Documentation for GPML Matlab Code version 4.2

1) What?

The code provided here originally demonstrated the main algorithms from Rasmussen and Williams: Gaussian Processes for Machine Learning. It has since grown to allow more likelihood functions, further inference methods and a flexible framework for specifying GPs. Other GP packages can be found here.

The code is written by Carl Edward Rasmussen and Hannes Nickisch; it runs on both Octave 3.2.x and Matlab® 7.x and later. The code is based on previous versions written by Carl Edward Rasmussen and Chris Williams.

2) Download, Install and Documentation

All the code including demonstrations and html documentation can be downloaded from gitlab or in a tar or zip archive file.

Minor changes and incremental bugfixes to the current version are documented in the changelog, changes from previous versions are documented in README.

Please read the copyright notice.

After unpacking the tar or zip file you will find 7 subdirectories: cov, doc, inf, lik, mean, prior and util. It is not necessary to install anything to get started, just run the `startup` script to set your path.

Details about the directory contents and on how to compile mex files can be found in the README. The getting started guide is the remainder of the html file you are currently reading (also available at http://gaussianprocess.org/gpml/code/matlab/doc). A Developer's Guide containing technical documentation is found in `manual.pdf`, but for the casual user, the guide is below.

3) Getting Started

Gaussian Processes (GPs) can conveniently be used for Bayesian supervised learning, such as regression and classification. In its simplest form, GP inference can be implemented in a few lines of code. However, in practice, things typically get a little more complicated: you might want to use complicated covariance functions and mean functions, learn good values for hyperparameters, use non-Gaussian likelihood functions (rendering exact inference intractable), use approximate inference algorithms, or combinations of many or all of the above. This is what the GPML software package does.

The remainder of section 3 first presents some essential components of the software in the next subsection. This enables understand the usage for the `gp` function described in section 3b). A practical example follows in 3c), and the section concludes with a more detailed overview in 3d).

3a) Some Essential Components

Before going straight to the examples, just a brief note about the organization of the package. There are four essential types of objects which you need to know about:

Gaussian Process

A Gaussian Process is fully specified by a *mean function* and a *covariance function*. These functions are specified separately, and consist of a specification of a functional form as well as a set of parameters called *hyperparameters*, see below.

Mean functions

Several mean functions are available, an overview is provided by the `meanFunctions` help function (type `help meanFunctions` to get help), and an example is the `meanLinear` function.

Covariance functions

Several covariance functions are available, an overview is provided by the `covFunctions` help function (type `help covFunctions` to get help), and an example is the `covSEard` "Squared Exponential with Automatic Relevance Determination" covariance function.

For a more comprehensive overview of mean and covariance functions, see section 3d) below.

Hyperparameters

GPs are specified using mean and covariance functions which typically have free parameters called *hyperparameters*. Also likelihood functions may have such parameters. Hyperparameters are represented in a struct with the fields `mean`, `cov` and `lik` (some of which may be empty). It is important that the number of elements in each of the fields in the hyperparameter struct matches the specification of the mean, covariance and likelihood functions.

Likelihood Functions

The likelihood function specifies the probability of the observations given the GP (and the hyperparameters). Several likelihood functions are available, an overview is provided by the `likFunctions` help function (type `help likFunctions` to get help).

Example likelihood functions include `likGauss` the Gaussian likelihood for regression and `likLogistic` the logistic likelihood for classification.

Inference Methods

The inference methods specify how to compute with the model, i.e. how to infer the (approximate) posterior process, how to find hyperparameters, evaluate the log marginal likelihood and how to make predictions. Several inference methods are avaiable, and overview is provided by the `infMethods` help file (type `help infMethods` to get help). An example inference method is `infGaussLik` for exact inference (regression with Gaussian likelihood).

Covariance approximations

The covariance approximation as used by `apx` determines an important computational aspect in GP inference: the scalability with the number of inputs. We offer four options here:
a) Exact covariance computations serving as default option (`demoRegression`, `demoClassification`),
b) sparse covariance approximations exploiting inducing points and conditional independence (`apxSparse`, `demoSparse`),
c) grid-based covariance approximations using interpolation from a rectilinear grid of inducing points and exploiting the resulting Kronecker and Toeplitz property of covariance matrices (`apxGrid`, `demoGrid1d`, `demoGrid2d`), and
d) state space covariance approximations exploiting a state space representation of univariate GPs (`apxState`, `demoState`).

3b) The gp Function

Using the GPML package is simple, there is only one single function to call: gp, it does posterior inference, learns hyperparameters, computes the marginal likelihood and makes predictions. Generally, the gp function takes the following arguments: a hyperparameter struct, an inference method, a mean function, a covariance function, a likelihood function, training inputs, training targets, and possibly test cases. The exact computations done by the function is controlled by the number of input and output arguments in the call. Here is part of the help message for the gp function (follow the link to see the whole thing):

```
function [varargout] = gp(hyp, inf, mean, cov, lik, x, y, xs, ys)

[ ... snip ... ]

Two modes are possible: training or prediction: if no test cases are
supplied, then the negative log marginal likelihood and its partial
derivatives wrt 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);

[ ... snip ... ]
```

Here `x` and `y` are training inputs and outputs, and `xs` and `ys` are test set inputs and outputs, `nlZ` is the negative log marginal likelihood and `dnlZ` its partial derivatives wrt the hyperparameters (which are used for training the hyperparameters). The prediction outputs are `ymu` and `ys2` for test output mean and covariance, and `fmu` and `fs2` are the equivalent quenteties for the corresponding latent variables. Finally, `lp` are the test output log probabilities.

