The GPML Toolbox version 4.0

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Abstract

The GPML toolbox is an Octave 3.2.x and Matlab 7.x implementation of inference and prediction in Gaussian process (GP) models. It implements algorithms discussed in Rasmussen & Williams: Gaussian Processes for Machine Learning, the MIT press, 2006 and Nickisch & Rasmussen: Approximations for Binary Gaussian Process Classification, JMLR, 2008.

The strength of the function lies in its flexibility, simplicity and extensibility. The function is flexible as firstly it allows specification of the properties of the GP through definition of mean function and covariance functions. Secondly, it allows specification of different inference procedures, such as e.g. exact inference and Expectation Propagation (EP). Thirdly it allows specification of likelihood functions e.g. Gaussian or Laplace (for regression) and e.g. cumulative Logistic (for classification). Simplicity is achieved through a single function and compact code. Extensibility is ensured by modular design allowing for easy addition of extension for the already fairly extensive libraries for inference methods, mean functions, covariance functions and likelihood functions.

This document is a technical manual for a developer containing many details. If you are not yet familiar with the GPML toolbox, the user documentation and examples therein are a better way to get started.
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1 Gaussian Process Training and Prediction

The \texttt{gpml} toolbox contains a single user function \texttt{gp} described in section 2. In addition there are a number of supporting structures and functions which the user needs to know about, as well as an internal convention for representing the posterior distribution, which may not be of direct interest to the casual user.

Inference Methods: An inference method is a function which computes the (approximate) posterior, the (approximate) negative log marginal likelihood and its partial derivatives w.r.t.. the hyperparameters, given a model specification (i.e., GP mean and covariance functions and a likelihood function) and a data set. Inference methods are discussed in section 3. New inference methods require a function providing the desired inference functionality and possibly extra functionality in the likelihood functions applicable.

Hyperparameters: The hyperparameters is a struct controlling the properties of the model, i.e., the GP mean and covariance function and the likelihood function. The hyperparameters is a struct with the three fields \texttt{mean}, \texttt{cov} and \texttt{lik}, each of which is a vector. The number of elements in each field must agree with number of hyperparameters in the specification of the three functions they control (below). If a field is either empty or non-existent it represents zero hyperparameters. When working with FITC approximate inference, the inducing inputs \( x_u \) can also be treated as hyperparameters for some common stationary covariances.

Hyperparameter Prior Distributions: When optimising the marginal likelihood w.r.t. hyperparameters, it is sometimes useful to softly constrain the hyperparameters by means of prior knowledge. A \texttt{prior} is a probability distribution over individual or a group of hyperparameters, section 7.

Likelihood Functions: The likelihood function specifies the form of the likelihood of the GP model and computes terms needed for prediction and inference. For inference, the required properties of the likelihood depend on the inference method, including properties necessary for hyperparameter learning, section 4.

Mean Functions: The mean function is a cell array specifying the GP mean. It computes the mean and its derivatives w.r.t. the part of the hyperparameters pertaining to the mean. The cell array allows flexible specification and composition of mean functions, discussed in section 5. The default is the zero function.

Covariance Functions: The covariance function is a cell array specifying the GP covariance function. It computes the covariance and its derivatives w.r.t. the part of the hyperparameters pertaining to the covariance function. The cell array allows flexible specification and composition of covariance functions, discussed in section 6.

Inference methods, see section 3, compute (among other things) an approximation to the posterior distribution of the latent variables \( f_i \) associated with the training cases, \( i = 1, \ldots, n \). This approximate posterior is assumed to be Gaussian, and is communicated via a struct \texttt{post} with the fields \texttt{post.alpha}, \texttt{post.sW} and \texttt{post.L}. Often, starting from the Gaussian prior \( p(f) = \mathcal{N}(f|m, K) \) the approximate posterior admits the form

\[
q(f|D) = \mathcal{N}(f|\mu = m + K\alpha, V = (K^{-1} + W)^{-1}), \text{ where } W \text{ diagonal with } W_{ii} = s_i^2. \tag{1}
\]

In such cases, the entire posterior can be computed from the two vectors \texttt{post.alpha} and \texttt{post.sW}; the inference method may optionally also return \( L = \text{chol(diag(s)K diag(s) + I}) \). If on the other hand the posterior doesn’t admit the above form, then \texttt{post.L} returns the matrix
\[ L = -(K + W^{-1})^{-1} \] (and post.sW is unused). In addition, a sparse representation of the posterior may be used, in which case the non-zero elements of the post.alpha vector indicate the active entries.
2 The \texttt{gp} Function

The \texttt{gp} function is typically the only function the user would directly call.

\begin{verbatim}
 function [varargout] = gp(hyp, inf, mean, cov, lik, x, y, xs, ys)
 % Gaussian Process inference and prediction. The gp function provides a
 % flexible framework for Bayesian inference and prediction with Gaussian
 % processes for scalar targets, i.e. both regression and binary
 % classification. The prior is Gaussian process, defined through specification
 % of its mean and covariance function. The likelihood function is also
 % specified. Both the prior and the likelihood may have hyperparameters
 % associated with them.
 % Two modes are possible: training or prediction: if no test cases are
 % supplied, then the negative log marginal likelihood and its partial
 % derivatives w.r.t. the hyperparameters is computed; this mode is used to fit
 % the hyperparameters. If test cases are given, then the test set predictive
 % probabilities are returned. Usage:
 % training: [nlZ dnlZ ] = gp(hyp, inf, mean, cov, lik, x, y);
 % prediction: [ymu ys2 fmu fs2 ] = gp(hyp, inf, mean, cov, lik, x, y, xs);
 % or: [ymu ys2 fmu fs2 lp] = gp(hyp, inf, mean, cov, lik, x, y, xs, ys);
 % where:
 % hyp struct of column vectors of mean/cov/lik hyperparameters
 % inf function specifying the inference method
 % mean prior mean function
 % cov prior covariance function
 % lik likelihood function
 % x n by D matrix of training inputs
 % y column vector of length n of training targets
 % xs ns by D matrix of test inputs
 % ys column vector of length nn of test targets
 % nlZ returned value of the negative log marginal likelihood
 % dnlZ struct of column vectors of partial derivatives of the negative
 % log marginal likelihood w.r.t. mean/cov/lik hyperparameters
 % ymu column vector (of length ns) of predictive output means
 % ys2 column vector (of length ns) of predictive output variances
 % fmu column vector (of length ns) of predictive latent means
 % fs2 column vector (of length ns) of predictive latent variances
 % lp column vector (of length ns) of log predictive probabilities

 % if nargin==7 % if no test cases are provided
 varargout = {nlZ, dnlZ, post}; % report -log marg lik, derivatives and post
 else
 % compute test predictions
 end
\end{verbatim}

It offers facilities for training the hyperparameters of a GP model as well as predictions at unseen inputs as detailed in the following help.

\begin{verbatim}
\end{verbatim}

\begin{verbatim}
\end{verbatim}

\begin{verbatim}
\end{verbatim}
Depending on the number of input parameters, \texttt{gp} knows whether it is operated in training or in prediction mode. The high-level structure of the code is as follows. After some initialisations, we perform inference and decide whether test set predictions are needed or only the result of the inference is demanded.

If the number of input arguments is incorrect, we echo a minimalist usage and return.

Set some useful default values for empty arguments, and convert \texttt{inf} and \texttt{lik} to function handles and mean and \texttt{cov} to cell arrays if necessary. Initialize variables.
Check that the sizes of the hyperparameters supplied in hyp match the sizes expected. The three parts hyp.mean, hyp.cov and hyp.lik are checked separately, and define empty entries if they don’t exist.

\[
\begin{align*}
\text{check hyperparameters} & \equiv \text{\eqref{check-hyperparameters}} \equiv \text{\eqref{inference}} \\
& \begin{align*}
1 & \text{if } \neg \text{isfield(hyp, 'mean'), hyp.mean = []; end} \quad \% \text{ check the hyp specification} \\
2 & \text{if } \text{eval(feval(mean{:}))} \neq \text{numel(hyp.mean)} \\
3 & \text{error('Number of mean function hyperparameters disagree with mean function')} \\
4 & \text{end} \\
5 & \text{if } \neg \text{isfield(hyp, 'cov'), hyp.cov = []; end} \\
6 & \text{if } \text{eval(feval(cov{:}))} \neq \text{numel(hyp.cov)} \\
7 & \text{error('Number of cov function hyperparameters disagree with cov function')} \\
8 & \text{end} \\
9 & \text{if } \neg \text{isfield(hyp, 'lik'), hyp.lik = []; end} \\
10 & \text{if } \text{eval(feval(lik{:}))} \neq \text{numel(hyp.lik)} \\
11 & \text{error('Number of lik function hyperparameters disagree with lik function')} \\
12 & \text{end}
\end{align*}
\end{align*}
\]

Inference is performed by calling the desired inference method \text{inf}. In training mode, we accept a failure of the inference method (and issue a warning), since during hyperparameter learning, hyperparameters causing a numerical failure may be attempted, but the \text{minimize} function may gracefully recover from this. During prediction, failure of the inference method is an error.

\[
\begin{align*}
\text{inference} & \equiv \text{\eqref{inference}} \equiv \text{\eqref{check-hyperparameters}} \\
& \begin{align*}
1 & \text{try} \quad \% \text{ call the inference method} \\
2 & \text{if } \text{strcmp(lstr,'likErf')} || \text{strcmp(lstr,'likLogistic')} \\
3 & \quad \text{if } \neg \text{isstruct(y)} \\
4 & \quad \quad \text{uy = unique(y);} \\
5 & \quad \quad \text{if } \text{any( uy"=+1 & uy"=-1 )} \\
6 & \quad \quad \text{warning('You try classification with labels different from \{+1,-1\}')} \\
7 & \quad \text{end} \\
8 & \text{end} \\
9 & \text{if } \text{nargin>7} \quad \% \text{ compute marginal likelihood and its derivatives only if needed} \\
10 & \quad \text{if } \text{isstruct(y)} \\
11 & \quad \quad \text{post = y;} \quad \% \text{ reuse a previously computed posterior approximation} \\
12 & \quad \text{else} \\
13 & \quad \quad \text{post = feval(inf{:}, hyp, mean, cov, lik, x, y);} \\
14 & \quad \text{end} \\
15 & \quad \text{else} \\
16 & \quad \quad \text{if } \text{nargout<=1} \\
17 & \quad \quad \quad \text{[post nlZ] = feval(inf{:}, hyp, mean, cov, lik, x, y); dnlZ = {};} \\
18 & \quad \quad \quad \text{else} \\
19 & \quad \quad \quad \quad \text{[post nlZ dnlZ] = feval(inf{:}, hyp, mean, cov, lik, x, y);} \\
20 & \quad \quad \text{end} \\
21 & \quad \text{end} \\
22 & \text{catch} \\
23 & \quad \text{msgstr = lasterr;} \\
24 & \text{if } \text{nargin>7, error('Inference method failed \[%s\]', msgstr); else} \\
25 & \quad \text{warning('Inference method failed \[%s\] .. attempting to continue',msgstr)} \\
26 & \quad \quad \text{varargout = \{NaN, vec2any(hyp,zeros(numel(any2vec(hyp)),1))\}; return} \\
27 & \text{end} \\
28 & \text{end}
\end{align*}
\end{align*}
\]

We copy the already computed negative log marginal likelihood to the first output argument, and if desired report its partial derivatives w.r.t. the hyperparameters if running in inference mode.

Predictions are computed in a loop over small batches to avoid memory problems for very large test...
sets.

\[(\text{compute test predictions}) \equiv\]

\[
\begin{align*}
\text{if issparse(alpha) & L = full(L(nz,nz)); end & convert L and sW if necessary} \\
\text{if issparse(sW), sW = full(sW(nz)); end}
\end{align*}
\]

\[
\text{else nz = true(size(alpha,1),1); end & non-sparse representation}
\]

\[
\text{if isempty(L) & in case L is not provided, we compute it}
\]

\[
\begin{align*}
K &= \text{feval(cov{:}, hyp.cov, x(nz,:));} \\
L &= \text{chol(eye(sum(nz)) + sW*sW'*K);}
\end{align*}
\]

\[
\text{if nargin<9}
\]

\[
\text{else}
\]

\[
\text{end}
\]

\[
\text{In every iteration of the above loop, we compute the predictions for all test points of the batch.}
\]

\[(\text{make predictions}) \equiv\]

\[
\begin{align*}
\text{if strcmp(cstr,'covFITC') || strcmp(cstr,'apxSparse') & cross-covariances} \\
Ks &= \text{feval(cov{:}, hyp.cov, x, xs(id,:)); Ks = Ks(nz,:); & res indep. of x}
\end{align*}
\]

\[
\text{else}
\]

\[
\text{end}
\]

\[
\text{V = L'\text{repmat(sW,1,length(id)).*Ks);} & \text{predictive means}
\]

\[
\text{if Lchol & L contains chol decompo => use Cholesky parameters (alpha,sW,L)}
\]

\[
\text{else}
\]

\[
\text{end}
\]

\[
\text{fs2(id) = max(fs2(id),0); & remove numerical noise i.e. negative variances}
\]

\[
\text{Fs2 = repmat(fs2(id),1,N); & we have multiple values in case of sampling}
\]

\[
\text{if nargin<9}
\]

\[
\text{else}
\]

\[
\text{end}
\]
lp(id) = sum(reshape(Lp, [],N),2)/N; % log probability; sample averaging
ymu(id) = sum(reshape(Ymu, [],N),2)/N; % predictive mean ys|y and ..
ys2(id) = sum(reshape(Ys2, [],N),2)/N; % .. variance
3 Inference Methods

Inference methods are responsible for computing the (approximate) posterior \( p \), the (approximate) negative log marginal likelihood \( n1Z \) and its partial derivatives \( dn1Z \) w.r.t. the hyperparameters \( hyp \). The arguments to the function are hyperparameters \( hyp \), mean function \( mean \), covariance function \( cov \), likelihood function \( lik \) and training data \( x \) and \( y \). Several inference methods are implemented and described this section.

\[\text{infMethods.m} \equiv\]
\begin{verbatim}
1 % Inference methods: Compute the (approximate) posterior for a Gaussian process.
2 % Methods currently implemented include:
3 %
4 % infGaussLik       Exact inference (only possible with Gaussian likelihood)
5 % infLaplace       Laplace’s Approximation
6 % infEP            Expectation Propagation
7 % infKL           Kullback-Leibler optimal Approximation
8 % infMCMC        Markov Chain Monte Carlo and Annealed Importance Sampling
9 % infLOO        Leave-One-Out predictive probability and Least-Squares Approxim.
10 % infPrior       Perform inference with hyperparameter prior.
11 %
12 % The interface to the approximation methods is the following:
13 %
14 % function [post n1Z dn1Z] = inf..(hyp, cov, lik, x, y)
15 %
16 % where:
17 %
18 % hyp is a struct of hyperparameters
19 % cov is the name of the covariance function (see covFunctions.m)
20 % lik is the name of the likelihood function (see likFunctions.m)
21 % x is a n by D matrix of training inputs
22 % y is a (column) vector (of size n) of targets
23 %
24 % n1Z is the returned value of the negative log marginal likelihood
25 % dn1Z is a (column) vector of partial derivatives of the negative
26 % log marginal likelihood w.r.t. each hyperparameter
27 % post struct representation of the (approximate) posterior containing
28 % alpha is a (sparse or full column vector) containing inv(K)*(mu-m),
29 % where K is the prior covariance matrix, m the prior mean,
30 % and mu the approx posterior mean
31 % sW is a (sparse or full column) vector containing diagonal of sqrt(W)
32 % L is a (sparse or full) triangular matrix, L = chol(sW*K*sW+eye(n)),
33 % or a full matrix, L = -inv(K+inv(W)),
34 % or a function L(A) of a matrix A such that -(K+inv(W))*L(A) = A
35 % Usually, the approximate posterior to be returned admits the form
36 % N(mu=m+K*alpha, W=inv(K+inv(W)), where alpha is a vector and W is diagonal.
37 %
38 % For more information on the individual approximation methods and their
39 % implementations, see the separate inf???.m files. See also gp.m.
\end{verbatim}
Not all inference methods are compatible with all likelihood functions, e.g., exact inference is only possible with Gaussian likelihood. In order to perform inference, each method needs various properties of the likelihood functions, section 4.

### 3.1 Exact Inference with Gaussian likelihood

For Gaussian likelihoods, GP inference reduces to computing mean and covariance of a multivariate Gaussian which can be done exactly by simple matrix algebra. The program `inf/infExact.m` does exactly this. If it is called with a likelihood function other than the Gaussian, it issues an error. The Gaussian posterior $q(f|D) = \mathcal{N}(f|\mu, V)$ is exact.

