, and several compactly supported (CS) covariance functions. For example, CS+FIC can be used with the following modification to the model initialization.

```
gpcf2 = gpcf_ppcs2('nin', nin, 'lengthScale', 5, 'magnSigma2', 1);
gp = gp_set('type','CS+FIC','lik',lik,'cf',{gpcf,gpcf2},'X_u',Xu)
```

In the first line, a CS covariance function, piecewise polynomial of second order, is created. It is then given to the GP structure together with inducing inputs (`Xu`) and sparse GP type definition.

We can tailor the above model, for example, by replacing the Gaussian observation model with a more robust Student-t observation model (Jylänki et al., 2011).

```
lik = lik_t('nu', 4, 'sigma2', 10, 'nu_prior', prior_logunif);
gp = gp_set('lik', lik, 'cf', gpcf, 'jitterSigma2', 1e-6, 'latent_method', 'EP');
```

Here we set explicitly the prior for the degrees of freedom parameter, ν in the Student-t distribution, add jitter on the diagonal of the covariance matrix and define EP as the means to approximate the marginal likelihood.

GPstuff has wide variety of observation models (see Table 1) of which we want to highlight implementations of recently proposed multinomial probit with EP (Riihimäki et al., 2013) and logistic GP density estimation and regression with Laplace approximation (Riihimäki and Vehtari, 2012).

The constructed models could be compared, for example, with deviance information criterion (DIC), widely applicable information criterion (WAIC), leave-one-out or k-fold cross-validation (LOO/kf-CV) (Vehtari and Ojanen, 2012) with functions `gp_dic`, `gp_waic`, `gp_loopred` and `gp_kfcv`.

New models can be implemented by modifying the existing model blocks, such as covariance functions. Adding new inference methods is more laborious since they require summaries from model blocks which may not be provided by the current version of GPstuff. A thorough introduction to GPstuff is provided by demo programs and Vanhatalo et al. (2013).

3. Related Software

Perhaps the best known GP software packages are the Gaussian processes for Machine Learning (GPML) (Rasmussen and Nickisch, 2010) and the flexible Bayesian modelling (FBM) (Neal, 1998). Overviews of alternatives are provided by the Gaussian processes website (`http://www.gaussianprocess.org/`) and the R Archive Network (`http://cran.r-project.org/`). The main advantage of GPstuff over the other GP software is its versatile collection of models and computational tools. Its most important features and comparison to GPML and FBM are presented in Table 1. GPstuff project was started in 2006 based on the MCMCstuff-toolbox (`http://becs.aalto.fi/en/research/bayes/mcmcstuff/`), which was based on Netlab (Nabney, 2001) and influenced by FBM. The INLA software (Rue et al., 2009) and the book by Rasmussen and Williams (2006) have motivated some of the technical details in GPstuff. In addition, the implementation of sparse matrix routines, used with the CS covariance functions, rely on the SuiteSparse toolbox (Davis, 2005).

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	GPstuff	GPML	FBM
Covariance functions			
number of elementary functions	13	10	4
sums of elements, masking of inputs	x	x	x
delta distance	x		x
products, positive scaling of elements	x	x	
Mean functions			
number of elementary functions	4	4	0
sums of elements, masking of inputs	x	x	
products, power, scaling of elements		x	
marginalized parameters	x		
Single latent likelihood/observation models			
Gaussian	x	x	x
logistic/logit, erf/probit	x	x	MCMC
Poisson	x	LA/EP/MCMC	MCMC
Gaussian scale mixture	MCMC		MCMC
Student-*t*	x	LA/VB/MCMC	
Laplacian		EP/VB/MCMC	
mixture of likelihoods		LA/EP/MCMC	
sech-squared, uniform for classification		x	
derivative observations	for sexp covf only		
binomial, negative binomial, zero-trunc. negative binomial, log-Gaussian Cox process; Weibull, log-Gaussian and log-logistic with censoring	x		
quantile regression	MCMC/EP		
Multilatent likelihood/observation models			
multinomial, Cox proportional hazard model, density estimation, density regression, input dependent noise, input dependent overdispersion in Weibull, zero-inflated negative binomial	MCMC/LA		
multinomial logit (softmax)	MCMC/LA		MCMC
multinomial probit	EP		MCMC
Priors for parameters (ϑ)			
several priors, hierarchical priors	x		x
Sparse models			
FITC	x	exact/EP/LA	
CS, FIC, CS+FIC, PIC, VAR, DTC, SOR	x		
PASS-GP	LA/EP		
Latent inference			
exact (Gaussian only)	x	x	x
scaled Metropolis, HMC	x		x
LA, EP, elliptical slice sampling	x	x	
variational Bayes (VB)		x	
scaled HMC (with inverse of prior cov.)		x	
scaled HMC (whitening with approximate posterior covariance)	x		
parallel EP, robust EP	x		
marginal corrections (cm2 and fact)	x		
Hyperparameter inference			
type II ML	x	x	x
type II MAP, Metropolis, HMC	x		x
LOO-CV for Gaussian	x	x	
least squares LOO-CV for non-Gaussian		some likelihoods	
LA/EP LOO-CV for non-Gaussian, k-fold CV	x		
NUTS, slice sampling (SLS), surrogate SLS, shrinking-rank SLS, covariance-matching SLS, grid, CCD, importance sampling	x		
Model assessment			
marginal likelihood	MAP,ML	ML	
LOO-CV for fixed hyperparameters	x	x	
LOO-CV for integrated hyperparameters, k-fold CV, WAIC, DIC	x		
average predictive comparison	x		

Table 1: The comparison of features in GPstuff (v4.1), GPML (v3.2) and FBM (2004-11-10) toolboxes. In case of model blocks the notation x means that it can be inferred with any inference method (EP, LA (Laplace), MCMC and in case of GPML also with VB). In case of sparse approximations, inference methods and model assessment methods x means that the method is available for all model blocks.

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