3c) A Practical Example

To get started, let's consider the simple example of one-dimensional non-linear regression on data corrupted by Gaussian noise. Our data set is

```
x = gpml_randn(0.8, 20, 1);                 % 20 training inputs
y = sin(3*x) + 0.1*gpml_randn(0.9, 20, 1);  % 20 noisy training targets
xs = linspace(-3, 3, 61)';                  % 61 test inputs
```

We need specify the mean, covariance and likelihood functions

```
meanfunc = [];                    % empty: don't use a mean function
covfunc = @covSEiso;              % Squared Exponental covariance function
likfunc = @likGauss;              % Gaussian likelihood
```

Finally we initialize the hyperparameter struct

```
hyp = struct('mean', [], 'cov', [0 0], 'lik', -1);
```

Note, that the hyperparameter struct must have the three fields `mean, cov and lik`. Each field must have the number of elements which corresponds to the functions specified. In our case, the mean function is empty, so takes no parameters. The covariance function is `covSEiso`, the squared exponential with isotropic distance measure, which takes two parameters (see `help covSEiso`). As explained in the help for the function, the meaning of the hyperparameters is "log of the length-scale" and the "log of the signal std dev". Initializing both of these to zero, corresponds to length-scale and signal std dev to be initialized to one. The Gaussian likelihood function has a single parameter, which is the log of the noise standard deviation, setting the log to zero corresponds to a standard deviation of `exp(-1)=0.37`.

A common situation with modeling with GPs is that approprate settings of the hyperparameters are not known a priori. The situation is reflected in the above initialization of the hyperparameters, where the values values are specified without careful justification, perhaps based on some vague notions of the magnitudes likely to be involved. Thus, a common task is to set hyperparameters by optimizing the (log) marginal likelihood. This is done as follows

```
hyp2 = minimize(hyp, @gp, -100, @infGaussLik, meanfunc, covfunc, likfunc, x, y);
```

The `minimize` function minimizes the negative log marginal likelihood, which is returned by the `gp` function, together with the partial derivatives wrt the hyperparameters. The inference method is specified to be `infGaussLik` exact inference. The minimize function is allowed a computational budget of 100 function evaluations. The hyperparameters found are

```
hyp2 =
  mean: []
   cov: [-0.6352 -0.1045]
   lik: -2.3824
```

showing that the covariance characteristic length-scale is `exp(-0.6352)=0.53`, the signal std dev is `exp(-0.1045)=0.90` and the noise std dev is `exp(-2.3824)=0.092` in good agreement with the data generating process.

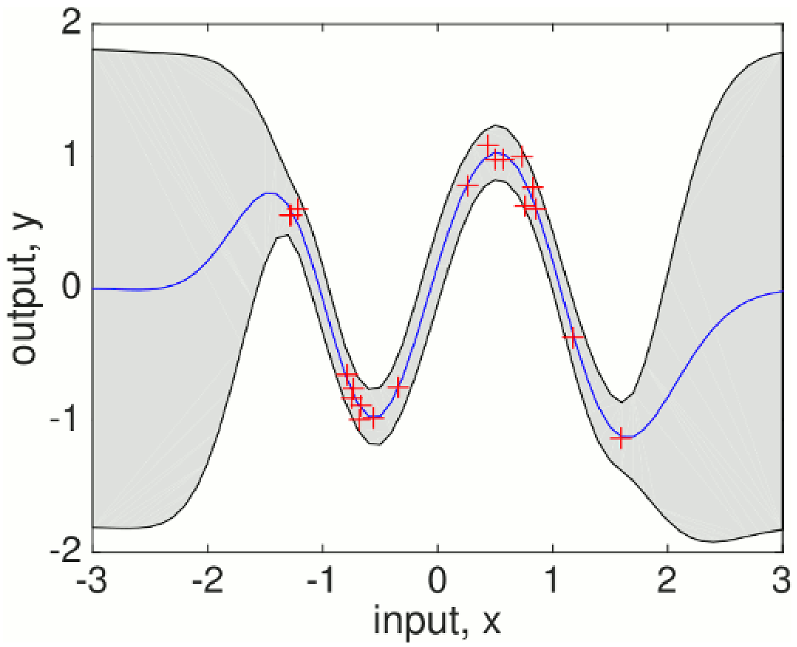
To make predictions using these hyperparameters

```
[mu s2] = gp(hyp2, @infGaussLik, meanfunc, covfunc, likfunc, x, y, xs);
```

To plot the predictive mean at the test points together with the predictive 95% confidence bounds and the training data

```
f = [mu+2*sqrt(s2); flipdim(mu-2*sqrt(s2),1)];
fill([xs; flipdim(xs,1)], f, [7 7 7]/8)
hold on; plot(xs, mu); plot(x, y, '+')
```

which produces a plot like this



3d) A More Detailed Overview

The previous section shows a minimalist example, using the central concepts of GPML. This section provides a less simplistic overview, mainly through a number of useful comments and pointers to more complete treatments.

In order to be able to find things, the toolbox is organized into the following directories `mean` for mean functions, `cov` for covariance functions, `lik` for likelihood functions, `inf` for inference methods `prior` for priors and `mcmc` for Markov Chain monte Carlo tools, `doc` for documentation and `util` for general utilities.