#### infGaussLik.m

```matlab
function [post nlZ dnlZ] = infGaussLik(hyp, mean, cov, lik, x, y, opt)

% Exact inference for a GP with Gaussian likelihood. Compute a parametrization
% of the posterior, the negative log marginal likelihood and its derivatives
% w.r.t. the hyperparameters. See also "help infMethods".

if nargin<7, opt = []; end % make sure parameter exists
if iscell(lik), likstr = lik{1}; else likstr = lik; end
if ~ischar(likstr), likstr = func2str(likstr); end
if ~strcmp(likstr,'likGauss') % NOTE: no explicit call to likGauss
    error('Exact inference only possible with Gaussian likelihood');
end

[n, D] = size(x);
[m, dm] = feval(mean{:}, hyp.mean, x); % evaluate mean vector and deriv
sn2 = exp(2*hyp.lik); W = ones(n,1)/sn2; % noise variance of likGauss
K = apx(hyp,cov,x,opt); % set up covariance approximation
[ldB2,solveKiW,dW,dhyp,post.L] = K.fun(W); % obtain functionality depending on W
alpha = solveKiW(y-m);
post.alpha = K.P(alpha); % return the posterior parameters
post.sW = sqrt(W); % sqrt of noise precision vector
if nargout>1 % do we want the marginal likelihood?
    nlZ = (y-m)'*alpha/2 + ldB2 + n*log(2*pi*sn2)/2; % -log marginal likelihood
    if nargout>2 % do we want derivatives?
        dnlZ = dhyp(alpha); dnlZ.mean = -dm(alpha);
        dnlZ.lik = -sn2*(alpha'*alpha) - 2*sum(dW)/sn2 + n;
    end
end
```

### 3.2 Laplace's Approximation

For differentiable likelihoods, Laplace's approximation, approximates the posterior by a Gaussian centered at its mode and matching its curvature `inf/infLaplace.m`.

More concretely, the mean of the posterior $q(f|D) = \mathcal{N}(f|\mu, V)$ is – defining $\ell_i(f_i) = \ln p(y_i|f_i)$ and
\( \ell(f) = \sum_{i=1}^{n} \ell_i(f_i) \) – given by

\[
\mu = \arg \min_f \phi(f), \text{ where } \phi(f) = \frac{1}{2} (f - m)^\top K^{-1} (f - m) - \ell(f) \leq -\ln[p(f)p(y|f)],
\]

which we abbreviate by \( \mu \leftarrow \mathcal{L}(\ell) \). The curvature \( \frac{\partial^2 \phi}{\partial f^2} = K^{-1} + W \) with \( W_{ii} = -\frac{\partial^2}{\partial f_i^2} \ln p(y_i|f_i) \) serves as precision for the Gaussian posterior approximation \( V = (K^{-1} + W)^{-1} \) and the marginal likelihood \( Z = \int p(f)p(y|f)df \) is approximated by \( \bar{Z} = \int \hat{\phi}(f)df \) where we use the 2nd order Taylor expansion at the mode \( \mu \) given by \( \hat{\phi}(f) = \phi(\mu) + \frac{1}{2} (f - \mu)^\top V^{-1} (f - \mu) \approx \phi(f) \).

Laplace’s approximation needs derivatives up to third order for the mode fitting procedure (Newton method)

\[
d_k = \frac{\partial^k}{\partial f^k} \log p(y|f), \quad k = 0, 1, 2, 3
\]

and

\[
d_k = \frac{\partial}{\partial \rho_i} \frac{\partial^k}{\partial f^k} \log p(y|f), \quad k = 0, 1, 2
\]

evaluated at the latent location \( f \) and observed value \( y \). The likelihood calls (see section \[4\])

- \([d_0, d_1, d_2, d_3] = \text{lik(hyp, y, f, []}, \ '\text{infLaplace}')\)

and

- \([d_0, d_1, d_2] = \text{lik(hyp, y, f, []}, \ '\text{infLaplace'}, i)\)

return exactly these values.

### 3.3 Expectation Propagation

The basic idea of Expectation Propagation (EP) as implemented in \textsf{inf/infEP.m} is to replace the non-Gaussian likelihood terms \( p(y_i|f_i) \) by Gaussian functions \( t(f_i; \nu_i, \tau_i) = \exp(\nu_i f_i - \frac{1}{2} \tau_i f_i^2) \) and to adjust the natural parameters \( \nu_i, \tau_i \) such that the following identity holds:

\[
\frac{1}{Z_{t,i}} \int r_k q_{-i}(f) \cdot t(f; \nu_i, \tau_i) df = \frac{1}{Z_{p,i}} \int r_k q_{-i}(f) \cdot p(y_i|f) df, \quad k = 1, 2
\]

with the so-called cavity distributions \( q_{-i}(f) = N(f|\mu, K) \prod_{j \neq i} t(f_j; \nu_j, \tau_j) \propto N(f|\mu, V)/t(f_i; \nu_i, \tau_i) \) equal to the posterior divided by the \( i \)th Gaussian approximation function and the two normalisers \( Z_{t,i} = \int q_{-i}(f) \cdot t(f_i; \nu_i, \tau_i) df \) and \( Z_{p,i} = \int q_{-i}(f) \cdot p(y_i|f_i) df \). The moment matching corresponds to minimising the following local KL-divergence

\[
\nu_i, \tau_i = \arg \min_{\nu, \tau} \text{KL}[q_{-i}(f)p(y_i|f_i)/Z_{p,i} || q_{-i}(f)t(f_i; \nu, \tau)/Z_{t,i}].
\]

In order to apply the moment matching steps in a numerically safe way, EP requires the derivatives of the expectations w.r.t. the Gaussian mean parameter \( \mu \)

\[
d_k = \frac{\partial^k}{\partial \mu^k} \int p(y|f)N(f|\mu, \sigma^2) df, \quad k = 0, 1, 2
\]

and the \( i \)th likelihood hyperparameter \( \rho_i \)

\[
d = \frac{\partial}{\partial \rho_i} \int p(y|f)N(f|\mu, \sigma^2) df
\]

which can be obtained by the likelihood calls (see section \[4\])
\[
\begin{align*}
\text{• } [d0, d1, d2] &= \text{lik}(\text{hyp}, y, \mu, s2, \text{'infEP'}) \\
\text{and} \\
\text{• } d &= \text{lik}(\text{hyp}, y, \mu, s2, \text{'infEP'}, i).
\end{align*}
\]

### 3.4 Kullback Leibler Divergence Minimisation

Another well known approach to approximate inference implemented in \text{inf/infKL.m} in attempts to directly find the closest Gaussian \(q(f|\mathcal{D}) = N(f|\mu, V)\) to the exact posterior \(p(f|\mathcal{D})\) w.r.t. to some proximity measure or equivalently to maximise a lower bound \(Z(\mu, V)\) to the marginal likelihood as described in Nickisch & Rasmussen [Approximations for Binary Gaussian Process Classification] JMLR, 2008. In particular, one minimises \(\text{KL}(N(f|\mu, V)||p(f|\mathcal{D}))\) which amounts to minimising \(-\ln Z(\mu, V)\) as defined by:

\[
-\ln Z = -\ln \int p(f)p(y|f)df = -\ln \int q(f|\mathcal{D}) \frac{p(f)}{q(f|\mathcal{D})} p(y|f)df
\]

\[
\leq \int q(f|\mathcal{D}) \ln \frac{q(f|\mathcal{D})}{p(f)} df - \int q(f|\mathcal{D}) \ln p(y|f)df =: -\ln Z(\mu, V)
\]

\[
= \text{KL}(N(f|\mu, V)||N(f|m, K)) - \sum_{i=1}^{n} N(f_i|\mu_i, v_{ii}) \ln p(y_i|f_i)df_i, v_{ii} = |V|_{ii}
\]

\[
= \frac{1}{2} \left( \text{tr}(VK^{-1} - I) - \ln |VK^{-1}| \right) + \frac{1}{2} (\mu - m)^\top K^{-1} (\mu - m) - \sum_{i=1}^{n} \ell^K_{KL}(\mu_i, v_{ii})
\]

where \(\ell^K_{KL}(\mu_i) = \int N(f_i|\mu_i, v_{ii}) \ell_i(f_i) df_i\) is the convolution of the log likelihood \(\ell_i\) with the Gaussian \(N\) and \(v = \text{dg}(V)\). Equivalently, one can view \(\ell^K_{KL}\) as a smoothed version of \(\ell\) with univariate smoothing kernel \(N\).

From Challis & Barber [Concave Gaussian Variational Approximations for Inference in Large Scale Bayesian Linear Models] AISTATS, 2011 we know that the mapping \((\mu, L) \mapsto -\ln Z(\mu, L^\top L)\) is jointly convex whenever the likelihoods \(f_i \mapsto P(y_i|f_i)\) are log concave. In particular, this implies that every \((\mu_i, s_i) \mapsto -\ell^K_{KL}(\mu_i, s_i^2)\) is jointly convex.

We use an optimisation algorithm similar to EP (section 3.3) where we minimise the local KL-divergence the other way round \(\mu, s_i = \arg \min_{\mu, s_i} \text{KL}(N(f|\mu, s^2)||q_{-i}(f)p(y_i|f_i)/Z_{p,i})\). This view was brought forward by Tom Minka [Convex Divergence measures and message passing], MSR-TR, 2005. The KL-minimisation constitutes a jointly convex 2d optimisation problem solved by \(\text{klmin}\) using a scaled Newton approach which is included as a sub function in \text{inf/infKL.m}. The smoothed likelihood \(\ell^K_{KL}(\mu_i, v_{ii})\) is implemented as a meta likelihood in \text{likKL} it uses Gaussian-Hermite quadrature to compute the required integrals. Note that – as opposed to EP – Gaussian-Hermite quadrature is appropriate since we integrate against the \(\ln P(y_i|f_i)\) (which can be well approximated by a polynomial) instead of \(P(y_i|f_i)\) itself. The algorithm is – again unlike EP – provably convergent for log-concave likelihoods (e.g. \text{likGauss}, \text{likLaplace}, \text{likSech2}, \text{likLogistic}, \text{likPoisson}) since it can be regarded as coordinate descent with guaranteed decrease in the objective in every step. Due to the complex update computations, \text{infKL} can be quite slow although it has the same \(O(n^3)\) asymptotic complexity as EP and Laplace.

### 3.5 Variational Bayes

One can drive the bounding even further by means of local quadratic lower bounds to the log likelihood \(\ell(f) = \ln p(y|f)\). Suppose that we use a super-Gaussian likelihood \(p(y|f)\) i.e. likelihoods
that can be lower bounded by Gaussians of any width \( w \) (e.g. likLaplace, likT, likLogistic, likSech2). Formally, that means that there are \( b, z \in \mathbb{R} \) such that

\[
\rho(f) = \ln p(y|f - z) - bf
\]

is symmetric and \( \sqrt{t} \mapsto \rho(f) \) is a convex function for all \( f \geq 0 \). As a result, we obtain the following exact representation of the likelihood

\[
\ell(f) = \ln p(y|f) = \max_{w>0} \left( (b + wz)f - \frac{wf^2}{2} - \frac{1}{2} h(\gamma) \right),
\]

which can be derived by convex duality and assuming the likelihoods to be super-Gaussian. Details can be found in papers by Palmer et al. [Variational EM Algorithms for Non-Gaussian Latent Variable Models, NIPS, 2006 and Nickisch & Seeger [Convex Variational Bayesian Inference for Large Scale Generalized Linear Models, ICML, 2009].

The bottom line is that we can treat the variational bounding as a sequence of Laplace approximations with the “variational Bayes” log likelihood

\[
\ell_{VB}(f_i) = \ell(g_i) + b_i(f_i - g_i), \quad g = \text{sgn}(f - z) \odot \sqrt{(f - z)^2 + v + z}
\]

instead of the usual likelihood \( \ell(f_i) = \ln p(y_i|f_i) \) i.e. we solve \( \mu \leftarrow \mathcal{L}(\ell_{VB}) \) instead of \( \mu \leftarrow \mathcal{L}(\ell) \). See section 3.2. In the code of inf/infVB.m, the likelihood is implemented in the function likVB.

At the end, the optimal value of \( W \) can be obtained analytically via \( w_i = |b_i - \ell'(g_i)|/|g_i - z_i| \).

For the minimisation in inf/infVB.m, we use a provably convergent double loop algorithm, where in the inner loop a nonlinear least squares problem (convex for log-concave likelihoods) is solved using inf/infLaplace.m such that \( \mu \leftarrow \mathcal{L}(\ell_{VB}) \) and in the outer loop, we compute \( \nu \leftarrow \text{dg}((K^{-1} + W)^{-1}) \).

The only requirement to the likelihood function is that it returns the values \( b, z \) required by the bound which are delivered by the call (see section 4)

- \([b,z] = \text{lik}(\text{hyp}, y, [], \text{ga}, 'infVB')\)

The negative marginal likelihood upper bound \(-\ln Z_{VB}\) is obtained by integrating the prior times the exact representation of the likelihood

\[
p(y|f) = \max_{\gamma>0} q(y|f, \gamma), \quad q(y|f, \gamma) = N(f|\nu, \gamma) \exp \left( -\frac{h(\gamma)}{2} - \frac{\nu^2}{2\gamma} \right) \sqrt{2\pi\gamma}, \quad \gamma = \frac{1}{w}, \quad \nu = b\gamma + z
\]

w.r.t. the latent variables \( f \) yielding

\[
-\ln Z_{VB} = -\ln \int N(f|m, K) \prod_{i=1}^{n} q_i(y_i|f_i, \gamma_i) df
\]

\[
= -\ln N(m|\nu, K + \Gamma) + \frac{1}{2} \left( h(\gamma) - \nu^\top \nu^2 - 1^\top \ln 2\pi\gamma \right).
\]

### 3.6 Compatibility Between Inference Methods and Covariance Approximations

Another kind of approximation is needed to render an inference method scalable. We have two approximation schemes which in fact approximate the covariance to make it amenable to large number of training data points. The following table shows the compatibility between some inference methods and two major groups of covariance approximations we will discuss in the next two sections.
3.7 Sparse Covariance Approximations

One of the main problems with GP models is the high computational load for inference computations. In a setting with \( n \) training points \( x \), exact inference with Gaussian likelihood requires \( O(n^3) \) effort; approximations like Laplace or EP consist of a sequence of \( O(n^3) \) operations.

There is a line of research with the goal to alleviate this burden by using approximate covariance functions \( \tilde{k} \) instead of \( k \). A review is given by Candela and Rasmussen\(^\text{[1]}\). One basic idea in those approximations is to work with a set of \( m \) inducing inputs \( u \) with a reduced computational load of \( O(nm^2) \). In the following, we will provide a rough idea of the FITC approximation used in the toolbox. Let \( K \) denote the \( n \times n \) covariance matrix between the training points \( x \), \( K_u \) the \( m \times n \) covariance matrix between the \( n \) training points and the \( m \) inducing points, and \( K_{uu} \) the \( m \times m \) covariance matrix between the \( m \) inducing points. The FITC approximation to the covariance is given by

\[
K \approx \tilde{K} = Q + G, \quad G = \text{diag}(g), \quad g = \text{diag}(K - Q), \quad Q = K_u^\top Q_{uu}^{-1} K_u, \quad Q_{uu} = K_{uu} + \sigma^2_{n_u} I,
\]

where \( \sigma_{n_u} \) is the noise from the inducing inputs. Note that \( \tilde{K} \) and \( K \) have the same diagonal elements \( \text{diag}(\tilde{K}) = \text{diag}(K) \); all off-diagonal elements are the same as for \( Q \). Internally, the necessary covariance evaluations are performed by a meta covariance function \( \text{cov/apxSparse.m} \). The toolbox offers FITC versions for regression with Gaussian likelihood \( \text{inf/infGaussLik.m} \), as well as for Laplace's approximation \( \text{inf/infLaplace.m} \).

The user can decide whether to treat the inducing inputs \( u \) as fixed or as hyperparameters. The latter allows to adjust the inducing inputs \( u \) w.r.t. the marginal likelihood. As detailed in the documentation of \( \text{inf/apx.m} \), \( u \) is treated as fixed if it is passed as the 2nd parameter of \( \text{apxSparse(cov, xu, ..)} \). If the hyperparameter structure \( \text{hyp} \) contains a field \( \text{hyp.xu} \) in inference method calls such as \( \text{infGaussLik(hyp, ..)} \) or inference/prediction calls like \( \text{gp(hyp, @infGaussLik, ..)} \) the inducing inputs \( u \) are treated as hyperparameters and can be optimised. See \( \text{doc/demoSparse.m} \) for an illustration.

3.8 Grid-Based Covariance Approximations

Another way to bring down computational costs is to take advantage of grid structure \( x \). For example, in geostatistics or image processing, the training data \( x \in \mathbb{R}^{n \times D} \) could be a complete 2d lattice of size \( n_1 \times n_2 \) as given by the axes \( g_1 \in \mathbb{R}^{n_1}, g_2 \in \mathbb{R}^{n_2} \) so that \( n = N = n_1 \cdot n_2, D = 2 \) and \( x = [\text{vec}(g_1 g_1^\top), \text{vec}(g_2 g_2^\top)] \). In general, a p-dimensional grid \( U \in \mathbb{R}^{N \times D} \) is specified by a set of axis matrices \( \{g_i \in \mathbb{R}^{n_i \times D}\}_{i=1}^p \), so that \( N = \prod_{i=1}^p n_i \) and \( D = \sum_{i=1}^p D_i \) where the axes do not need to be 1d nor do their components need to be sorted. As a consequence, \( U \) represents a Cartesian product of its axes \( U = g_1 \times g_2 \times \cdots \times g_p \). The \( \text{cov/apxGrid.m} \) covariance function represents a Kronecker product covariance matrix

\[
K_{UU} = K_p \otimes \cdots \otimes K_2 \otimes K_1
\]

whose factorisation structure is given by the grid \( x_g \). The gain in computational efficiency is due to the fact that matrix-vector product, determinant, inverse and eigenvalue computations decompose so that many operations with an overall cost of \( O(N^3) \) now only cost \( O(\sum_{i=1}^p n_i^3) \).