In addition to this structure, the naming of functions within some of these directories also start with the letters `mean`, `cov`, `lik` and `inf` as a further mnemonic aid.

The following paragraphs contain useful further details about some of the concepts we have already used.

Mean functions and **covariance functions**. As detailed in `meanFunctions` and `covFunctions` there are actually two types of these, simple and composite. Composite functions are used to compose simple functions into more expressive structures. For example

```
  meanfunc = {@meanSum, {@meanLinear, @meanConst}};
```

specifies a mean function which is a sum of a linear and a constant part. Note how composite functions are specified using cell arrays. Note also, that the corresponding mean hyperparameter will consist of a vector containing the concatenation of the different parts of the mean function. If you call a mean or covariance function without arguments, they will return a string indicating the number of hyperparameters expected; this also works for composite covariance functions; the letter `D` in the string designates the dimension of the inputs.

Likelihood functions. As detailed in `likFunctions` there are also simple and composite likelihood functions; the only composite likelihood function is `likMix`, which implements a mixture of multiple likelihoods.

Inference methods.

Whereas all mean functions and covariance functions may be used in any context, there are some restrictions on which likelihood functions may be used with which inference method. An exhaustive compatibility matrix between likelihoods (rows) and inference methods (columns) is given in the table below:

Plain Regression Likelihoods										
	Cov. approxim.: `dense`, `sparse`, `grid` or `state`	✓	✓	✓	(✓)*				type, output domain	alternative names
Inference / Likelihood	GPML name	Gaussian noise infGaussLik	Laplace infLaplace	Variational Bayes infVB	EP infEP	Kullback Leibler infKL	Sampling infMCMC	LOO infLOO		
Gaussian	likGauss	✓	✓	✓	✓	✓	✓	✓	regression, IR	
Warped Gaussian	likGaussWarp		✓	✓	✓	✓	✓	✓	regression, IR	
Gumbel	likGumbel		✓			✓	✓	✓	regression, IR	extremal value regression
Sech squared	likSech2		✓	✓	✓	✓	✓	✓	regression, IR	logistic distribution
Laplacian	likLaplace			✓	✓	✓	✓	✓	regression, IR	double exponential
Student's t	likT		✓	✓		✓	✓	✓	regression, IR	
Classification Likelihoods										
Uniform	likUni		✓	✓	✓	✓	✓	✓	classification, ±1	label noise
Error function	likErf		✓		✓	✓	✓	✓	classification, ±1	probit regression
Logistic function	likLogistic		✓	✓	✓	✓	✓	✓	classification, ±1	logistic regression logit regression
Generalized Linear Model Likelihoods										
	Cov. approxim.: `dense`, `sparse`, `grid` or `state`	✓	✓	✓	(✓)*				type, output domain	alternative names
Inference / Likelihood	GPML name	Gaussian noise infGaussLik	Laplace infLaplace	Variational Bayes infVB	EP infEP	Kullback Leibler infKL	Sampling infMCMC	LOO infLOO		
Weibull	likWeibull		✓				✓	✓	positive data, IR+\{0}	nonnegative regression
Gamma	likGamma		✓				✓	✓	positive data, IR+\{0}	nonnegative regression
Exponential	likExp		✓				✓	✓	positive data, IR+\{0}	nonnegative regression

Inverse Gaussian	likInvGauss		✓				✓	✓	positive data, IR+\{0}	nonnegative regression
Poisson	likPoisson		✓		(✓)**	✓	✓	✓	count data, IN	Poisson regression
Negative Binomial	likNegBinom		✓				✓	✓	count data, IN	negative binomial regression
Beta	likBeta		✓				✓	✓	interval data, [0,1]	range regression
Composite Likelihoods										
Mixture	likMix		✓		✓	✓	✓	✓	classification, ±1 and regression, IR	mixing meta likelihood

* EP supports FITC via a separate function. No support for the generic covariance approximations.
** EP might not converge in some cases since quadrature is used.

All of the objects described above are written in a modular way, so you can add functionality if you feel constrained despite the considerable flexibility provided. Details about how to do this are provided in the developer documentation.

Inference by MCMC sampling is the only inference method that cannot be used as a black box. Also gradient-based marginal likelihood optimisation is not possible with MCMC. Please see usageSampling for a toy example illustrating the usage of the implemented samplers.

4) Practice

Instead of exhaustively explaining all the possibilities, we will give two illustrative examples to give you the idea; one for regression and one for classification. You can either follow the example here on this page, or using the two scripts demoRegression and demoClassification (using the scripts, you still need to follow the explanation on this page).

4a) Simple Regression

You can either follow the example here on this page, or use the script demoRegression.

This is a simple example, where we first generate `n=20` data points from a GP, where the inputs are scalar (so that it is easy to plot what is going on). We then use various other GPs to make inferences about the underlying function.

First, generate some data from a Gaussian process (it is not essential to understand the details of this):

```
clear all, close all

meanfunc = {@meanSum, {@meanLinear, @meanConst}}; hyp.mean = [0.5; 1];
covfunc = {@covMaterniso, 3}; ell = 1/4; sf = 1; hyp.cov = log([ell; sf]);
likfunc = @likGauss; sn = 0.1; hyp.lik = log(sn);

n = 20;
x = gpml_randn(0.3, n, 1);
K = feval(covfunc{:}, hyp.cov, x);
mu = feval(meanfunc{:}, hyp.mean, x);
y = chol(K)'*gpml_randn(0.15, n, 1) + mu + exp(hyp.lik)*gpml_randn(0.2, n, 1);

plot(x, y, '+')
```

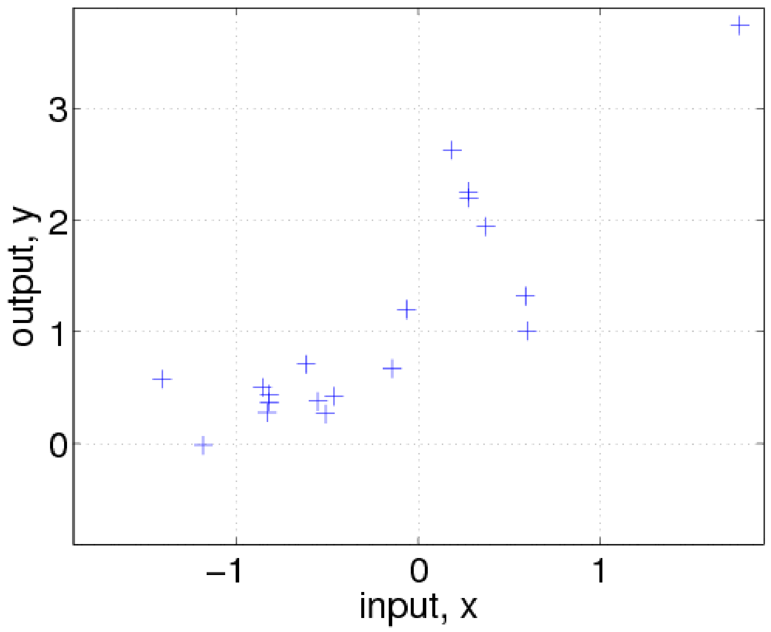
Above, we first specify the mean function `meanfunc`, covariance function `covfunc` of a GP and a likelihood function, `likfunc`. The corresponding hyperparameters are specified in the `hyp` structure:

The **mean function** is composite, adding (using `meanSum` function) a linear (`meanLinear`) and a constant (`meanConst`) to get an affine function. Note, how the different components are composed using cell arrays. The hyperparameters for the mean are given in `hyp.mean` and consists of a single (because the input will one dimensional, i.e. `D=1`) slope (set to 0.5) and an off-set (set to 1). The number and the order of these hyperparameters conform to the mean function specification. You can find out how many hyperparameters a mean (or covariance or likelihood function) expects by calling it without arguments, such as `feval(meanfunc{:})`. For more information on mean functions see meanFunctions and the directory mean/.

The **covariance function** is of the Matérn form with isotropic distance measure covMaterniso. This covariance function is also composite, as it takes a constant (related to the smoothness of the GP), which in this case is set to 3. The covariance function takes two hyperparameters, a characteristic length-scale `ell` and the standard deviation of the signal `sf`. Note, that these positive parameters are represented in `hyp.cov` using their logarithms. For more information on covariance functions see covFunctions and cov/.

Finally, the **likelihood function** is specified to be Gaussian. The standard deviation of the noise `sn` is set to 0.1. Again, the representation in the `hyp.lik` is given in terms of its logarithm. For more information about likelihood functions, see likFunctions and lik/.

Then, we generate a dataset with `n=20` examples. The inputs `x` are drawn from a unit Gaussian (using the `gpml_randn` utility, which generates unit Gaussian pseudo random numbers with a specified seed). We then evaluate the covariance matrix `K` and the mean vector `m` by calling the corresponding functions with the hyperparameters and the input locations `x`. Finally, the targets `y` are computed by drawing randomly from a Gaussian with the desired covariance and mean and adding Gaussian noise with standard deviation `exp(hyp.lik)`. The above code is a bit special because we explicitly call the mean and covariance functions (in order to generate samples from a GP); ordinarily, we would only directly call the gp function.

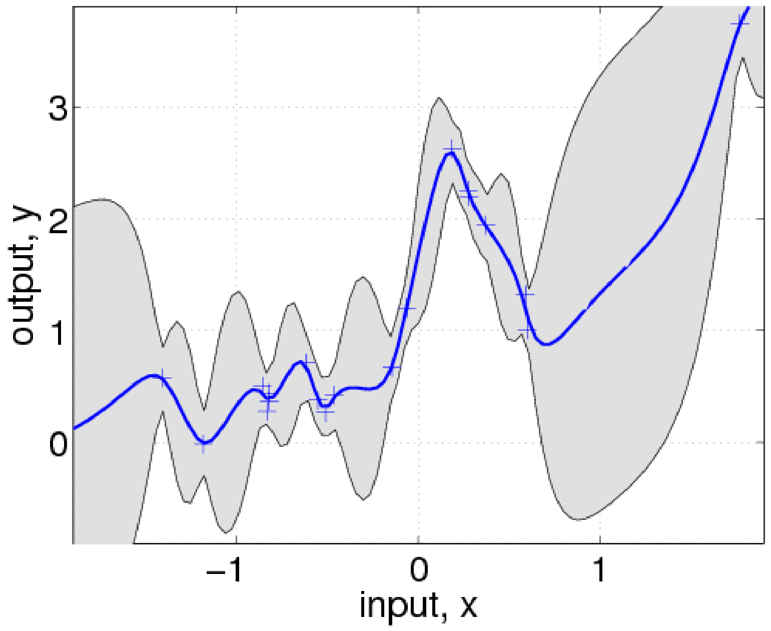


Let's ask the model to compute the (joint) negative log probability (density) `nlml` (also called marginal likelihood or evidence) and to generalize from the training data to other (test) inputs `z`:

```
nlml = gp(hyp, @infGaussLik, meanfunc, covfunc, likfunc, x, y)

z = linspace(-1.9, 1.9, 101)';
[m s2] = gp(hyp, @infGaussLik, meanfunc, covfunc, likfunc, x, y, z);

f = [m+2*sqrt(s2); flipdim(m-2*sqrt(s2),1)];
fill([z; flipdim(z,1)], f, [7 7 7]/8)
hold on; plot(z, m); plot(x, y, '+')
```