\( ^{\text{[1]}}\) A Unifying View of Sparse Approximate Gaussian Process Regression, JMLR, 2005
For off-grid data points, we can still take advantage of the computational properties of a grid-based covariance matrix $K_{UU}$ via the structured kernel interpolation (SKI) framework aka KISS-GP by Wilson and Nickisch\textsuperscript{2} with extensions\textsuperscript{3}. Here, the $n \times n$ covariance $K$ is obtained from the $N \times N$ grid covariance $K_{UU}$ by interpolation $K \approx W_X K_{UU} W_X^T$, where $K_{UU}$ is a covariance matrix formed by evaluating the user-specified kernel over a set of latent inducing inputs $U$, with locations that have been chosen to create algebraic structure in $K_{UU}$ that we can exploit for efficiency. Here, the interpolation matrix $W_X \in \mathbb{R}^{n \times N}$ is extremely sparse; i.e., for local cubic interpolation $W_X$ contains only $4^D$ nonzeros per row, where $D$ is the data dimension. In addition $W_X$ is row-normalised $W_X^1 = W_X N$. The structure in $K_{UU}$ alongside the sparsity of $W_X$, allows for very fast MVMs with the SKI approximate covariance matrix $K$ over the inputs $x$ enabling fast inference and prediction.

Internally, we use a meta covariance function `cov/apxGrid.m` to represent the Kronecker covariance matrix and a Gaussian regression inference method `inf/infGaussLik.m`. We also support incomplete grids where $n < N$. A good starting point is Yunus Saatçi’s PhD thesis\textsuperscript{4}. For incomplete grids, we use the interpolation-based extensions by Wilson et al\textsuperscript{5} where conjugate gradients and a determinant approximations are used. See `doc/demoGrid1d.m` and `doc/demoGrid2d.m` for an illustration. We also offer non-Gaussian likelihoods as described by Seth Flaxman\textsuperscript{6} so that `inf/infLaplace.m` can be used.

\textsuperscript{2}Kernel Interpolation for Scalable Structured Gaussian Processes, ICML, 2015
\textsuperscript{3}Thoughts on Massively Scalable Gaussian Processes, TR, 2015.
\textsuperscript{4}Scalable Inference for Structured Gaussian Process Models, University of Cambridge, 2011
\textsuperscript{5}Fast Kernel Learning for Multidimensional Pattern Extrapolation, NIPS, 2014
\textsuperscript{6}Fast Kronecker inference in Gaussian processes with non-Gaussian likelihoods, ICML, 2015
4 Likelihood Functions

A likelihood function \( p_\rho(y|f) \) (with hyperparameters \( \rho \)) is a conditional density \( \int p_\rho(y|f)dy = 1 \) defined for scalar latent function values \( f \) and outputs \( y \). In the GPML toolbox, we use iid. likelihoods \( p_\rho(y|f) = \prod_{i=1}^{n} p_\rho(y_i|f_i) \). The approximate inference engine does not explicitly distinguish between classification and regression likelihoods: it is fully generic in the likelihood allowing to use a single code in the inference step.

Likelihood functionality is needed both during inference and while predicting.

4.1 Prediction

A prediction at \( x_\ast \) conditioned on the data \( \mathcal{D} = (X, y) \) (as implemented in gp.m) consists of the predictive mean \( \mu_{y_\ast} \) and variance \( \sigma^2_{y_\ast} \), which are computed from the the latent marginal moments \( \mu_{f_\ast}, \sigma^2_{f_\ast} \) i.e. the Gaussian marginal approximation \( N(f_\ast|\mu_{f_\ast}, \sigma^2_{f_\ast}) \) via

\[
p(y_\ast|\mathcal{D}, x_\ast) = \int p(y_\ast|f_\ast)p(f_\ast|\mathcal{D}, x_\ast)df_\ast \approx \int p(y_\ast|f_\ast)N(f_\ast|\mu_{f_\ast}, \sigma^2_{f_\ast})df_\ast. \tag{3}
\]

The moments are given by \( \mu_{y_\ast} = \int y_\ast p(y_\ast|\mathcal{D}, x_\ast)dy_\ast \) and \( \sigma^2_{y_\ast} = \int (y_\ast - \mu_{y_\ast})^2 p(y_\ast|\mathcal{D}, x_\ast)dy_\ast \). The likelihood call

- \([lp, ymu, ys2] = \text{lik(hyp, []}, fmu, fs2)\)


doing exactly this. Evaluation of the logarithm of \( p_{y_*} = p(y_*|\mathcal{D}, x_\ast) \) for values \( y_* \) can be done via

- \([lp, ymu, ys2] = \text{lik(hyp, y, fmu, fs2})\)

where \( lp \) contains the number \( \ln p_{y_*} \).

Using the moments of the likelihood \( \mu_{f_\ast} = \int y_\ast p(y_\ast|f_\ast)dy_\ast \) and \( \sigma^2_{f_\ast} = \int (y_\ast - \mu_{f_\ast})^2 p(y_\ast|f_\ast)dy_\ast \), we obtain for the predictive moments the following (exact) expressions

\[
\mu_{y_\ast} = \int \mu_{f_\ast} p(f_\ast|\mathcal{D}, x_\ast)df_\ast, \quad \text{and}
\]

\[
\sigma^2_{y_\ast} = \int \left[ \sigma^2_{f_\ast} + (\mu_{f_\ast} - \mu_{y_\ast})^2 \right] p(f_\ast|\mathcal{D}, x_\ast)df_\ast.
\]

1. The binary case is simple since \( y_* \in \{-1, +1\} \) and \( 1 = p_{y_*} + p_{-y_*} \). Using \( \pi_* = p_{+1} \), we find

\[
p_{y_*} = \begin{cases} 
\pi_* & y_* = +1 \\
1 - \pi_* & y_* = -1
\end{cases}
\]

\[
\mu_{y_*} = \sum_{y_* = \pm 1} y_* p(y_*|\mathcal{D}, x_\ast) = 2 \cdot \pi_* - 1 \in [-1, 1], \quad \text{and}
\]

\[
\sigma^2_{y_*} = \sum_{y_* = \pm 1} (y_* - \mu_{y_*})^2 p(y_*|\mathcal{D}, x_\ast) = 4 \cdot \pi_* \pi_*(1 - \pi_*), \quad \text{in [0, 1]}
\]

2. The continuous case for homoscedastic likelihoods depending on \( r_* = y_* - f_* \) only and having noise variance \( \sigma^2_{f_\ast} = \sigma^2_{n} \) is also simple since the identity \( p(y_*|f_\ast) = p(y_* - f_*|0) \) allows to substitute \( y_* \leftarrow y_* + f_* \) yielding \( \mu(f_\ast) = f_* + \int y_* p(y_*|0)dy_* \) and assuming \( \int y_* p(y_*|0)dy_* = 0 \) we arrive at

\[
\mu_{y_*} = \mu_{f_*}, \quad \text{and}
\]

\[
\sigma^2_{y_*} = \sigma^2_{f_*} + \sigma^2_{n}.
\]
3. The generalised linear model (GLM) case is also feasible. Evaluation of the predictive distribution is done by quadrature

\[ p(y_*) \approx \int p(y_*|f_*)p(f_*|\mathcal{D}, x_*)df_* \approx \int p(y_*|f_*)N(f_*|\mu_{f_*}, \sigma_{f_*}^2)df_* \]

For GLMs the mean is given by \( \mu(f_*) = g(f_*) \) and the variance is usually given by a simple function of the mean \( \sigma^2(f_*) = v(g(f_*)) \), hence we use Gaussian-Hermite quadrature with \( N(f_*|\mu_{f_*}, \sigma_{f_*}^2) \approx p(f_*|\mathcal{D}, x_*) \) to compute

\[ \mu_{y_*} = \int g(f_*)p(f_*|\mathcal{D}, x_*)df_*, \text{ and} \]
\[ \sigma_{y_*}^2 = \int \left[ v(g(f_*)) + (g(f_*) - \mu_{y_*})^2 \right] p(f_*|\mathcal{D}, x_*)df_* = v(\mu_{y_*}) \]

4. Finally the warped Gaussian likelihood predictive distribution with strictly monotonically increasing warping function \( g \) is given by the expression

\[ p(y_*|\mathcal{D}, x_*) = g'(y_*) N(g(y_*)|\mu_{f_*}, \sigma_n^2 + \sigma_{f_*}^2) \]

so that the predictive moments can be computed by Gaussian-Hermite quadrature.

In the following, we will detail how and which likelihood functions are implemented in the GPML toolbox. Further, we will mention dependencies between likelihoods and inference methods and provide some analytical expressions in addition to some likelihood implementations.

### 4.2 Interface

The likelihoods are in fact the most challenging object in our implementation. Different inference algorithms require different aspects of the likelihood to be computed, therefore the interface is rather involved as detailed below.

```matlab
likFunctions.m

% likelihood functions are provided to be used by the gp.m function:
% likErf (Error function, classification, probit regression)
% likLogistic (Logistic, classification, logit regression)
% likUni (Uniform likelihood, classification)
% likGauss (Gaussian, regression)
% likGaussWarp (Warped Gaussian, regression)
% likGumbel (Gumbel likelihood for extremal values)
% likLaplace (Laplacian or double exponential, regression)
% likSech2 (Sech-square, regression)
% likT (Student’s t, regression)
% likPoisson (Poisson regression, count data)
% likGamma (Nonnegative regression, positive data)
% likInvGauss (Nonnegative regression, positive data)
% likBeta (Beta regression, interval data)
% likMix (Mixture of individual likelihood functions)

% The likelihood functions have three possible modes, the mode being selected
```
% as follows (where "lik" stands for any likelihood function in "lik/lik*.m"): 

% 1) With one or no input arguments: [REPORT NUMBER OF HYPERPARAMETERS]

  s = lik OR s = lik(hyp)

The likelihood function returns a string telling how many hyperparameters it 
expects, using the convention that "D" is the dimension of the input space. 
For example, calling "likLogistic" returns the string '0'.

% 2) With three or four input arguments: [PREDICTION MODE]

lp = lik(hyp, y, mu) OR [lp, ymu, ys2] = lik(hyp, y, mu, s2)

This allows to evaluate the predictive distribution. Let p(y_*|f_*) be the
likelihood of a test point and N(f_*|mu,s2) an approximation to the posterior 
margin p(f_*|x_*,x,y) as returned by an inference method. The predictive 
distribution p(y_*|x_*,x,y) is approximated by.

q(y_*) = \int N(f_*|mu,s2) p(y_*|f_*) df_*

lp = log( q(y) ) for a particular value of y, if s2 is [] or 0, this

 corresponds to log( p(y|mu) )

 ymu and ys2 the mean and variance of the predictive marginal q(y)

 note that these two numbers do not depend on a particular

 value of y

All vectors have the same size.

% 3) With five or six input arguments, the fifth being a string [INFERENCE MODE]

[varargout] = lik(hyp, y, mu, s2, inf) OR

[varargout] = lik(hyp, y, mu, s2, inf, i)

There are three cases for inf, namely a) infLaplace, b) infEP and c) infVB.
The last input i, refers to derivatives w.r.t. the ith hyperparameter.

% a1) [lp,dlp,d2lp,d3lp] = lik(hyp, y, f, [], 'infLaplace')

lp, dlp, d2lp and d3lp correspond to derivatives of the log likelihood 

log(p(y|f)) w.r.t. to the latent location f.

lp = log( p(y|f) )

dlp = d log( p(y|f) ) / df

d2lp = d^2 log( p(y|f) ) / df^2

d3lp = d^3 log( p(y|f) ) / df^3

% a2) [lp_dhyp,dlp_dhyp,d2lp_dhyp] = lik(hyp, y, f, [], 'infLaplace', i)

returns derivatives w.r.t. to the ith hyperparameter

lp_dhyp = d log( p(y|f) ) / ( dhyp_i)

dlp_dhyp = d^2 log( p(y|f) ) / (df dhyp_i)

d2lp_dhyp = d^3 log( p(y|f) ) / (df^2 dhyp_i)

% b1) [lZ,dlZ,d2lZ] = lik(hyp, y, mu, s2, 'infEP')

let Z = \int p(y|f) N(f|mu,s2) df then

lZ = log(Z)

dlZ = d log(Z) / dmu

d2lZ = d^2 log(Z) / dmu^2

%
4.3 Implemented Likelihood Functions

The following table enumerates all (currently) implemented likelihood functions that can be found at lik/lik<NAME>.m and their respective set of hyperparameters $\rho$.

| lik<NAME> | regression $y_i \in \mathbb{R}$ | $p(y_i | f_i) =$ | $\rho =$ |
|--------------|---------------------------------|----------------|----------------|
| Gauss        | Gaussian                        | $N(y_i | f_i, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(y_i - f_i)^2}{2\sigma^2}\right)$ | $\{ \ln \sigma \}$ |
| GaussWarp    | Warped Gaussian                 | $N(g(a_i) | f_i, \sigma^2)g_0(y_i)$ | $\{ \theta_1, ..., \theta_n, \ln \sigma \}$ |
| Gumbel       | Gumbel                          | $\frac{2}{\sigma^2} \exp\left(-z_i - e^{-z_i}\right), z_i = \gamma + \frac{\alpha(y_i - f_i)}{\sigma\sqrt{\pi}}$, $|z| = 1$ | $\{ \ln \sigma \}$ |
| Sech2        | Sech-squared                    | $\frac{1}{2 \cosh^2(y_i | f_i)}$ | $[\sigma]$ |
| Laplace      | Laplacian                       | $\frac{1}{\pi} \exp\left(-\frac{|y_i - f_i|}{b}\right), b = \frac{\sigma}{\sqrt{2}}$ | $[\ln \sigma]$ |
| T            | Student's t                     | $\frac{\Gamma\left(\frac{v+1}{2}\right)}{\Gamma\left(\frac{v}{2}\right)} \frac{1}{\sqrt{\pi \sigma^2}} \left(1 + \frac{(y_i - f_i)^2}{\sigma^2}\right)^{-\frac{v+1}{2}}$ | $[\ln (v - 1), \ln \sigma]$ |

| lik<NAME> | classification $y_i \in \{+1\}$ | $p(y_i | f_i) =$ | $\rho =$ |
|--------------|---------------------------------|----------------|----------------|
| Erf          | Error function                  | $\int_{-\infty}^{y_i} N(t)dt$ | $\emptyset$ |
| Logistic     | Logistic function               | $\frac{1}{1 + \exp(-u_i f_i)}$ | $\emptyset$ |
| Uni          | Label noise                     | $\emptyset$ | $\emptyset$ |

| lik<NAME> | count data $y_i \in \mathbb{N}$ | $p(y_i | f_i) =$ | $\rho =$ |
|--------------|---------------------------------|----------------|----------------|
| Poisson      | Poisson                         | $\mu \cdot e^{\frac{u_i}{\mu}}$, $\mu = \exp(1 + e^t)$ | $\emptyset$ |

| lik<NAME> | nonnegative data $y_i \in \mathbb{R}_+ \setminus \{0\}$ | $p(y_i | f_i) =$ | $\rho =$ |
|--------------|--------------------------------------------------------|----------------|----------------|
| Weibull      | Weibull, $\gamma_1 = \Gamma(1 + 1/k)$ | $\kappa \gamma_1 / \mu (\gamma_1 / \mu)^{k-1} \exp\left(-\frac{\gamma_1 y_i / \mu}{\mu}\right)$ | $[\ln k]$ |
| Gamma        | Gamma                                                  | $\frac{k_\alpha}{\Gamma(\alpha)} \mu^{-\alpha} \exp\left(-\frac{\gamma y_i / \mu}{\mu}\right)$ | $[\ln \alpha]$ |
| Exp          | Exponential                                            | $\mu^{-1} \exp\left(-\frac{u_i}{\mu}\right)$ | $\emptyset$ |
| InvGauss     | Inverse Gaussian                                      | $\frac{k_\lambda}{2 \sqrt{\pi \lambda}} \exp\left(-\frac{\lambda (y_i - \mu)^2}{2 \mu^2 \lambda}\right)$ | $[\ln \lambda]$ |

| lik<NAME> | interval data $y_i \in [0, 1]$ | $p(y_i | f_i) =$ | $\rho =$ |
|--------------|---------------------------------|----------------|----------------|
| Beta         | Beta                              | $\int_{0}^{\min(1, 1 - \mu \phi)} (1 - y)^{1-\mu} \phi^{-1}$ | $[\ln \phi]$ |

| Composite likelihood functions | $p(y_i | f_i)_1, p(y_i | f_i)_2, .. \Rightarrow p(y_i | f_i)$ | $\rho =$ |
|------------------------------|---------------------------------|----------------|
| Mix                          | Mixture                         | $\sum_{\alpha_i} \alpha_i p(y_i | f_i)$ | $[\ln \alpha_1, \ln \alpha_2, ..]$ |
4.4 Usage of Implemented Likelihood Functions

Some code examples taken from doc/usageLik.m illustrate how to use simple and composite likelihood functions to specify a GP model.

Syntactically, a likelihood function \(lf\) is defined by

\[
lf := 'func' | @func // simple
\]

\[
lf := \{lf\} | \{param, lf\} | \{lf, \{lf, ..., lf\}\} // composite
\]

i.e., it is either a string containing the name of a likelihood function, a pointer to a likelihood function or one of the former in combination with a cell array of likelihood functions and an additional list of parameters.

```
1 % demonstrate usage of likelihood functions
2 %
3 % See also likFunctions.m.
4 %
5 ⟨gpml copyright⟩
6 clear all, close all
7 n = 5; f = randn(n,1); % create random latent function values
8
9 % set up simple classification likelihood functions
10 yc = sign(f);
11 lc0 = {'likErf'}; hypc0 = []; % no hyperparameters are needed
12 lc1 = @likLogistic; hypc1 = []; % also function handles are OK
13 lc2 = {'likUni'}; hypc2 = [];
14 lc3 = {'likMix', {'likUni', @likErf}}; hypc3 = log([1;2]); %mixture
15
16 % set up simple regression likelihood functions
17 yr = f + randn(n,1)/20;
18 sn = 0.1; % noise standard deviation
19 lr0 = {'likGauss'}; hypr0 = log(sn);
20 lr1 = {'likLaplace'}; hypr1 = log(sn);
21 lr2 = {'likSech2'}; hypr2 = log(sn);
22 nu = 4; % number of degrees of freedom
23 lr3 = {'likT'}; hypr3 = [log(nu-1); log(sn)];
24 lr4 = {'likMix',{lr0,lr1}}; hypr4 = [log([1,2]);hypr0;hypr1];
25
26 a = 1; % set up warped Gaussian with \(g(y) = y + a*sign(y).*y.^2\)
27 lr5 = {'likGaussWarp','[poly2]'}; hypr5 = log([a;sn]);
28 lr6 = {'likGumbel','+'}; hypr6 = log(sn);
29
30 % set up Poisson regression
31 yp = fix(abs(f)) + 1;
32 lp0 = @likPoisson,'logistic'; hypp0 = [];
33 lp1 = @likPoisson,'logistic2',0.1}; hypp1 = [];
34 lp2 = @likPoisson,'exp'}; hypp2 = [];
35
36 % set up other GLM likelihoods for positive or interval regression
37 lg1 = @likGamma,'logistic'}; al = 2; hyp.lik = log(al);
38 lg2 = @likInvGauss,'exp'}; lam = 1.1; hyp.lik = log(lam);
39 lg3 = @likBeta,'expexp'}; phi = 2.1; hyp.lik = log(phi);
40 lg4 = @likBeta,'logit'}; phi = 4.7; hyp.lik = log(phi);
41 lg5 = @likWeibull,'logistic2',0.01}}; ka = 0.5; hyp.lik = log(ka);
42
43 % 0) specify the likelihood function
44 lik = lc0; hyp = hypc0; y = yc;
```
% lik = lr4; hyp = hypr4; y = yr;
% lik = lp1; hyp = hypp1; y = yp;
% 1) query the number of parameters
feval(lik{:})
% 2) evaluate the likelihood function on f
exp(feval(lik{:},hyp,y,f))
% 3a) evaluate derivatives of the likelihood
[lp,dlp,d2lp,d3lp] = feval(lik{:}, hyp, y, f, [], 'infLaplace');
% 3b) compute Gaussian integrals w.r.t. likelihood
mu = f; s2 = rand(n,1);
[lZ,dlZ,d2lZ] = feval(lik{:}, hyp, y, mu, s2, 'infEP');
% 3c) obtain lower bound on likelihood
ga = rand(n,1);
[b,z] = feval(lik{:}, hyp, y, [], ga, 'infVB');

4.5 Compatibility Between Likelihoods and Inference Methods

The following table lists all possible combinations of likelihood function and inference methods.

<table>
<thead>
<tr>
<th>Likelihood \ Inference</th>
<th>Gaussian Likelihood</th>
<th>Laplace</th>
<th>VB</th>
<th>EP</th>
<th>KL</th>
<th>MCMC</th>
<th>LOO</th>
<th>Type, Output Domain</th>
<th>Alternative Names</th>
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</table>

(✓)* EP might not converge in some cases since quadrature is used.

Exact inference is only tractable for Gaussian likelihoods. Expectation propagation together with Student’s t likelihood is inherently unstable due to non-log-concavity. Laplace’s approximation for Laplace likelihoods is not sensible because at the mode the curvature and the gradient is undefined due to the non-differentiable peak of the Laplace distribution. Special care has been taken for the non-convex optimisation problem imposed by the combination Student’s t likelihood and Laplace’s approximation.

4.6 Gaussian Likelihood

The Gaussian likelihood is the simplest likelihood because the posterior distribution is not only Gaussian but can be computed analytically. In principle, the Gaussian likelihood would only be operated in conjunction with the exact inference method but we chose to provide compatibility with
all other inference algorithms as well because it enables code testing and allows to switch between different regression likelihoods very easily.

\[ lik/likGauss.m \]

\begin{verbatim}
1 function [varargout] = likGauss(hyp, y, mu, s2, inf, i)
2 % likGauss - Gaussian likelihood function for regression. The expression for the
3 % likelihood is
4 % likGauss(t) = exp(-(t-y)^2/2*sn^2) / sqrt(2*pi*sn^2),
5 % where y is the mean and sn is the standard deviation.
6 %
7 % The hyperparameters are:
8 %
9 % hyp = [ log(sn) ]
10 %
11 % Several modes are provided, for computing likelihoods, derivatives and moments
12 % respectively, see likFunctions.m for the details. In general, care is taken
13 % to avoid numerical issues when the arguments are extreme.
14 %
15 % gpml copyright
16 % See also LIKFUNCTIONS.M.
17 %
18 if nargin<3, varargout = {'1'}; return; end % report number of hyperparameters
19 sn2 = exp(2*hyp);
20 if nargin<5 % prediction mode if inf is not present
21     % prediction mode if inf is not present
22 else
23     switch inf
24         case 'infLaplace'
25             % Laplace's method with Gaussian likelihood
26         case 'infEP'
27             % EP inference with Gaussian likelihood
28         case 'infVB'
29             % Variational Bayes inference with Gaussian likelihood
30     end
31 end
32
if isempty(y), y = zeros(size(mu)); end
s2zero = 1; if nargin>3&&numel(s2)>0&&norm(s2)>eps, s2zero = 0; end % s2==0 ?
lp = -(y-mu).^2./sn2/2-log(2*pi*sn2)/2; s2 = 0;
else
lp = likGauss(hyp, y, mu, s2, 'infEP'); % prediction
end
ymu = {}; ys2 = {};
if nargout>1
ymu = mu; % first y moment
if nargout>2
ys2 = s2 + sn2; % second y moment
end
end
varargout = {lp,ymu,ys2};
\end{verbatim}

The Gaussian likelihood function has a single hyperparameter $\rho$, the log of the noise standard deviation $\sigma_n$. 

\[ likGauss(t) = \exp\left(-\frac{(t-y)^2}{2\sigma_n^2}\right) / \sqrt{2\pi\sigma_n^2}, \]
4.6.1 Exact Inference

Exact inference doesn’t require any specific likelihood related code; all computations are done directly by the inference method, section 3.1.

4.6.2 Laplace's Approximation

\[
\text{Laplace's method with Gaussian likelihood} \quad 24a \equiv 23a \\
\text{if nargin<6} \quad \% \text{no derivative mode} \\
\text{if isempty(y), y=0; end} \\
ymmu = y-mu; dlp = {}; d2lp = {}; d3lp = {}; \\
lp = -ymmu.^2/(2*sn2) - \log(2*pi*sn2)/2; \\
\text{if nargout>1} \\
dlpmu = ymmu/sn2; \quad \% \text{dlp, derivative of log likelihood} \\
\text{if nargout>2} \quad \% \text{d2lp, 2nd derivative of log likelihood} \\
d2lp = -ones(size(ymmu))/sn2; \\
\text{if nargout>3} \quad \% \text{d3lp, 3rd derivative of log likelihood} \\
d3lp = zeros(size(ymmu)); \\
end \\
end \\
\text{varargout} = \{lp,dlp,d2lp,d3lp\}; \\
\text{else} \quad \% \text{derivative mode} \\
lp_dhyp = (y-mu).^2/sn2 - 1; \quad \% \text{derivative of log likelihood w.r.t. hypers} \\
dlp_dhyp = 2*(mu-y)/sn2; \quad \% \text{first derivative,} \\
d2lp_dhyp = 2*ones(size(mu))/sn2; \quad \% \text{and also of the second mu derivative} \\
\text{varargout} = \{lp_dhyp,dlp_dhyp,d2lp_dhyp\}; \\
end
\]

4.6.3 Expectation Propagation

\[
\text{EP inference with Gaussian likelihood} \quad 24b \equiv 23a \\
\text{if nargin<6} \quad \% \text{no derivative mode} \\
lZ = -(y-mu).^2./(sn2+s2)/2 - \log(2*pi*(sn2+s2))/2; \quad \% \text{log part function} \\
dlZ = {}; d2lZ = {}; \\
\text{if nargout>1} \\
dlZ = (y-mu)./(sn2+s2); \quad \% \text{1st derivative w.r.t. mean} \\
\text{if nargout>2} \\
d2lZ = -1./(sn2+s2); \quad \% \text{2nd derivative w.r.t. mean} \\
end \\
end \\
\text{varargout} = \{lZ,dlZ,d2lZ\}; \\
\text{else} \quad \% \text{derivative mode} \\
dlZhyp = ((y-mu).^2./(sn2+s2)-1) ./ (1+s2./sn2); \quad \% \text{deriv. w.r.t. hyp.lik} \\
\text{varargout} = \{dlZhyp\}; \\
end
\]

4.6.4 Variational Bayes

\[
\text{Variational Bayes inference with Gaussian likelihood} \quad 24c \equiv 23a \\
\% \text{variational lower site bound} \\
t(s) = \exp(-(y-s)^2/2sn2)/sqrt(2*pi*sn2) \\
\% \text{the bound has the form: (b+z/ga)*f - f.^2/(2*ga) - h(ga)/2} \\
n = numel(s2); b = zeros(n,1); y = y.*ones(n,1); z = y; \\
\text{varargout} = \{b,z\}; \\
\]
4.7 Warped Gaussian Likelihood

Starting from the likelihood \( p(y|f) \) we are sometimes facing the situation where the data \( y \in Y \subseteq \mathbb{R} \) is not distributed according to \( p(y|f) \) but some nonlinear transformation of the data \( g(y) = z \) so that \( z \sim p(z|f) \). Here, the warping function \( g : Y \rightarrow \mathbb{R} \) needs to be strictly monotonically increasing i.e. \( g'(y) > 0 \). Formally, we start from the fact that \( p(z|f) \) integrates to one and use the derivative \( dz = g'(y)dy \) to substitute

\[
\int p(z|f)dz = 1 = \int p_g(y|f)dy, \quad p_g(y|f) = p(g(y)|f)g'(y)
\]

where we have defined the log warped likelihood \( \ln p_g(y|f) = \ln p(g(y)|f) + \ln g'(y) \). The interesting bit is that approximate inference methods such as infExact, infLaplace, infEP, infVB, infKL remain fully feasible; only prediction and derivatives become more involved. The usual GP inference is \( \text{i.e.} \quad g = \text{likGauss} \), the predictive distribution is – for Gaussian likelihood – given by

\[
\text{Predictive moments}
\]

Hyperparameter derivatives for infLaplace are obtained as follows

\[
\frac{\partial}{\partial \theta} \ln \frac{\partial}{\partial f^k} p_g(y|f) = \frac{\partial}{\partial \theta} \ln \frac{\partial}{\partial f^k} p(g(y)|f) + \frac{\partial}{\partial \theta} \frac{\partial}{\partial f^k} \ln g'(y), \quad k = 0, 1, 2
\]

\[
= -\frac{\partial}{\partial f^k} \ln p(g(y)|f) \frac{\partial}{\partial \theta} g(y) + \frac{\partial}{\partial \theta} \frac{\partial}{\partial f^k} \ln g'(y).
\]

Similarly for infEP the derivatives are given by

\[
\frac{\partial}{\partial \theta} \ln \int p_g(y|f)N(f|\mu, \sigma^2)df = \frac{\partial}{\partial \theta} \ln \int p(g(y)|f)N(f|\mu, \sigma^2)df + \frac{\partial}{\partial \theta} \ln g'(y)
\]

\[
= -\frac{\partial}{\partial \mu} \ln \int p(g(y)|f)N(f|\mu, \sigma^2)df \frac{\partial}{\partial \theta} g(y) + \frac{\partial}{\partial \theta} \ln g'(y).
\]

This trick above works for any homoscedastic likelihood where \( p(y|f) = p(y + \beta|f + \beta) \) such as likGauss, likLaplace, likSech2 and likT.

Predictive moments

As detailed in [4] the predictive distribution is – for Gaussian likelihood – given by

\[
p(z_*|D, x_*) = \int p(z_*|f_*)p(f_*|D, x_*)df_* = \int N(z_*|f_*, \sigma_n^2)N(f_*|\mu_f, \sigma_f^2)df_*
\]

\[
= N(z_*|\mu_f, \sigma_n^2 + \sigma_f^2), \quad \text{where} \quad z_* = g(y_*)
\]

\[
p(y_*|D, x_*) = g'(y_*)N(g(y_*)|\mu_f, \sigma_n^2 + \sigma_f^2).
\]

Hence, the predictive moments are obtained by the 1d integrals

\[
\mu_{y_*} = \int y_* g'(y_*)N(g(y_*)|\mu_f, \sigma_n^2 + \sigma_f^2)dy_*
\]

\[
= \int g^{-1}(z_*)N(z_*|\mu_f, \sigma_n^2 + \sigma_f^2)dz_*, \quad \text{and}
\]

\[
\sigma_{y_*}^2 = \int (y_* - \mu_{y_*})^2 g'(y_*)N(g(y_*)|\mu_f, \sigma_n^2 + \sigma_f^2)dy_*
\]

\[
= \int (g^{-1}(z_*) - \mu_{y_*})^2 N(z_*|\mu_f, \sigma_n^2 + \sigma_f^2)dz_*.
\]
4.8 Gumbel Likelihood

Distributions of extrema are well captured by the Gumbel distribution

\[ p(y) = \frac{1}{\beta} \exp \left( -\frac{y - \eta}{\beta} \right), \quad z = s \frac{y - \eta}{\beta}, \quad s \in \{\pm 1\} \]

with mean \( \mu = \eta + \beta \gamma \) and variance \( \sigma^2 = \pi^2 \beta^2 / 6 \) where \( \gamma = 0.57721566490153 \) denotes Euler–Mascheroni’s constant. Skewness is approximately given by 1.1395 between left and right skewness and kurtosis is 12/5. The final expression for the Gumbel likelihood is

\[ p(y|f) = \frac{\pi}{\sigma \sqrt{6}} \exp \left( -\frac{y - \eta}{\sigma} \right), \quad z = \gamma + s \frac{\pi}{\sigma \sqrt{6}} (y - f), \quad s \in \{\pm 1\}. \]

4.9 Laplace Likelihood

Laplace’s Approximation

The following derivatives are needed:

\[
\frac{\partial \ln p(y|f)}{\partial f} = -\ln(2b) - \frac{|f - y|}{b},
\]

\[
\frac{\partial^2 \ln p(y|f)}{\partial f^2} = \text{sign}(f - y),
\]

\[
\frac{\partial^3 \ln p(y|f)}{\partial (\partial f)^2} = \frac{\partial^3 \ln p}{\partial (\partial f)^3} = \frac{\partial^3 \ln p}{\partial (\partial \sigma)^2} = 0,
\]

\[
\frac{\partial \ln p(y|f)}{\partial \ln \sigma_n} = \frac{|f - y|}{b} - 1.
\]

Expectation Propagation

Expectation propagation requires integration against a Gaussian measure for moment matching.