The `gp` function is called with a struct of hyperparameters `hyp`, and inference method, in this case @infGaussLik for exact inference and the mean, covariance and likelihood functions, as well as the inputs and outputs of the training data. With no test inputs, `gp` returns the negative log probability of the training data, in this example `nlml=11.97`.

To compute the predictions at test locations we add the test inputs `z` as a final argument, and `gp` returns the mean `m` variance `s2` at the test location. The program is using algorithm 2.1 from the GPML book. Plotting the mean function plus/minus two standard deviations (corresponding to a 95% confidence interval):

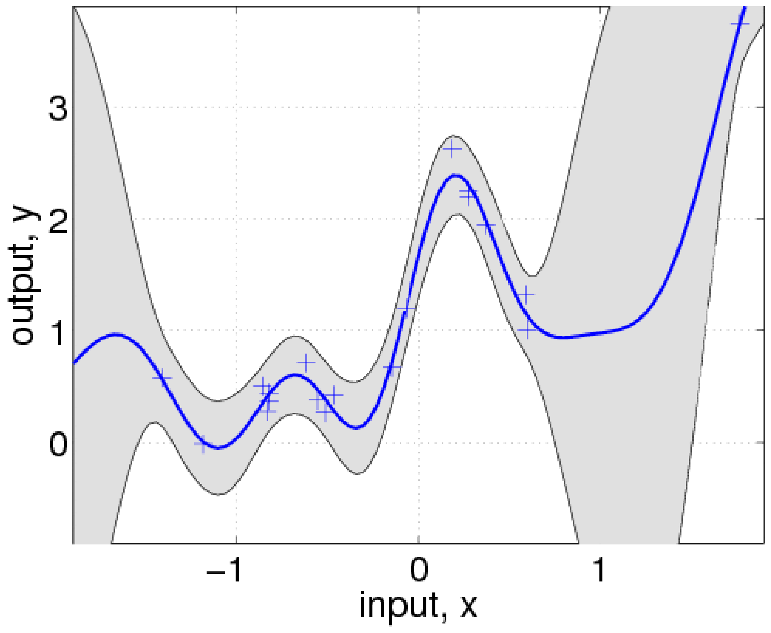


Typically, we would not a priori know the values of the hyperparameters `hyp`, let alone the form of the mean, covariance or likelihood functions. So, let's pretend we didn't know any of this. We assume a particular structure and learn suitable hyperparameters:

```
covfunc = @covSEiso; hyp2.cov = [0; 0]; hyp2.lik = log(0.1);

hyp2 = minimize(hyp2, @gp, -100, @infGaussLik, [], covfunc, likfunc, x, y);
exp(hyp2.lik)
nlml2 = gp(hyp2, @infGaussLik, [], covfunc, likfunc, x, y)

[m s2] = gp(hyp2, @infGaussLik, [], covfunc, likfunc, x, y, z);
f = [m+2*sqrt(s2); flipdim(m-2*sqrt(s2),1)];
fill([z; flipdim(z,1)], f, [7 7 7]/8)
hold on; plot(z, m); plot(x, y, '+')
```

First, we guess that a squared exponential covariance function `covSEiso` may be suitable. This covariance function takes two hyperparameters: a characteristic length-scale and a signal standard deviation (magnitude). These hyperparameters are non-negative and represented by their logarithms; thus, initializing `hyp2.cov` to zero, correspond to unit characteristic length-scale and unit signal standard deviation. The likelihood hyperparameter in `hyp2.lik` is also initialized. We assume that the mean function is zero, so we simply ignore it (and when in the following we call gp, we give an empty argument for the mean function).

In the following line, we optimize over the hyperparameters, by minimizing the negative log marginal likelihood w.r.t. the hyperparameters. The third parameter in the call to minimize limits the number of function evaluations to a maximum of 100. The inferred noise standard deviation is `exp(hyp2.lik)=0.15`, somewhat larger than the one used to generate the data (0.1). The final negative log marginal likelihood is `nlml2=14.13`, showing that the joint probability (density) of the training data is about `exp(14.13-11.97)=8.7` times smaller than for the setup actually generating the data. Finally, we plot the predictive distribution.