We need to evaluate \( \ln Z = \ln \int \mathcal{L}(y|f, \sigma_n^2) \mathcal{N}(f|\mu, \sigma^2) \, df \) as well as the derivatives \( \frac{\partial \ln Z}{\partial \mu} \) and \( \frac{\partial^2 \ln Z}{\partial \mu^2} \) where \( \mathcal{N}(f|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma^2} \exp \left( -\frac{(f - \mu)^2}{2\sigma^2} \right), \quad \mathcal{L}(y|f, \sigma_n^2) = \frac{1}{\sqrt{2\pi} \sigma_n^2} \exp \left( -\frac{(y - \eta)^2}{2\sigma^2} \right), \) and \( b = \frac{\sigma_n}{\sqrt{2}}. \) As a first step, we reduce the number of parameters by means of the substitution \( \hat{f} = \frac{f - \mu}{\sigma_n} \) yielding

\[
Z = \int \mathcal{L}(y|f, \sigma_n^2) \mathcal{N}(f|\mu, \sigma^2) \, df
\]

\[
= \frac{1}{\sqrt{2\pi}\sigma^2} \frac{\sqrt{2}}{2\sigma\sqrt{2\pi}} \int \exp \left( -\frac{(f - \mu)^2}{2\sigma^2} \right) \exp \left( -\sqrt{2} \frac{|y - \eta|}{\sigma_n} \right) \, df
\]

\[
= \frac{\sqrt{2}}{2\sigma\sqrt{2\pi}} \int \exp \left( -\frac{(\sigma_n \hat{f} + y - \mu)^2}{2\sigma^2} \right) \exp \left( -\sqrt{2} |\hat{f}| \right) \, d\hat{f}
\]

\[
= \frac{\sigma_n}{\sigma \sigma_n \sqrt{2\pi}} \int \exp \left( -\frac{\sigma_n^2 (\hat{f} - \mu)^2}{2\sigma^2} \right) \mathcal{L}(\hat{f}|0, 1) \, d\hat{f}
\]

\[
\ln Z = \ln \hat{Z} - \ln \sigma_n = \ln \int \mathcal{L}(f|0, 1) \mathcal{N}(f|\mu, \sigma^2) \, df - \ln \sigma_n
\]
with $\bar{\mu} = \frac{\mu - y}{\sigma_n}$ and $\bar{\sigma} = \frac{\sigma}{\sigma_n}$. Thus, we concentrate on the simpler quantity $\ln \tilde{Z}$.

\[
\ln Z = \ln \left[ \exp \left( -\frac{(f - \bar{\mu})^2}{2\bar{\sigma}^2} - \sqrt{2}f \right) \right] + C
\]

\[
\ln Z = \ln \left[ \exp \left( -\frac{(f - \bar{\mu})^2}{2\bar{\sigma}^2} + \sqrt{2}f \right) \right] + \int_0^\infty \exp \left( -\frac{(f - \bar{\mu})^2}{2\bar{\sigma}^2} - \sqrt{2}f \right) df + C
\]

Here, $\Phi(z) = \int_{-\infty}^z N(f|0, 1)\, df$ denotes the cumulative Gaussian distribution. Finally, we have

\[
\ln Z = \ln \left[ \exp \left( -\sqrt{2}\bar{\mu} \right) \Phi \left( \frac{m_+}{\bar{\sigma}} \right) - \exp \left( \frac{m_+^2}{2\bar{\sigma}} \right) \Phi \left( \frac{m_-}{\bar{\sigma}} \right) + \exp \left( \frac{m_-^2}{2\bar{\sigma}} \right) \right]
\]

where \( z_+ = \frac{\bar{\mu}}{\bar{\sigma}} + \sqrt{2} = \frac{\mu - y}{\sigma_n} + \sqrt{2}, z_- = \frac{\bar{\mu}}{\bar{\sigma}} - \sqrt{2} = \frac{\mu - y}{\sigma_n} - \sqrt{2} \) and $\bar{\mu} = \frac{\mu - y}{\sigma_n}, \bar{\sigma} = \frac{\sigma}{\sigma_n}$.

Now, using $\frac{d}{d\bar{\theta}} \ln \Phi(z) = \frac{1}{\Phi(z)} \frac{d}{d\bar{\theta}} \Phi(z) = \frac{N(z)}{\Phi(z)} \frac{dz}{d\bar{\theta}}$ we tackle first derivative

\[
\frac{\partial}{\partial \bar{\mu}} \ln Z = \frac{e^{a_+} \frac{\partial}{\partial \bar{\mu}} a_+ + e^{a_-} \frac{\partial}{\partial \bar{\mu}} a_-}{e^{a_+} + e^{a_-}}
\]

\[
\frac{\partial a_+}{\partial \bar{\mu}} = \frac{\partial}{\partial \bar{\mu}} \ln \Phi(-z_+) + \sqrt{2} \frac{\sigma}{\sigma_n}
\]

\[
= - \frac{N(-z_+)}{\sigma \Phi(-z_+)} + \sqrt{2} \frac{\sigma}{\sigma_n} = - \frac{q_+}{\sigma} + \sqrt{2} \frac{\sigma}{\sigma_n}
\]

\[
\frac{\partial a_-}{\partial \bar{\mu}} = \frac{\partial}{\partial \bar{\mu}} \ln \Phi(z_-) - \sqrt{2} \frac{\sigma}{\sigma_n}
\]

\[
= \frac{N(z_-)}{\sigma \Phi(z_-)} - \sqrt{2} \frac{\sigma}{\sigma_n} = \frac{q_-}{\sigma} - \sqrt{2} \frac{\sigma}{\sigma_n}
\]

\[
\frac{\partial a_\pm}{\partial \bar{\mu}} = \pm \frac{q_\pm}{\sigma} \pm \sqrt{2} \frac{\sigma}{\sigma_n}
\]

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as well as the second derivative

\[ \frac{\partial^2 \ln Z}{\partial \mu^2} = \frac{\partial}{\partial \mu} \left( \frac{e^{a_+} \partial a_+}{\partial \mu} + \frac{\partial a_-}{\partial \mu} \right) - \left( \frac{\partial \ln Z}{\partial \mu} \right)^2 \]

\[ \frac{\partial}{\partial \mu} \left( e^{a_+} \frac{\partial a_+}{\partial \mu} \right) = e^{a_+} \left( \frac{\partial a_+}{\partial \mu} \right)^2 + \frac{\partial^2 a_+}{\partial \mu^2} \]

\[ \frac{\partial^2 a_+}{\partial \mu^2} = -\frac{1}{\sigma} \frac{\partial}{\partial \mu} \frac{N(-z_+)}{\Phi^2(-z_+)} \]

\[ = -\frac{1}{\sigma} \frac{N(-z_+)}{\Phi^2(-z_+)} \frac{\partial^2 z_+}{\partial \mu^2} \]

\[ = -\frac{1}{\sigma^2} \frac{N(-z_+)}{\Phi^2(-z_+)} \frac{\partial^2 z_+}{\partial \mu^2} - N(-z_+) \frac{\partial -z_+}{\partial \mu} \]

\[ \frac{\partial^2 a_-}{\partial \mu^2} = \frac{1}{\sigma} \frac{\partial}{\partial \mu} \frac{N(z_-)}{\Phi^2(z_-)} \]

\[ = \frac{1}{\sigma} \frac{N(z_-)}{\Phi^2(z_-)} \frac{\partial^2 z_-}{\partial \mu^2} \]

\[ = \frac{1}{\sigma} \frac{N(z_-)}{\Phi^2(z_-)} - \frac{\partial^2 z_-}{\partial \mu^2} \]

\[ \frac{\partial^2 a_\pm}{\partial \mu^2} = -\frac{q^2_\pm + q_\pm z_\pm}{\sigma^2} \]

which can be simplified to

\[ \frac{\partial^2 \ln Z}{\partial \mu^2} = \frac{e^{a_+} b_+ + e^{a_-} b_-}{e^{a_+} + e^{a_-}} - \left( \frac{\partial \ln Z}{\partial \mu} \right)^2 \]

using

\[ b_\pm = \left( \frac{\partial a_\pm}{\partial \mu} \right)^2 + \frac{\partial^2 a_\pm}{\partial \mu^2} = \left( \frac{q_\pm}{\sigma} \pm \frac{\sqrt{2}}{\sigma_n} \right)^2 - \frac{q^2_\pm + q_\pm z_\pm}{\sigma^2} \]

\[ = \left( \frac{q_\pm}{\sigma} - \frac{\sqrt{2}}{\sigma_n} \right)^2 - \frac{2 \sigma_n}{\sigma^2} - \left( \frac{z_\pm}{\sigma_n} \pm \frac{\sqrt{2}}{\sigma^2} \right) q_\pm. \]

We also need

\[ \frac{\partial \ln Z}{\partial \ln \sigma_n} = \frac{e^{a_+} \frac{\partial a_+}{\partial \ln \sigma_n} + e^{a_-} \frac{\partial a_-}{\partial \ln \sigma_n}}{e^{a_+} + e^{a_-}} - \frac{2 \sigma_n^2}{\sigma^2_n} - 1. \]

**Variational Bayes**

We need \( h(\gamma) \) and its derivatives as well as \( \beta(\gamma) \):
\[ h(\gamma) = \frac{2}{\sigma_n^2} \gamma + \ln(2\sigma_n^2) + y^2\gamma^{-1} \]
\[ h'(\gamma) = \frac{2}{\sigma_n^2} - y^2\gamma^{-2} \]
\[ h''(\gamma) = 2y^2\gamma^{-3} \]
\[ \beta(\gamma) = y\gamma^{-1} \]

### 4.10 Student’s t Likelihood

The likelihood has two hyperparameters (both represented in the log domain to ensure positivity): the degrees of freedom \( \nu \) and the scale \( \sigma_n \) with mean \( y \) (for \( \nu > 1 \)) and variance \( \frac{\nu}{\nu - 2} \sigma_n^2 \) (for \( \nu > 2 \)).

\[
p(y|f) = Z \cdot \left( 1 + \frac{(f - y)^2}{\nu \sigma_n^2} \right)^{-\frac{\nu+1}{2}}, \quad Z = \frac{\Gamma \left( \frac{\nu+1}{2} \right)}{\Gamma \left( \frac{\nu}{2} \right) \sqrt{\nu \pi \sigma_n^2}}
\]

### Laplace’s Approximation

For the mode fitting procedure, we need derivatives up to third order; the hyperparameter derivatives at the mode require some mixed derivatives. All in all, using \( r = y - f \), we have

\[
\ln p(y|f) = \ln \Gamma \left( \frac{\nu+1}{2} \right) - \ln \Gamma \left( \frac{\nu}{2} \right) - \frac{1}{2} \ln \nu \pi \sigma_n^2 - \frac{\nu + 1}{2} \ln \left( 1 + \frac{r^2}{\nu \sigma_n^2} \right)
\]

\[
\frac{\partial \ln p}{\partial f} = (\nu + 1) \frac{r}{r^2 + \nu \sigma_n^2}
\]

\[
\frac{\partial^2 \ln p}{(\partial f)^2} = (\nu + 1) \frac{r^2 - \nu \sigma_n^2}{(r^2 + \nu \sigma_n^2)^2}
\]

\[
\frac{\partial^3 \ln p}{(\partial f)^3} = 2(\nu + 1) \frac{r^3 - 3r \nu \sigma_n^2}{(r^2 + \nu \sigma_n^2)^3}
\]

\[
\frac{\partial \ln p}{\partial \ln \nu} = \frac{\partial Z}{\partial \ln \nu} - \frac{\nu}{2} \ln \left( 1 + \frac{r^2}{\nu \sigma_n^2} \right) + \frac{\nu + 1}{2} \cdot \frac{r^2}{r^2 + \nu \sigma_n^2}
\]

\[
\frac{\partial Z}{\partial \ln \nu} = \nu \frac{d \ln \Gamma \left( \frac{\nu+1}{2} \right)}{d \ln \nu} - \nu \frac{d \ln \Gamma \left( \frac{\nu}{2} \right)}{d \ln \nu} - \frac{1}{2}
\]

\[
\frac{\partial^3 \ln p}{(\partial \ln \nu)(\partial f)^2} = \nu \frac{r^2 (r^2 - 3(\nu + 1) \sigma_n^2) + \nu \sigma_n^2}{(r^2 + \nu \sigma_n^2)^3}
\]

\[
\frac{\partial \ln p}{\partial \ln \sigma_n} = (\nu + 1) \frac{r^2}{r^2 + \nu \sigma_n^2} - 1
\]

\[
\frac{\partial^3 \ln p}{(\partial \ln \sigma_n)(\partial f)^2} = 2 \nu \sigma_n^2 (\nu + 1) \frac{\nu \sigma_n^2 - 3r^2}{(r^2 + \nu \sigma_n^2)^3}
\]

### 4.11 Cumulative Logistic Likelihood

The likelihood has one hyperparameter (represented in the log domain), namely the standard deviation \( \sigma_n \)

\[
p(y|f) = Z \cdot \cosh^{-2} (\tau (f - y)) \text{, } \tau = \frac{\pi}{2 \sigma_n \sqrt{3}}, \quad Z = \frac{\pi}{4 \sigma_n \sqrt{3}}
\]
Laplace’s Approximation

The following derivatives are needed where \( \phi(x) \equiv \ln(\cosh(x)) \)

\[
\frac{\ln p(y|f)}{\partial f} = \ln(\tau) - \ln(4\sigma_n \sqrt{3}) - 2\phi(\tau(f-y))
\]

\[
\frac{\partial \ln p}{\partial f} = 2\tau\phi'(\tau(f-y))
\]

\[
\frac{\partial^2 \ln p}{(\partial f)^2} = -2\tau^2\phi''(\tau(f-y))
\]

\[
\frac{\partial^3 \ln p}{(\partial f)^3} = 2\tau^3\phi'''(\tau(f-y))
\]

\[
\frac{\partial^3 \ln p}{(\partial \ln \sigma_n)(\partial f)^2} = 2\tau^2 \left( 2\phi''(\tau(f-y)) + \tau(f-y)\phi'''(\tau(f-y)) \right)
\]

\[
\frac{\partial \ln p}{\partial \ln \sigma_n} = 2\tau(\gamma(y-f)/\mu - \phi'((f-y))/\mu) - 1
\]

4.12 GLM Likelihoods: Poisson, Weibull, Gamma, Exponential, Inverse Gaussian and Beta

Data \( y \) from a space other than \( \mathbb{R} \) e.g. \( \mathbb{N}, \mathbb{R}_+ \) or \([0,1]\) can be modeled using generalised linear model likelihoods \( p(y|f) \) where the expected value \( E[y] = \mu \) is related to the underlying Gaussian process \( f \) by means of an inverse link function \( \mu = g(f) \). Typically, the likelihoods are from an exponential family, hence the variance \( V[y] = v(\mu) \), is a simple function of the mean \( \mu \) as well as higher order moments such as skewness \( S[y] = s(\mu) \) and kurtosis \( K[y] = k(\mu) \).

Here, we directly specify the inverse link function \( \mu = g(f) \) defining the mapping from the GP \( f \) to the mean intensity \( \mu \). For numerical reasons, we work with the log of the inverse link function \( h(f) = \ln g(f) \) and use its derivatives \( h' \), \( h'' \) and \( h''' \) for subsequent computations. In the table below, we have summarised the GLM likelihood expressions, the moments, the range of their variables and the applicable inverse link functions.

### 4.12.1 Inverse Link Functions

Possible inverse link functions and their properties (\( \cup \) convex, \( \cap \) concave, \( \uparrow \) monotone) are summarised below:

<table>
<thead>
<tr>
<th>Likelihood</th>
<th>( \mu = )</th>
<th>( g : \mathbb{R} \rightarrow )</th>
<th>( g ) is</th>
<th>( h(f) = \ln \mu = )</th>
<th>( h ) is</th>
</tr>
</thead>
<tbody>
<tr>
<td>exp</td>
<td>( e^f )</td>
<td>( \mathbb{R}_+ )</td>
<td>( \cup, \uparrow )</td>
<td>( f )</td>
<td>( \cup, \cap, \uparrow )</td>
</tr>
<tr>
<td>logistic</td>
<td>( \ell(f) = \ln(1 + e^f) )</td>
<td>( \mathbb{R}_+ )</td>
<td>( \cup, \uparrow )</td>
<td>( \ln(\ln(1 + e^f)) )</td>
<td>( \cap, \uparrow )</td>
</tr>
<tr>
<td>logistic2</td>
<td>( \ell(f + \alpha f) )</td>
<td>( \mathbb{R}_+ )</td>
<td>( \uparrow )</td>
<td>( \ln(\ell(f + \alpha f)) )</td>
<td>( \cap, \uparrow )</td>
</tr>
<tr>
<td>expexp</td>
<td>( \exp(-e^{-f}) )</td>
<td>([0,1])</td>
<td>( \uparrow )</td>
<td>( -e^{-f} )</td>
<td>( \cup, \uparrow )</td>
</tr>
<tr>
<td>logit</td>
<td>( 1/(1 + e^{-f}) )</td>
<td>([0,1])</td>
<td>( \uparrow )</td>
<td>( -\ln(1 + e^{-f}) )</td>
<td>( \cup, \uparrow )</td>
</tr>
</tbody>
</table>
Please see doc/usageLik.m for how to specify the pair likelihood function and link function in GPML.

**Exponential inverse link:** $\exp$

For $g(f) = e^f$ things are simple since $h(f) = f$, $h'(f) = 1$ and $h''(f) = h'''(f) = 0$.

**Logistic inverse link:** $\logistic$

For $g(f) = \ln(1 + e^f)$ the derivatives of $h(f)$ are given by

\[
\begin{align*}
    h(f) &= \ln(\ln(1 + e^f)) \\
    h'(f) &= \frac{1}{\ln(1 + e^f)} s(-f), \quad s(f) = \frac{1}{1 + e^f}, \quad s'(f) = \frac{-e^f}{(1 + e^f)^2} = -s(-f)s(f) \\
    h''(f) &= \frac{1}{\ln(1 + e^f)} \frac{e^{-f}}{(1 + e^{-f})^2} - \frac{1}{\ln^2(1 + e^f)} \frac{e^f}{1 + e^f} \frac{1}{1 + e^{-f}} \\
    &= h'(f) [s(f) - h'(f)] \\
    h'''(f) &= h''(f) [s(f) - h'(f)] + h'(f) \left[ \frac{-e^f}{(1 + e^f)^2} - h''(f) \right] \\
    &= h''(f) [s(f) - 2h'(f)] - h'(f) s(f)s(-f).
\end{align*}
\]

Note that $g(f) = e^{h(f)} = \ln(1 + e^f)$ is convex and $h(f) = \ln(\ln(1 + e^f))$ with

\[
h''(f) = \frac{1}{\ln(1 + e^f)} \left( 1 - \frac{e^f}{\ln(1 + e^f)} \right) \frac{1}{1 + e^f} \frac{1}{1 + e^{-f}} < 0
\]

is concave since $e^f \geq \ln(1 + e^f)$ for all $f \in \mathbb{R}$.

**Twice logistic inverse link:** $\logistic^2$

Note that $h(f) = \ln(\ell(f + af\ell(f)))$ is – according to Seeger et al.\[^7\] – concave.

**Double negative exponential inverse link:** $\exp\exp$

For $g(f) = \exp(-e^{-f})$ the derivatives of $h(f)$ are given by

\[
\begin{align*}
    h(f) &= -e^{-f} \\
    h'(f) &= -h(f) \\
    h''(f) &= h(f) \\
    h'''(f) &= -h(f)
\end{align*}
\]

\[^7\text{Bayesian Intermittent Demand Forecasting, NIPS, 2016}\]
Logit regression inverse link: \texttt{logit}

For \( g(f) = 1/(1 + e^{-f}) \) the derivatives of \( h(f) \) can be computed using the logistic inverse link function \( h_\ell(f) \) since \( h(f) = f - \exp(h_\ell(f)) \)

\[
\begin{align*}
    h(f) &= f - e^{h_\ell(f)} \\
    h'(f) &= 1 - e^{h_\ell(f)} h'_\ell(f) \\
    h''(f) &= -e^{h_\ell(f)} [h'_\ell(f)^2 + h''_\ell(f)] = e^{h_\ell(f)} s_\ell(-f) s'_\ell(f) \\
    h'''(f) &= -e^{h_\ell(f)} [h'_\ell(f)^3 + 3h''_\ell(f) h'_\ell(f) + h'''_\ell(f)]
\end{align*}
\]

4.12.2 Poisson Likelihood

Count data \( y \in \mathbb{N} \) can be modeled in the GP framework using the Poisson distribution \( p(y) = \mu^y e^{-\mu}/y! \) with mean/variance \( \mathbb{E}[y] = \mathbb{V}[y] = \mu \), skewness \( s[y] = 1/\sqrt{\mu} \) and kurtosis \( k[y] = 1/\mu \) leading to the likelihood

\[
p(y|f) = \mu^y \exp(-\mu)/y!, \quad \mu = g(f)
\]

\( \Leftrightarrow \ln p(y|f) = y \cdot \ln g(f) - g(f) - \ln \Gamma(y + 1). \)

For Laplace’s method to work, we need the first three derivatives of the log likelihood \( \ln p(y|f) \), where \( h(f) = \ln g(f) \)

\[
\begin{align*}
    \ln p(y|f) &= y \cdot h(f) - \exp(h(f)) - \ln \Gamma(y + 1) \\
    \frac{\partial}{\partial f} \ln p(y|f) &= h'(f) [y - \exp(h(f))] \\
    \frac{\partial^2}{\partial f^2} \ln p(y|f) &= h''(f) [y - \exp(h(f))] - [h'(f)]^2 \exp(h(f)) \\
    \frac{\partial^3}{\partial f^3} \ln p(y|f) &= h'''(f) [y - \exp(h(f))] - 3h'(f) \cdot h''(f) \exp(h(f)) - [h'(f)]^3 \exp(h(f)) \\
    &+ h'''(f) [y - \exp(h(f))] - h'(f) [h'(f)^2 + 3h''(f)] \exp(h(f)).
\end{align*}
\]

Note that if \( \ln \mu = h(f) \) is concave and \( \mu = g(f) \) is convex then the Poisson likelihood \( p(y|f) \) is log-concave in \( f \) which is the case for both \exp and \texttt{logistic}.

4.12.3 Weibull Likelihood

Nonnegative data \( y \in \mathbb{R}_+ \) such as time-to-failure can be modeled in the GP framework using the Weibull distribution \( p(y) = \kappa/\lambda(y/\lambda)^{\kappa-1} e^{-(y/\lambda)^\kappa} \) with shape parameter \( \kappa > 0 \), scale parameter \( \lambda > 0 \), mean \( \mathbb{E}[y] = \lambda \gamma_1 = \mu \) where \( \gamma_j = \Gamma(1 + j/\kappa) \), variance \( \mathbb{V}[y] = \lambda^2 \gamma_2 - \mu^2 = \mu^2 (\gamma_2/\gamma_1^2 - 1) \), skewness \( s[y] = (\gamma_3 - 3\gamma_1 \gamma_2 + 2 \gamma_1^3)/(\gamma_2 - \gamma_1^2)^{3/2} \) and kurtosis \( k[y] = (\gamma_4 - 4\gamma_1\gamma_3 + 12 \gamma_1^2 \gamma_2 - 3\gamma_2^2 - 6 \gamma_1^4)/(\gamma_2 - \gamma_1^2)^2 \). Using the substitution \( \mu = \lambda \gamma_1 \Leftrightarrow 1/\lambda = \gamma_1/\mu \), we obtain

\[
p(y|f) = \gamma_1 \frac{\kappa}{\mu} \left( \gamma_1 \frac{y}{\mu} \right)^{\kappa-1} \exp \left( - \left( \gamma_1 \frac{y}{\mu} \right)^\kappa \right), \quad \mu = g(f) > 0
\]

\( \Leftrightarrow \ln p(y|f) = \ln \left( \gamma_1 \frac{\kappa}{\mu} \right) + (\kappa - 1) \ln \left( \gamma_1 \frac{y}{\mu} \right) - \left( \gamma_1 \frac{y}{\mu} \right)^\kappa. \)

Note that the Weibull likelihood \( p(y|f) \) is log-concave in \( f \) neither for the \exp nor for the \texttt{logistic} inverse link.
4.12.4 Gamma Likelihood

Nonnegative data \( y \in \mathbb{R}_+ \) can be modeled in the GP framework using the Gamma distribution 
\[
p(y) = y^{-\alpha} \Gamma(\alpha) e^{-y/\theta} \quad \text{with shape parameter } \alpha > 0, \text{ scale parameter } \theta > 0,
\]
mean \( \mathbb{E}[y] = \alpha \theta = \mu \), variance \( \mathbb{V}[y] = \alpha \theta^2 = \mu^2/\alpha \), skewness \( \mathbb{S}[y] = 2/\sqrt{\alpha} \) and kurtosis \( \mathbb{K}[y] = 6/\alpha \). Using the substitution \( \mu = \alpha \theta \), we obtain

\[
p(y|f) = \frac{\alpha \mu^{\alpha-1}}{\Gamma(\alpha)} \mu^{-\alpha} \exp\left(-\frac{y\mu}{\mu}\right), \quad \mu = g(f) > 0
\]

\[
\Leftrightarrow \ln p(y|f) = -\alpha \left(\ln \mu + \frac{y}{\mu}\right) - \ln Z_\alpha(y), \quad \ln Z_\alpha(y) = \ln \Gamma(\alpha) - \alpha \ln \alpha + (1 - \alpha) \ln y.
\]

Note that if \( \ln \mu = h(f) \) was convex and \( \mu = g(f) \) was concave then the Gamma likelihood \( p(y|f) \) would be log-concave in \( f \) which is not the case for both exp and logistic.

4.12.5 Exponential Likelihood

Nonnegative data \( y \in \mathbb{R}_+ \) can be modeled in the GP framework using the Exponential distribution 
\[
p(y) = e^{-y/\theta} \quad \text{with scale parameter } \theta > 0,
\]
mean \( \mathbb{E}[y] = \theta = \mu \), variance \( \mathbb{V}[y] = \mu^2 \), skewness \( \mathbb{S}[y] = 3 \sqrt{\mu/\lambda} \) and kurtosis \( \mathbb{K}[y] = 15 \mu/\lambda \). We obtain

\[
p(y|f) = \mu^{-1} \exp\left(-\frac{y}{\mu}\right), \quad \mu = g(f) > 0
\]

\[
\Leftrightarrow \ln p(y|f) = -\ln \mu - \frac{y}{\mu}.
\]

Note that for exp (but not for logistic) the likelihood is log-concave. The exponential distribution corresponds to the Gamma distribution with \( \alpha = 1 \) and the Weibull distribution with \( \kappa = 1 \).

4.12.6 Inverse Gaussian Likelihood

Nonnegative data \( y \in \mathbb{R}_+^n \) can be modeled in the GP framework using the Inverse Gaussian distribution 
\[
p(y) = \lambda/(2\pi y^3) \exp(-\lambda(y - \mu)^2/(2\mu^2 y)) \quad \text{with shape parameter } \lambda > 0, \text{ mean parameter } \mu > 0,
\]
mean \( \mathbb{E}[y] = \mu \), variance \( \mathbb{V}[y] = \mu^3/\lambda, \text{ skewness } \mathbb{S}[y] = 3 \sqrt{\mu/\lambda} \text{ and kurtosis } \mathbb{K}[y] = 15 \mu/\lambda. \) We obtain

\[
p(y|f) = \sqrt{\frac{\lambda}{2\pi y^3}} \exp\left(-\frac{\lambda(y - \mu)^2}{2\mu^2 y}\right), \quad \mu = g(f) > 0
\]

\[
\Leftrightarrow \ln p(y|f) = -\frac{\lambda(y - \mu)^2}{2\mu^2 y} - \ln Z_\alpha(y), \quad \ln Z_\alpha(y) = -\frac{1}{2} (\ln \lambda - \ln 2\pi y^3).
\]

The inverse Gaussian likelihood is in general not log-concave in \( f \) for both exp and logistic.

4.12.7 Beta Likelihood

Interval data \( y \in [0, 1]^n \) can be modeled in the GP framework using the Beta distribution 
\[
p(y) = y^{\alpha-1}(1-y)^{\beta-1}/B(\alpha, \beta) \quad \text{with shape parameters } \alpha, \beta > 0, \text{ mean } \mathbb{E}[y] = \alpha/(\alpha + \beta) \text{ and variance } \mathbb{V}[y] = \alpha \beta/([\alpha + \beta]^2(\alpha + \beta + 1)) \text{ and } 1/B(\alpha, \beta) = \Gamma(\alpha + \beta)/[\Gamma(\alpha)\Gamma(\beta)]. \) Reparametrising using
the mean parameter $\mu = \mathbb{E}[y] = \alpha/(\alpha + \beta)$, the shape parameter $\phi = \alpha + \beta$, the variance $\mathbb{V}[y] = \mu(1 - \mu)/(1 + \phi)$ and hence
\[
p(y|f) = \frac{\Gamma(\phi)}{\Gamma(\mu\phi)\Gamma((1 - \mu)\phi)} y^{\mu\phi - 1}(1 - y)^{(1 - \mu)\phi - 1}, \quad \mu = g(f) > 0
\]
\[
\Leftrightarrow \ln p(y|f) = \ln \Gamma(\phi) - \ln \Gamma(\mu\phi) - \ln \Gamma((1 - \mu)\phi) + (\mu\phi - 1) \ln y + ((1 - \mu)\phi - 1) \ln(1 - y).
\]

The Beta likelihood is in general not log-concave in $f$ for both exp and logistic.
5 Mean Functions

A mean function $m_\phi : X \to \mathbb{R}$ (with hyperparameters $\phi$) of a GP $f$ is a scalar function defined over the whole domain $X$ that computes the expected value $m(x) = \mathbb{E}[f(x)]$ of $f$ for the input $x$.

5.1 Interface

In the GPML toolbox, a mean function $m : X \to \mathbb{R}$ needs to implement evaluation $m = m_\phi(X)$ and first derivatives $m_i = \frac{\partial}{\partial \phi_i} m$ with respect to the components $i$ of the parameter $\phi \in \Phi$ as detailed below.

```matlab
35 〈meanFunctions.m35〉≡
1 % Mean functions to be use by Gaussian process functions. There are two
2 % different kinds of mean functions: simple and composite:
3 %
4 % Simple mean functions:
5 %
6 % meanZero - zero mean function
7 % meanOne - one mean function
8 % meanConst - constant mean function
9 % meanLinear - linear mean function
10 % meanPoly - polynomial mean function
11 % meanDiscrete - precomputed mean for discrete data
12 % meanGP - predictive mean of another GP
13 % meanGPexact - predictive mean of a regression GP
14 % meanNN - nearest neighbor mean function
15 % meanWSPC - weighted sum of projected cosines
16 %
17 % Composite mean functions (see explanation at the bottom):
18 %
19 % meanScale - scaled version of a mean function
20 % meanSum - sum of mean functions
21 % meanProd - product of mean functions
22 % meanPow - power of a mean function
23 % meanMask - mask some dimensions of the data
24 % meanPref - difference mean for preference learning
25 % meanWarp - warped mean function
26 %
27 % Naming convention: all mean functions are named "mean/mean*.m".
28 %
29 % 1) With no or only a single input argument:
30 %
31 % s = meanNAME or s = meanNAME(hyp)
32 %
33 % The mean function returns a string s telling how many hyperparameters hyp it
34 % expects, using the convention that "D" is the dimension of the input space.
35 % For example, calling "meanLinear" returns the string 'D'.
36 %
37 % 2) With two input arguments and one output argument:
38 %
39 % m = meanNAME(hyp, x)
40 %
41 % The function computes and returns the mean vector m with components
42 % $m(i) = m(x(i,:))$ where hyp are the hyperparameters and $x$ is an $n \times D$ matrix
43 % of data, where $D$ is the dimension of the input space. The returned mean
```
% vector m is of size n by 1.

% 3) With two input arguments and two output arguments:

[m, dm] = meanNAME(hyp, x)

The function computes and returns the mean vector m as in 2) above.

In addition to that, the (linear) directional derivative function dm is returned. The call dhyp = dm(q) for a direction vector q of size n by 1 returns a vector of directional derivatives dhyp = d (q'*m(x)) / d hyp of the same size as the hyperparameter vector hyp. The components of dhyp are defined as follows: dhyp(i) = q'*( d m(x) / d hyp(i) ).

See also doc/usageMean.m.

5.2 Implemented Mean Functions

We offer simple and composite mean functions producing new mean functions m(x) from existing mean functions µ_j(x). All code files are named according to the pattern mean/mean<NAME>.m for simple identification. This modular specification allows to define affine mean functions m(x) = c + a'x or polynomial mean functions m(x) = (c + a'x)^2. All currently available mean functions are summarised in the following table.

### Simple mean functions m(x)

<table>
<thead>
<tr>
<th>&lt;NAME&gt;</th>
<th>Meaning</th>
<th>m(x) =</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zero</td>
<td>mean vanishes always</td>
<td>0</td>
</tr>
<tr>
<td>Const</td>
<td>mean equals a constant</td>
<td>c</td>
</tr>
<tr>
<td>Linear</td>
<td>mean linearly depends on x ∈ X ⊆ R^D</td>
<td>a'x</td>
</tr>
<tr>
<td>Poly</td>
<td>mean polynomially depends on x ∈ X ⊆ R^D</td>
<td>\sum_d a_d x^d</td>
</tr>
<tr>
<td>Discrete</td>
<td>precomputed mean for discrete data x ∈ X ⊆ N</td>
<td>µ_x</td>
</tr>
<tr>
<td>GP</td>
<td>predictive mean of another GP</td>
<td>\int y · p(y</td>
</tr>
<tr>
<td>GPexact</td>
<td>predictive mean of a regression GP</td>
<td>\int y · p(y</td>
</tr>
<tr>
<td>NN</td>
<td>nearest neighbor for a set {(z_j, m_j) \in X \times R }</td>
<td>m_i, i = \arg\min_j d(x, z_j)</td>
</tr>
<tr>
<td>WSPC</td>
<td>weighted sum of d projected cosines x ∈ X ⊆ R^D</td>
<td>a' \cos(Wx + b)</td>
</tr>
</tbody>
</table>

### Composite mean functions \[\mu_1(x), \mu_2(x), .. \mapsto m(x)\]

<table>
<thead>
<tr>
<th>&lt;NAME&gt;</th>
<th>meaning</th>
<th>m(x) =</th>
</tr>
</thead>
<tbody>
<tr>
<td>Scale</td>
<td>scale a mean</td>
<td>a\mu(x)</td>
</tr>
<tr>
<td>Sum</td>
<td>add up mean functions</td>
<td>\sum_i \mu_i(x)</td>
</tr>
<tr>
<td>Prod</td>
<td>multiply mean functions</td>
<td>\prod_i \mu_i(x)</td>
</tr>
<tr>
<td>Pow</td>
<td>raise a mean to a power</td>
<td>\mu(x)^\alpha</td>
</tr>
<tr>
<td>Mask</td>
<td>act on components I ⊆ {1, 2, .., D} of x ∈ X ⊆ R^D only</td>
<td>\mu(x_I)</td>
</tr>
<tr>
<td>Pref</td>
<td>preference learning mean x = [x_1; x_2], x_i ∈ R^{D/2}</td>
<td>\mu(x_1) - \mu(x_2)</td>
</tr>
<tr>
<td>Warp</td>
<td>warped mean</td>
<td>q[\mu(x)]</td>
</tr>
</tbody>
</table>

5.3 Usage of Implemented Mean Functions

Some code examples taken from doc/usageMean.m illustrate how to use simple and composite mean functions to specify a GP model.