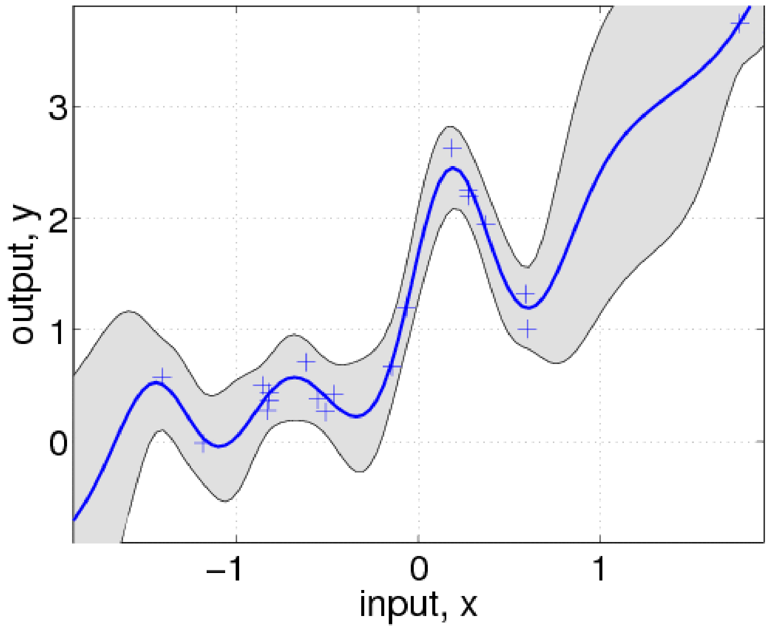


This plot shows clearly, that the model is indeed quite different from the generating process. This is due to the different specifications of both the mean and covariance functions. Below we'll try to do a better job, by allowing more flexibility in the specification.

Note that the confidence interval in this plot is the confidence for the distribution of the (noisy) *data*. If instead you want the confidence region for the underlying *function*, you should use the 3rd and 4th output arguments from gp as these refer to the latent process, rather than the data points.

```
hyp.cov = [0; 0]; hyp.mean = [0; 0]; hyp.lik = log(0.1);
hyp = minimize(hyp, @gp, -100, @infGaussLik, meanfunc, covfunc, likfunc, x, y);
[m s2] = gp(hyp, @infGaussLik, meanfunc, covfunc, likfunc, x, y, z);

f = [m+2*sqrt(s2); flipdim(m-2*sqrt(s2),1)];
fill([z; flipdim(z,1)], f, [7 7 7]/8)
hold on; plot(z, m); plot(x, y, '+');
```

Here, we have changed the specification by adding the affine mean function. All the hyperparameters are learnt by optimizing the marginal likelihood.



This shows that a much better fit is achieved when allowing a mean function (although the covariance function is still different from that of the generating process).

Guiding marginal likelihood optimisation with a hyperprior

It can be usefull to put a prior distribution on (a part of) the hyperparameters. Sometimes, one may want to exclude some hyperparameters from the optimisation i.e. fix their values beforehand and treat them as constants.

In these cases, a hyperprior comes to bear. A hyperprior is specified by augmenting the `inf` parameter of `gp.m` In the regression before, we had `inf = @infGaussLik;`. To put a Gaussian prior on the first mean hyperparameter `hyp.mean(1)` and a Laplacian prior on the second mean hyperparameter `hyp.mean(2)` and wished to fix the noise variance hyperparameter `hyp.lik`, we simple need to set up the corresponding `prior` structure as detailed below.

```
  mu = 1.0; s2 = 0.01^2;
  prior.mean = {{@priorGauss,mu,s2}; {'priorLaplace',mu,s2}};
  prior.lik = {{@priorDelta}};
  inf = {@infPrior,@infGaussLik,prior};
  hyp = minimize(hyp, @gp, -100, inf, meanfunc, covfunc, likfunc, x, y);
```

Further examples are provided in usagePrior.

4b) Sparse Approximate Regression based on inducing inputs

In case the number of training inputs x exceeds a few thousands, exact inference takes too long. We offer the sparse approximations to deal with these cases. The general idea is to use inducing points u and to base the computations on cross-covariances between training, test and inducing points only. See demoSparse for a quick overview over possible options.

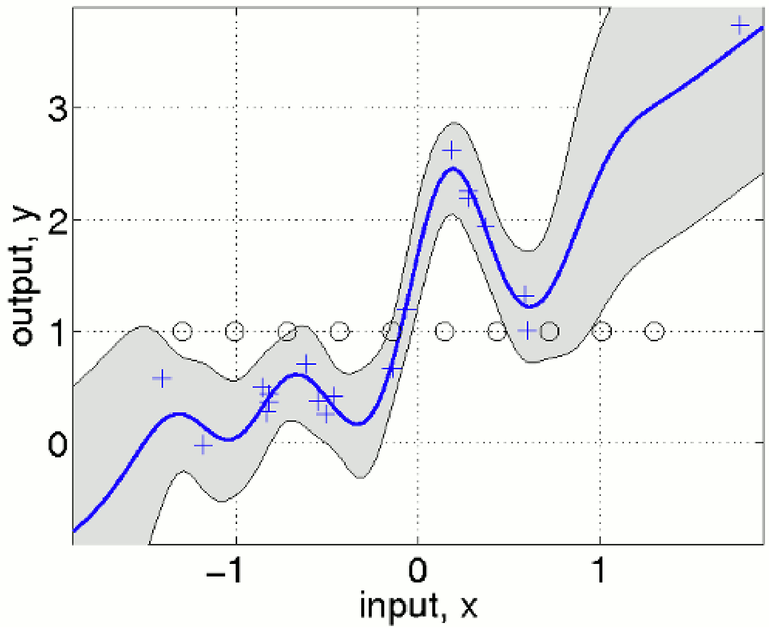
Using sparse approximations is very simple, we just have to wrap the covariance function `covfunc` into apxSparse.m and call gp.m with the inference method infGaussLik.m as demonstrated by the following lines of code.

```
  nu = fix(n/2); u = linspace(-1.3,1.3,nu)';
  covfuncF = {@apxSparse, {covfunc}, u};
  inf = @(varargin) infGaussLik(varargin{:}, struct('s', 0.0));
  [mF s2F] = gp(hyp, inf, meanfunc, covfuncF, likfunc, x, y, z);
```

In this code, a sparse approximate covariance function is defined by composing the `apxSparse` function with a covariance function and a set of inducing inputs. Further, an inference method `inf` is defined by concatenating the `struct('s', 0.0)` to the `infGaussLik` inference method. The value of the appended `s` can be used to chose between `s=1` for Fully Independent Training Conditional (FITC) approximation, or `s=0` corresponding the Variational Free Energy (VFE) approximation, or intermediate values of `0<s<1` corresponding to Sparse Power Expectation Propagation (SPEP).

We define equispaced inducing points `u` that are shown in the figure as black circles. Note that the predictive variance is overestimated outside the support of the inducing inputs. In a multivariate example where densely sampled inducing inputs are infeasible, one can simply use a random subset of the training points.

```
  nu = fix(n/2); iu = randperm(n); iu = iu(1:nu); u = x(iu,:);
```



Another possibility is to specify the inducing inputs as a part of the hyperparmeters using the field `hyp.xu`

```
hyp.xu = u;
```

in which case optimization of the hyperparameters will also optimize the inducing inputs (note that, when inducing inputs are given as a field in the hyperparameters, then these take precedence over inducing inputs specified in to the `apxSparse` function).

4c) Large scale regression exploiting grid structure

A covariance function factorising over coordinate axes evaluated on a rectilinear (not necessarily equispaced) grid of data points leads to a covariance matrix with Kronecker structure. This can be exploited to scale GPs beyond the O(n^3) limit. Observations not located on the grid can be interpolated from the grid values. The example below contains the most relevant code from the script demoGrid2d, where we extrapolate a pixel image beyond its boundaries. An instructive example in 1d can be found in demoGrid1d.

For a comprehensive set of examples and more resources, see a website by Andrew Wilson.

We start off by setting up the training data and the GP on a [-2,2]x[-3,3] lattice with 15600 pixels -- a size where a usual dense GP would be computationally infeasible. We use a lattice only for the purpose of visualisation.

```
x1 = linspace(-2,2,120); x2 = linspace(-3,3,130);
x = apxGrid('expand',{x1',x2'});
y = sin(x(:,2)) + x(:,1) + 0.1*gpml_randn(1,[size(x,1),1]);
```

Then, we define the locations where we would like to have the predictions i.e. a [-4,4]x[-6,6] lattice to see the result of the extrapolation.

```
xs1 = linspace(-4,4,100); xs2 = linspace(-6,6,110);
xs = apxGrid('expand',{xs1',xs2'});
```

Next, we construct the grid for KISS/SKI GP using an auxiliary function so that both training data `x` and the test data `xs` are properly covered.

```
xg = apxGrid('create',[x;xs],true,[50,70]);
```

Now that the data set is well-defined, we specify our GP model along with initial values for the hyperparameter by wrapping the covariance functions into `apxGrid`, GPML's grid-based covariance approximation method.

```
cov = {{@covSEiso},{@covSEiso}}; covg = {@apxGrid,cov,xg};
mean = {@meanZero}; lik = {@likGauss};
hyp.cov = zeros(4,1); hyp.mean = []; hyp.lik = log(0.1);
```

As a next step, we perform hyperparameter optimisation as with a usual GP model using the inference method `infGaussLik` which only supports `likGauss`. In order to do so, we specify parameters for the LCG: the maximum number of iterations and the convergence threshold via the `opt` variable.

```
opt.cg_maxit = 200; opt.cg_tol = 5e-3;
infg = @(varargin) infGaussLik(varargin{:},opt);
hyp = minimize(hyp,@gp,-50,infg,[],covg,[],x,y);
```

Finally, we make use of grid interpolation to compute predictions very rapidly with the `post.predict` utility provided by the `infGrid` method.

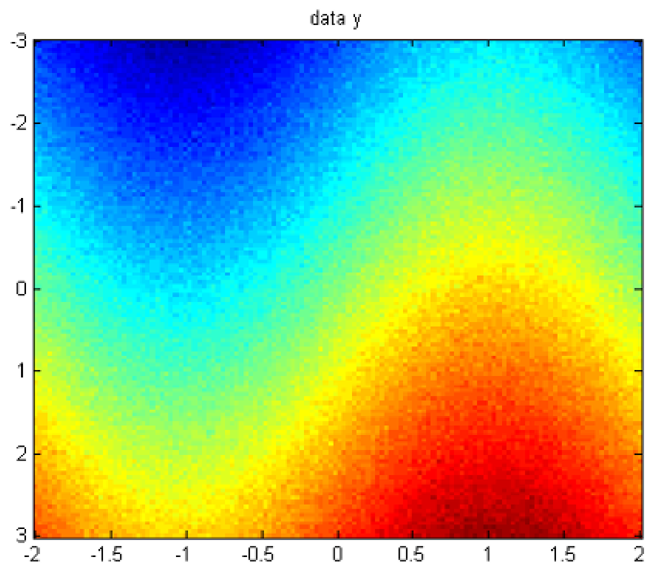
```
[post,nlZ,dnlZ] = infGrid(hyp,{@meanZero},covg,{@likGauss},x,y,opt);
[fm,fs2,ym,ys2] = post.predict(xs);
```