Syntactically, a mean function \texttt{mf} is defined by

\texttt{mn := 'func' | @func // simple}
mf := \{mn\} | \{mn, \{param, mf\}\} | \{mn, \{mf, .., mf\}\} // composite

i.e., it is either a string containing the name of a mean function, a pointer to a mean function or one of the former in combination with a cell array of mean functions and an additional list of parameters.

```matlab
function doc/usageMean.m[37]

% demonstrate usage of mean functions
% See also meanFunctions.m.
% gpml copyright
% clear all, close all
n = 5; D = 2; x = randn(n,D);

% set up simple mean functions
m0 = {'meanZero'}; hyp0 = [];
% no hyperparameters are needed
m1 = {'meanOne'}; hyp1 = [];
% no hyperparameters are needed
mc = @meanConst; hypc = 2;
% also function handles are possible
ml = @meanLinear; hypl = [2;3];
% m(x) = 2*x1 + 3*x2
mp = @meanPoly,2; hypp = [1;1;2;3];
% m(x) = x1+x2+2*x1^2+3*x2^2
mn = @meanNN,[1,0; 0,1],[0.9,0.5]; hypn = [];
% nearest neighbor
s = 12; hypd = randn(s,1);
md = {'meanDiscrete',s};

% GP predictive mean
xt = randn(2*n,D); yt = sign(xt(:,1)-xt(:,2));
% training data
mg = @meanGP,hyp,@infEP,@meanZero,@covSEiso,@likErf,xt,yt;
hype = [0;0; log(0.1)];
% regression GP predictive mean
xt = randn(2*n,D); yt = xt(:,1).*xt(:,2);
% training data
me = @meanGPexact,@meanZero,@covSEiso,xt,yt;

% set up composite mean functions
msc = {'meanScale',{m1}}; hypsc = [3; hyp1];
% scale by 3
msu = {'meanSum',{m0,mc,ml}}; hypsu = [hyp0; hypc; hypl];
% sum
mpr = @meanProd,{mc,ml}; hyppr = [hypc; hypl];
% product
mpo = {'meanPow',3,msu}; hyppo = hypsu;
% third power
mask = [false,true];
% mask excluding all but the 2nd component
mma = {'meanMask',mask,ml}; hypma = hypl(mask);
mpf = @meanPref,ml; hyppf = 2;
% linear pref with slope
mwp = @meanWarp,ml,@sin,@cos; hypwp = 2;
% sin of linear

% 0) specify mean function
mean = md; hyp = hypd; x = randi([1,s],n,1);
mean = mn; hyp = hypn;
mean = mg; hyp = hypg;
mean = me; hyp = hype;
mean = m0; hyp = hyp0;
mean = msu; hyp = hypc,
mean = mpr; hyp = hyppr;
mean = mp0; hyp = hypo;
mean = mpf; hyp = hyppf;

% 1) query the number of parameters
feval(mean{:})

% 2) evaluate the function on x
feval(mean{:},hyp,x)

% 3) compute the derivatives w.r.t. to hyperparameter i
i = 2; feval(mean{:},hyp,x,i)
```

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6 Covariance Functions

A covariance function $k_\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ (with hyperparameters $\psi$) of a GP $f$ is a scalar function defined over the whole domain $\mathcal{X}^2$ that computes the covariance $k(x, z) = \nabla[f(x), f(z)] = \mathbb{E}[(f(x) - m(x))(f(z) - m(z))]$ of $f$ between the inputs $x$ and $z$.

6.1 Interface

Again, the interface is simple since only evaluation of the full covariance matrix $K = k_\psi(X)$ and its derivatives $K_i = \frac{\partial}{\partial \psi_i} K$ as well as cross terms $k_\ast = k_\psi(X, x_\ast)$ and $k_{\ast\ast} = k_\psi(x_\ast, x_\ast)$ for prediction are required.

```matlab
% Covariance functions to be use by Gaussian process functions. There are two
different kinds of covariance functions: simple and composite:

1) Elementary and standalone covariance functions:
   covZero - zero covariance function
covEye - unit covariance function
covOne - unit constant covariance function
covDiscrete - precomputed covariance for discrete data

2) Composite covariance functions:
   covScale - scaled version of a covariance function
covSum - sums of covariance functions
covProd - products of covariance functions
covMask - mask some dimensions of the data
covPref - difference covariance for preference learning
covPER - make stationary covariance periodic
covADD - additive covariance function

3) Mahalanobis distance based covariances and their modes
   covMaha - generic "mother" covariance
covGE - Gamma exponential covariance
covMatern - Matern covariance function with nu=1/2, 3/2 or 5/2
covPP - piecewise polynomial covariance function (compact support)
covRQ - rational quadratic covariance function
covSE - squared exponential covariance function
   * eye - unit length scale
   * iso - isotropic length scale
   * ard - automatic relevance determination
   * pro - (low-rank) projection in input space
   * fac - factor analysis covariance
   * vle - spatially varying length scale

4) Dot product based covariances and their modes
   covDot - generic "mother" covariance
covLIN - linear covariance function
covPoly - polynomial covariance function
   * eye - unit length scale
   * iso - isotropic length scale
   * ard - automatic relevance determination

5) Standalone covariances
   covNNone - neural network covariance function
   covLINNone - linear covariance function with bias
```
%covPeriodic - smooth periodic covariance function (1d)
%covPeriodicNoDC - as above but with zero DC component and properly scaled
%covCos - sine periodic covariance function (1d) with unit period
%covGabor - Gabor covariance function

6) Shortcut covariances assembled from library
%covConst - covariance for constant functions
%covNoise - independent covariance function (i.e. white noise)
%covPERiso - make isotropic stationary covariance periodic
%covPERard - make ARD stationary covariance periodic
%covMaterniso - Matern covariance function with nu=1/2, 3/2 or 5/2
%covMaternard - Matern covariance function with nu=1/2, 3/2 or 5/2 with ARD
%covPPiso - piecewise polynomial covariance function (compact support)
%covPPard - piecewise polynomial covariance function (compact support)
%covRQiso - isotropic rational quadratic covariance function
%covRQard - rational quadratic covariance function with ARD
%covSEiso - isotropic squared exponential covariance function
%covSEisoU - same as above but without latent scale
%covSEard - squared exponential covariance function with ARD
%covSEvlen - spatially varying lengthscale squared exponential
%covSEproj - projection squared exponential covariance function
%covLINiso - linear covariance function
%covLINard - linear covariance function with ARD
%covGaborard - Gabor covariance function with ARD
%covSM - spectral mixture covariance function

7) Special purpose (approximation) covariance functions
%apxSparse - sparse approximation: to be used for large scale inference
%apxGrid - grid interpolation: to be used for large scale inference

The covariance functions are written according to a special convention where
the exact behaviour depends on the number of input and output arguments
passed to the function. If you want to add new covariance functions, you
should follow this convention if you want them to work with the function gp.
There are four different ways of calling the covariance functions:

1) With no (or one) input argument(s):

   s = cov

2) With two input arguments and one output argument:

   K = cov(hyp, x) equivalent to K = cov(hyp, x, [])

3) With three input arguments and one output argument:
\texttt{Kz} = \texttt{cov(hyp, x, z)}

\texttt{kx} = \texttt{cov(hyp, x, 'diag')}

The function computes test set covariances; \texttt{kx} is a vector of self covariances for the test cases in \texttt{x} (of length \texttt{n}) and \texttt{Kz} is an (\texttt{n} by \texttt{nz}) matrix of cross covariances between training cases \texttt{x} and test cases \texttt{z}.

4) With two output arguments:

\texttt{[K,dK] = cov(hyp, x)} equivalent to \texttt{[K,dK] = cov(hyp, x, [])}

\texttt{[K,dK] = cov(hyp, x, z)}

\texttt{[K,dK] = cov(hyp, x, 'diag')}  

The function computes and returns the covariances \texttt{K} as in 3) above. In addition to that, the (linear) directional derivative function \texttt{dK} is returned. The two possible calls \texttt{dhyp = dK(Q)} and \texttt{[dhyp,dx] = dK(Q)} for a direction \texttt{Q} of the same size as \texttt{K} are possible. The return arguments \texttt{dhyp} and \texttt{dx} are the directional derivatives \texttt{dhyp = d trace(Q'*K) / d hyp} and \texttt{dx = d trace(Q'*K) / d x} are of the same size as the hyperparameter vector \texttt{hyp} and the input data \texttt{x}, respectively. The components of \texttt{dhyp} and \texttt{dx} are defined as follows: \texttt{dhyp(i) = trace(Q'*( d K / d hyp(i) ))} and \texttt{dx(i,j) = trace(Q'*( d K / d x(i,j) ))}.

Covariance functions can be specified in two ways: either as a string containing the name of the covariance function or using a cell array. For example:

\texttt{cov = 'covRQard'};

\texttt{cov = {'covRQard'}};

\texttt{cov = {@covRQard}};

are supported. Only the second and third form using the cell array can be used for specifying composite covariance functions, made up of several contributions. For example:

\texttt{cov = {'covScale', {'covRQiso'}}};

\texttt{cov = {'covSum', {'covRQiso'},'covSEard','covNoise'}};

\texttt{cov = {'covProd', {'covRQiso'},'covSEard','covNoise'}};

\texttt{cov = {'covMask',{mask,'covSEiso'}}}

\texttt{q=1; cov = {'covPPiso',q}};

\texttt{d=3; cov = {'covPoly',d}};

\texttt{cov = {'covADD',[[1,2],'covSEiso']}};

\texttt{cov = {@apxSparse,{@covSEiso},u}}; where \texttt{u} are the inducing inputs

specifies a covariance function which is the sum of three contributions. To find out how many hyperparameters this covariance function requires, we do:

\texttt{feval(cov{:})}

which returns the string `'3+(D+1)+1'` (i.e. the 'covRQiso' contribution uses 3 parameters, the 'covSEard' uses D+1 and 'covNoise' a single parameter).

See also doc/usageCov.m.

\texttt{gpml copyright 6a}
### 6.2 Implemented Covariance Functions

Similarly to the mean functions, we provide a whole algebra of covariance functions \( k: \mathbb{X} \times \mathbb{X} \to \mathbb{R} \) with the same generic name pattern `cov/cov<NAME>.m` as before.

Besides a long list of simple covariance functions, we also offer a variety of composite covariance functions as shown in the following table.

<table>
<thead>
<tr>
<th>1) Elementary and standalone covariance functions ( k(\mathbf{x}, \mathbf{z}) )</th>
<th>2) Composite covariance functions ( k_{c1}(\mathbf{x}, \mathbf{z}), k_{c2}(\mathbf{x}, \mathbf{z}), \ldots \to k(\mathbf{x}, \mathbf{z}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>(&lt;NAME&gt;) meaning</td>
<td>( k(\mathbf{x}, \mathbf{z}) = )</td>
</tr>
<tr>
<td>Zero</td>
<td>covariance vanishes always</td>
</tr>
<tr>
<td>Eye</td>
<td>unit additive measurement noise ( u(\mathbf{x}) )</td>
</tr>
<tr>
<td>Line</td>
<td>unit constant ( l(\mathbf{x}) )</td>
</tr>
<tr>
<td>Discrete</td>
<td>precomputed covariance for discrete data ( \mathbf{x} \in \mathbb{X} \subseteq \mathbb{N} ) as before.</td>
</tr>
</tbody>
</table>

| 3) Covariance functions based on Mahalanobis distances \( k(\mathbf{x}, \mathbf{z}) = k(\mathbf{x}, \mathbf{z}) - \mathbf{F}^{\top} \mathbf{F} \), where \( \mathbf{x}, \mathbf{z} \in \mathbb{X} \subseteq \mathbb{R}^{n} \) | 4) Covariance functions based on Euclidean dot products \( k(\mathbf{x}, \mathbf{z}) = k(\mathbf{x}, \mathbf{z}) \), \( \mathbf{x} = \mathbf{F}^{\top} \mathbf{z} \), where \( \mathbf{x}, \mathbf{z} \in \mathbb{X} \subseteq \mathbb{R}^{m} \) |
| 3| 4| |
| \(<NAME>\) shared generic *mother* covariance function \( k(\mathbf{r}) = \) | \( \Phi \) |
| SE | gamma exponential | \( \exp(-|\mathbf{r}|^\gamma), \gamma \in (0, 2) \) |
| Matern | Matérn, \( f_1(t) = 1, f_2(t) = 1 + t, f_3(t) = f_2(t) + \frac{t^2}{2} \) | \( \exp(-|\mathbf{r}|^{\gamma}) \) |
| PP | compact support, piecewise polynomial \( f_{\gamma}(\mathbf{r}) \) | \( \max(0, 1 - |\mathbf{r}|^{\gamma}) \) |
| RQ | rational quadratic | \( (1 + |\mathbf{r}|^{\gamma}/\psi) \) |
| SE | squared exponential | \( \exp(-|\mathbf{r}|^2) \) |
| eye | unit lengthscale | \( \mathbf{F} = \mathbf{I} \) |
| iso | isotropic lengthscale | \( \mathbf{F} = \mathbf{C}_{\mathbf{I}} \), \( \mathbf{F} \in \mathbb{R}^{n \times n} \) |
| ard | automatic relevance determination | \( \mathbf{P} = \mathbf{A}_{\mathbf{R}}, \mathbf{A} = \text{diag}(\lambda), \lambda \in \mathbb{R}^{n} \) |
| proj | low-rank projection in input space | \( \mathbf{P} = \mathbf{F}_{\mathbf{U}} \mathbf{F}^{\top}_{\mathbf{U}}, \mathbf{U} \in \mathbb{R}^{n \times \ell} \) |
| fact | factor analysis | \( \mathbf{F}^\top = \mathbf{L}, \mathbf{L} = \text{diag}(\lambda), \mathbf{L} \in \mathbb{R}^{n \times \ell} \) |
| vlen | spatially varying lengthscale, \( \mathbf{k}(\mathbf{x}, \mathbf{z}) = \left( \frac{t(x_{\mathbf{x}})}{|x_{\mathbf{x}}^{\top} x_{\mathbf{x}}|} \right)^{v_2} \) | \( \Phi \) |

| 5) Standalone covariance functions \( k(\mathbf{x}, \mathbf{z}) = \) |  |
| \(<NAME>\) meaning | \( k(\mathbf{x}, \mathbf{z}) = \) |
| RBFone | neural net, \( \mathbb{X} \subseteq \mathbb{R}^{D} \) | \( \sigma_{\mathbf{r}} \sin^{-1} \left( \frac{x_{\mathbf{x}}^{\top} x_{\mathbf{z}}}{\sqrt{|x_{\mathbf{x}}^{\top} x_{\mathbf{x}}|} |x_{\mathbf{z}}|} \right) \) |
| LIFone | linear with bias, \( \mathbb{X} \subseteq \mathbb{R}^{D} \) | \( (x_{\mathbf{x}}^{\top} z^{\top})^{\gamma} \) |
| Periodic | periodic, \( \mathbb{X} \subseteq \mathbb{R}^{D} \) | \( \sigma_{\mathbf{r}} \exp \left(-\frac{x_{\mathbf{x}}^{\top} x_{\mathbf{z}}}{p/2} \right) \) |
| PeriodicRBFDC | periodic, rescaled, DC component removed, \( \mathbb{X} \subseteq \mathbb{R}^{D} \) | \( \sigma_{\mathbf{r}} \exp \left(-\frac{x_{\mathbf{x}}^{\top} x_{\mathbf{z}}}{p/2} \right) \) |
| Cos | periodic cosine, \( \mathbb{X} \subseteq \mathbb{R}^{D} \) | \( \sigma_{\mathbf{r}} \cos(p(x_{\mathbf{x}} - z_{\mathbf{z}})) \) |
| Gabor | Gabor function, \( \mathbb{X} \subseteq \mathbb{R}^{D}, \lambda, p \in \mathbb{R}^{D} \) | \( \exp \left(-j x_{\mathbf{x}}^{\top} A^{-2} t \right) \cos \left(2 \pi p^{\top} t \right), t_{\mathbf{p}} = \frac{t}{p} \) |
The spectral mixture covariance `covSM` was introduced by Wilson & Adams [Gaussian Process Kernels for Pattern Discovery and Extrapolation], ICML, 2013.

The periodic covariance function `covPER` starts from a stationary covariance function that depends on the data only through a distance $r^2 = (x - x')^T \Lambda^{-2} (x - x')$ such as `covMatern`, `covPP`, `covRQ`, `covSE` and turns them into a periodic covariance function by embedding the data $x \in \mathbb{R}^D$ into a periodic high-dimensional space $x_p = u(x) \in \mathbb{R}^{2D}$ by a function $u(x) = 2\pi \text{diag}(p^{-1}) x$.

The additive covariance function `covADD` starts from a one-dimensional covariance function $k(x_i, x'_i, \psi_i)$ acting on a single component $i \in \{1, \ldots, D\}$ of $x$. From that, we define covariance functions $k_i(x_1, x_1) = \prod_{i=1}^D k(x_i, x'_i, \psi_i)$ acting on vector-valued inputs $x_1$. The sums of exponential size can efficiently be computed using the Newton-Girard formulae. Samples functions drawn from a GP with additive covariance are additive functions. The number of interacting variables $|I|$ is a measure of how complex the additive functions are.

### 6.3 Usage of Implemented Covariance Functions

Some code examples taken from `doc/usageCov.m` illustrate how to use simple and composite covariance functions to specify a GP model.

Syntactically, a covariance function `cf` is defined by

```matlab
cv := 'func' | @func // simple
cf := {cv} | {cv, {param, cf}} | {cv, cf, .., cf} // composite
```

i.e., it is either a string containing the name of a covariance function, a pointer to a covariance function or one of the former in combination with a cell array of covariance functions and an additional list of parameters.

### 6.4 Implementation Details

The spectral mixture covariance `covSM` was introduced by Wilson & Adams [Gaussian Process Kernels for Pattern Discovery and Extrapolation], ICML, 2013.

The periodic covariance function `covPER` starts from a stationary covariance function that depends on the data only through a distance $r^2 = (x - x')^T \Lambda^{-2} (x - x')$ such as `covMatern`, `covPP`, `covRQ`, `covSE` and turns them into a periodic covariance function by embedding the data $x \in \mathbb{R}^D$ into a periodic high-dimensional space $x_p = u(x) \in \mathbb{R}^{2D}$ by a function $u(x) = 2\pi \text{diag}(p^{-1}) x$.

The additive covariance function `covADD` starts from a one-dimensional covariance function $k(x_i, x'_i, \psi_i)$ acting on a single component $i \in \{1, \ldots, D\}$ of $x$. From that, we define covariance functions $k_i(x_1, x_1) = \prod_{i=1}^D k(x_i, x'_i, \psi_i)$ acting on vector-valued inputs $x_1$. The sums of exponential size can efficiently be computed using the Newton-Girard formulae. Samples functions drawn from a GP with additive covariance are additive functions. The number of interacting variables $|I|$ is a measure of how complex the additive functions are.

### 6.5 Usage of Implemented Covariance Functions

Some code examples taken from `doc/usageCov.m` illustrate how to use simple and composite covariance functions to specify a GP model.

Syntactically, a covariance function `cf` is defined by

```matlab
cv := 'func' | @func // simple

cf := {cv} | {cv, {param, cf}} | {cv, cf, .., cf} // composite
```

i.e., it is either a string containing the name of a covariance function, a pointer to a covariance function or one of the former in combination with a cell array of covariance functions and an additional list of parameters.
% set up simple covariance functions
7 cn = {'covNoise'}; sn = .1; hypn = log(sn);  % one hyperparameter
8 cc = @covConst; sf = 2; hypc = log(sf);  % function handles OK
9 ce = @covEye; hype = [];  % identity
10 cl = @covLIN; hypl = [];  % linear is parameter-free
11 cla = {'covLINard'}; L = rand(D,1); hypla = log(L);  % linear (ARD)
12 cli = {'covLINiso'}; l = rand(1); hypli = log(l);  % linear iso
13 cp = @covPoly,3; c = 2; hypp = log([c;sf]);  % third order poly
14 cga = {'covSEard'}; hypga = log([L;sf]);  % Gaussian with ARD
15 cgi = {'covSEiso'}; hypgi = log([ell;sf]);  % isotropic Gaussian
16 cgu = {'covSEisoU'}; hypgu = log(ell);  % isotropic Gauss no scale
17 cli = {'covRQard'}; al = 2; hypra = log([L;sf;al]);  % rational quadratic
18 cpa = {'covRQiso'}; hypri = log([ell;sf;al]);  % isotropic
19 cma = {'covMaternard',5}; hypma = log([ell;sf]);  % Matern class d=5
20 cmi = {'covMaterniso',3}; hypmi = log([ell;sf]);  % Matern class d=3
21 cnn = {'covNNone'}; hypnn = log([L;sf]);  % neural network
22 cpe = {'covPeriodic'}; p = 2; hyppe = log([ell;p;sf]);  % periodic
23 cvl = {'covSEvlen',{@meanLinear}}; hypvl = [1;2;1;0];  % var lenscale
24 cds = @covDiscrete,s; hypds = L(triu(true(s)));
25 cgg = {'covGaboriso'}; ell = 1; p = 1.2; hypgb = log([ell;p]);  % Gabor
26 cga = {'covScale',cgu}; hypsc = [log(3); hypgu];  % scale by 9
27 csm = @covSM,Q; hypsm = log([w;m(:);v(:)]);  % Spectral Mixture
28 cma = {'covMask',mask,cgi{:}}; hypma = hypgi;
29 cpr = {'covPERiso',cvi}; hyppr = [0;0];  % isotropic periodic rational quadratic
30 cma = {'covPERard',cvi};  % periodic Matern with ARD
31 cad = {'covADD',[]};  % additive based on SEiso using unary and pairwise interactions
32 cpr = {'covPref',cvi}; hyppr = [0;0];  % preference covariance with squared exponential base covariance
33 xp = rand(n,2*D); xsp = rand(3,2*D);
34 0) specify a covariance function
35 cov = cma; hyp = hypma;
36 cov = cci; hyp = hypcc;
37 cov = csp; hyp = hypsm;
38 cov = cds; hyp = hypds; x = xd; xs = xsd;
39 1) query the number of parameters
40 feval(cov{1})
7 Hyperpriors

A hyperprior \( p(\theta) \) with \( \theta = [\rho, \phi, \psi] \) is a joint probability distribution over the likelihood hyperparameters \( \rho \), the mean hyperparameters \( \phi \) and the covariance hyperparameters \( \psi \). We concentrate on factorial priors \( p(\theta) = \prod_j p_j(\theta_j) \). Hyperpriors can be used to regularise the optimisation of the hyperparameters via the marginal likelihood \( Z(\theta) \) so that \( p(\theta)Z(\theta) \) is maximised instead. As we wish to perform unconstrained optimisation, we require (mainly) smooth hyperpriors with infinite support.

7.1 Interface

In the GPML toolbox, a prior distribution \( p(\theta) \) needs to implement the evaluation of the log density \( \ln p(\theta) \) and its first derivative \( \frac{\partial}{\partial \theta} \ln p(\theta) \). In addition, we require sampling capabilities i.e. the generation of \( \theta \sim p(\theta) \).

\[\text{priorDistributions.m}\]

1 \% prior distributions to be used for hyperparameters of Gaussian processes
2 \% using infPrior.
3 \% There are two different kinds of prior distributions: simple and composite:
4 \% simple prior distributions:
5 \% priorGauss - univariate Gaussian
6 \% priorLaplace - univariate Laplace
7 \% priorT - univariate Student’s t
8 \% priorSmoothBox1 - univariate interval (linear decay in log domain)
9 \% priorSmoothBox2 - univariate interval (quadr. decay in log domain)
10 \% priorGamma - univariate Gamma, IR+
11 \% priorWeibull - univariate Weibull, IR+
12 \% priorInvGauss - univariate Inverse Gaussian, IR+
13 \% priorLogNormal - univariate Log-normal, IR+
14 \% priorClamped or - fix hyperparameter to its current value by setting
derivatives to zero, no effect on marginal likelihood
15 \% priorDelta derivatives to zero, no effect on marginal likelihood
16 \% priorGaussMulti - multivariate Gauss
17 \% priorLaplaceMulti - multivariate Laplace
18 \% priorTMulti - multivariate Student’s t
19 \% priorClampedMulti or - fix hyperparameter to its current value by setting
derivatives to zero, no effect on marginal likelihood
20 \% priorDeltaMulti derivatives to zero, no effect on marginal likelihood
21 \% priorEqualMulti or - make several hyperparameters have the same value by
22 \% priorSameMulti same derivative, no effect on marginal likelihood

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% composite prior distributions (see explanation at the bottom):

% priorMix - nonnegative mixture of priors
% priorTransform - prior on g(t) rather than t

% Naming convention: all prior distributions are named "prior/prior*.m".

% 1) With only a fixed input arguments:

% r = priorNAME(par1,par2,parN)

% The function returns a random sample from the distribution for e.g.
% random restarts, simulations or optimisation initialisation.

% 2) With one additional input arguments:

% [lp,dlp] = priorNAME(par1,par2,parN, t)

% The function returns the log density at location t along with its first
% derivative.

% See also doc/usagePrior.m, inf/infPrior.m.

% gpml copyright
7.2 Implemented Hyperpriors

All code files are named according to the pattern prior/prior<NAME>.m for simple identification. All currently available hyperpriors are summarised in the following table.

<table>
<thead>
<tr>
<th>Simple univariate priors p(θ)</th>
<th>Univariate hyperpriors defined over the whole reals with mean µ and variance σ²</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;NAME&gt;</td>
<td>Meaning</td>
</tr>
<tr>
<td>Gauss</td>
<td>normally distributed hyperparameter θ ∈ R</td>
</tr>
<tr>
<td>Laplace</td>
<td>double exponentially distributed hyperparameter θ ∈ R</td>
</tr>
<tr>
<td>T</td>
<td>Student's t distributed hyperparameter θ ∈ R</td>
</tr>
</tbody>
</table>

| SmoothBox1          | interval hyperparameter θ ∈ R i.e. θ ∈ [a, b] | \( \frac{1}{\pi\sigma^2} \exp \left( -\frac{(\theta - \mu)^2}{\sigma^2} \right) \) | a ∈ [−∞, +∞), b ∈ R Registry, η ∈ R⁺ |
| SmoothBox2          | localised hyperparameter θ ∈ R i.e. θ ∈ [a, b] | \( \frac{1}{\pi\sigma^2} \exp \left( -\frac{(\theta - \mu)^2}{\sigma^2} \right) \) | a ∈ [−∞, +∞), b ∈ R Registry, η ∈ R⁺ |

<table>
<thead>
<tr>
<th>Univariate hyperpriors supported only over the positive reals</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gamma</td>
</tr>
<tr>
<td>Weibull</td>
</tr>
<tr>
<td>InverseGauss</td>
</tr>
<tr>
<td>LogNormal</td>
</tr>
</tbody>
</table>

| Multivariate hyperpriors supported all over \( R^D \) with \( \mu \) and covariance \( \Sigma \) |
|---------------------------------|-------------------------------------------------|-----------------|
| GaussMulti                     | multivariate normal distribution \( \theta \in R^D \) | \( \frac{1}{(2\pi\Sigma)^{D/2}} \exp \left( -\frac{1}{2} (\theta - \mu)^\Sigma (\theta - \mu) \right) \) | µ ∈ R⁺, Σ ∈ R⁺⊗≠D |
| LaplaceMulti                   | multivariate Laplace distribution \( \theta \in R^D \) | \( \frac{1}{\sqrt{D}!} \exp \left( -\frac{1}{2} \|L^{–1}(\theta - \mu)\|_1 \right) \) | L = Σ, Σ ∈ R⁺⊗≠D |
| TMulti                         | multivariate Student's t distribution \( \theta \in R^D \) | \( \frac{1}{\Gamma(D/2)\Gamma(\nu/2)} \left( 1 + \frac{(\theta - \mu)^2}{\nu} \right)^{-\nu/2} \) | µ ∈ R⁺, Σ ∈ R⁺⊗≠D, ν ∈ R⁺ |

<table>
<thead>
<tr>
<th>Univariate hyperpriors supported only over the real line</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Delta Clamped</td>
<td>clamped hyperparameter ( \theta = \theta_0 \in R )</td>
<td>( \delta(\theta - \theta_0) )</td>
</tr>
<tr>
<td>DeltaMulti</td>
<td>clamped hyperparameter ( \theta = \theta_0 \in R^D )</td>
<td>( \delta(\theta - \theta_0) )</td>
</tr>
<tr>
<td>ClampedMulti</td>
<td>same hyperparameter ( \theta = \theta_0 \in R^D )</td>
<td>( \delta \left( \theta - \theta_0 \right) )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Composite hyperpriors ([\eta_1(0), \eta_2(0), \ldots] \rightarrow p(\theta))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transform</td>
</tr>
<tr>
<td>Mix</td>
</tr>
</tbody>
</table>

The priorSmoothBox2 is a Gauss-uniform sandwich obtained by complementing a uniform distribution on \([a, b]\) with two Gaussian halves at each side. The parameter \( \eta \) balances the probability mass between the constituents so that \( \eta/(\eta + 1) \) is used for the box and \( 1/(\eta + 1) \) for the Gaussian sides. Its brother priorSmoothBox1 is the product of two sigmoidal functions.

The priorDelta or equivalently priorClamped can be used to exclude some hyperparameters from the optimisation. Their values are clamped to \( \theta_0 \) and the derivative vanishes. There are also multivariate counterparts priorDeltaMulti and priorClampedMulti.

7.3 Usage of Implemented Hyperpriors

Some code examples taken from doc/usagePrior.m illustrate how to use univariate, multivariate and composite priors on hyperparameters. Syntactically, a hyperprior hp is defined by

```matlab
func := Dist // prior distributions in prior/
| Clamped | Delta // predefined for fixing the hyperparameter
pr := 'func' | @func // univariate hyperprior
```

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i.e., it is either a string containing the name of a hyperprior function, a pointer to a hyperprior function or one of the former in combination with a cell array of hyperprior functions and an additional list of parameters. Furthermore, we have multivariate hyperprior variants and 2 (equivalent) predefined hyperpriors allowing to exclude variables from optimisation.

```matlab
clear all, close all

% 1) specify some priors
% a) univariate priors
mu = 1.0; s2 = 0.01^2; nu = 3;
pg = {@priorGauss,mu,s2}; % Gaussian prior
pl = {'priorLaplace',mu,s2}; % Laplace prior
pt = {@priorT,mu,s2,nu}; % Student’s t prior
p1 = {@priorSmoothBox1,0,3,15}; % smooth box constraints lin decay
p2 = {@priorSmoothBox2,0,2,15}; % smooth box constraints qua decay
pd = {'priorDelta'}; % fix value of prior exclude from optim
pc = {@priorClamped}; % equivalent to above
lam = 1.05; k = 2.5;
pw = {@priorWeibull,lam,k}; % Weibull prior

% b) meta priors
pmx = {@priorMix,[0.5,0.5],{pg,pl}}; % mixture of two priors
g = @exp; dg = @exp; ig = @log;
ptr = {@priorTransform,g,dg,ig,pg}; % Gaussian in the exp domain

% c) multivariate priors
m = [1;2]; V = [2,1;1,2];
pG = {@priorGaussMulti,m,V}; % 2d Gaussian prior
pD = {'priorDeltaMulti'}; % fix value of prior exclude from optim
PC = {@priorClampedMulti}; % equivalent to above

% 2) evaluation
% pri = pt; hp = randn(1,3);
% pri = pmx; hp = randn(1,3);
% pri = ptr; hp = randn(1,3);
pri = pG; hp = randn(2,3);

% a) draw a sample from the prior
feval(pri{:})

% b) evaluate prior and derivative if requires
[lp,dlp] = feval(pri{:},hp)

% 3) comprehensive example
x = (0:0.1:10)'; y = 2*x+randn(size(x)); % generate training data
mean = {@meanSum,{@meanConst,@meanLinear}}; % specify mean function
cov = {@covSEiso}; lik = {@likGauss}; % specify covariance and lik
hyp.cov = [log(1);log(1.2)]; hyp.lik = log(0.9); hyp.mean = [2;3];
```
par = {mean, cov, lik, x, y}; mfun = @minimize; % input for GP function

% a) plain marginal likelihood optimisation (maximum likelihood)
im = @infExact; % inference method
hyp_plain = feval(mfun, hyp, @gp, -10, im, par{:}); % optimise

% b) regularised optimisation (maximum a posteriori) with 1d priors
prior.mean = {pg; pc}; % Gaussian prior for first, clamp second par
prior.cov = {p1; []}; % box prior for first, nothing for second par
im = {@infPrior, @infExact, prior}; % inference method
hyp_p1 = feval(mfun, hyp, @gp, -10, im, par{:}); % optimise

% c) regularised optimisation (maximum a posteriori) with Nd priors
prior = []; % clear the structure
prior.multi{1} = {@priorTMulti, [mu; mu], diag([s2, s2]), nu,...
structure('mean', [1, 2])}; % use hyper struct
prior.multi{1} = {@priorTMulti, mu, s2, nu, structure('mean', [1, 2])}; % equivalent shortcut
prior.multi{2} = {@priorGaussMulti, [mu; mu], diag([s2, s2]),... [1, 3]}; % use unwrapped hyper vector
prior.multi{2} = {@priorGaussMulti, mu, s2, [1, 3]}; % equivalent shortcut
im = {@infPrior, @infExact, prior}; % inference method
hyp_pN = feval(mfun, hyp, @gp, -10, im, par{:}); % optimise

[any2vec(hyp), any2vec(hyp_plain), any2vec(hyp_p1), any2vec(hyp_pN)]