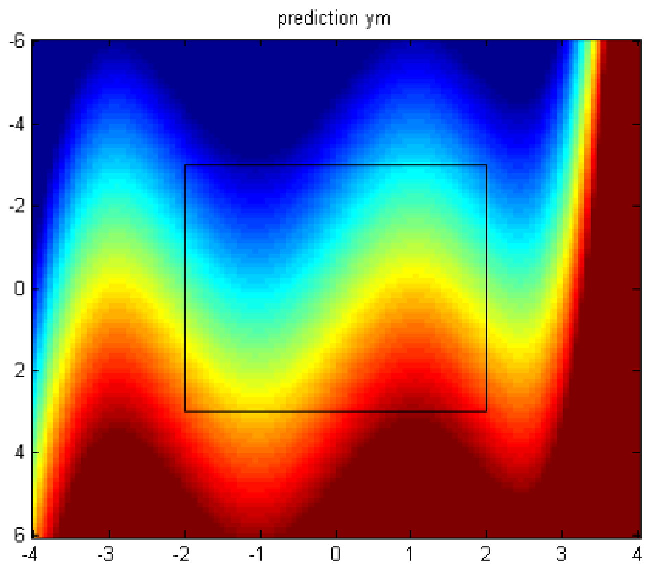
Alternatively, we can use the usual pathway based on `gp`,

```
post.L = @(a) zeros(size(a));
ym = gp(hyp,infg,[],covg,[],x,post,xs);
```

where we have switched of the predictive variance computations as they are very demanding to evaluate on an entire lattice. If the are required for a larger set of test points `xs`, one can resort to sampling-based estimates.

The figure below summarizes what we have done. On the left, we see the training data and on the right the GP predictive mean.





4d) Exercises for the reader

Inference Methods

Try using Expectation Propagation instead of exact inference in the above, by exchanging `@infGaussLik` with `@infEP`. You get exactly identical results, why?

Mean or Covariance

Try training a GP where the affine part of the function is captured by the *covariance function* instead of the *mean function*. That is, use a GP with no explicit mean function, but further additive contributions to the covariance. How would you expect the marginal likelihood to compare to the previous case?

4e) Classification

You can either follow the example here on this page, or use the script demoClassification.

The difference between regression and classification isn't of fundamental nature. We can use a Gaussian process latent function in essentially the same way, it is just that the Gaussian likelihood function often used for regression is inappropriate for classification. And since exact inference is only possible for Gaussian likelihood, we also need an alternative, approximate, inference method.

Here, we will demonstrate binary classification, using two partially overlapping Gaussian sources of data in two dimensions. First we generate the data:

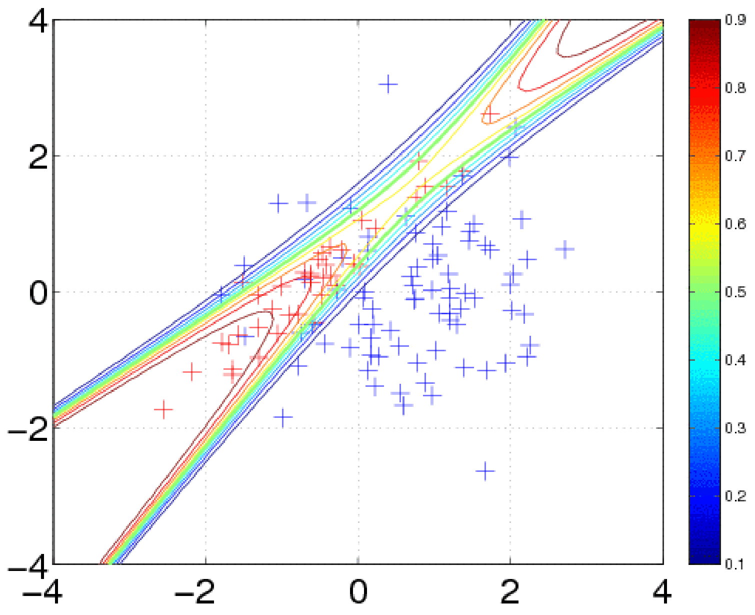
```
clear all, close all

n1 = 80; n2 = 40;                   % number of data points from each class
S1 = eye(2); S2 = [1 0.95; 0.95 1];           % the two covariance matrices
m1 = [0.75; 0]; m2 = [-0.75; 0];                            % the two means

x1 = bsxfun(@plus, chol(S1)'*gpml_randn(0.2, 2, n1), m1);
x2 = bsxfun(@plus, chol(S2)'*gpml_randn(0.3, 2, n2), m2);

x = [x1 x2]'; y = [-ones(1,n1) ones(1,n2)]';
plot(x1(1,:), x1(2,:), 'b+'); hold on;
plot(x2(1,:), x2(2,:), 'r+');
```

120 data points are generated from two Gaussians with different means and covariances. One Gaussian is isotropic and contains 2/3 of the data (blue), the other is highly correlated and contains 1/3 of the points (red). Note, that the labels for the targets are ±1 (and **not** 0/1).

In the plot, we superimpose the data points with the posterior equi-probability contour lines for the probability of class two given complete information about the generating mechanism

```
[t1 t2] = meshgrid(-4:0.1:4,-4:0.1:4);
t = [t1(:) t2(:)]; n = length(t);                 % these are the test inputs
tmm = bsxfun(@minus, t, m1');
p1 = n1*exp(-sum(tmm*inv(S1).*tmm/2,2))/sqrt(det(S1));
tmm = bsxfun(@minus, t, m2');
```

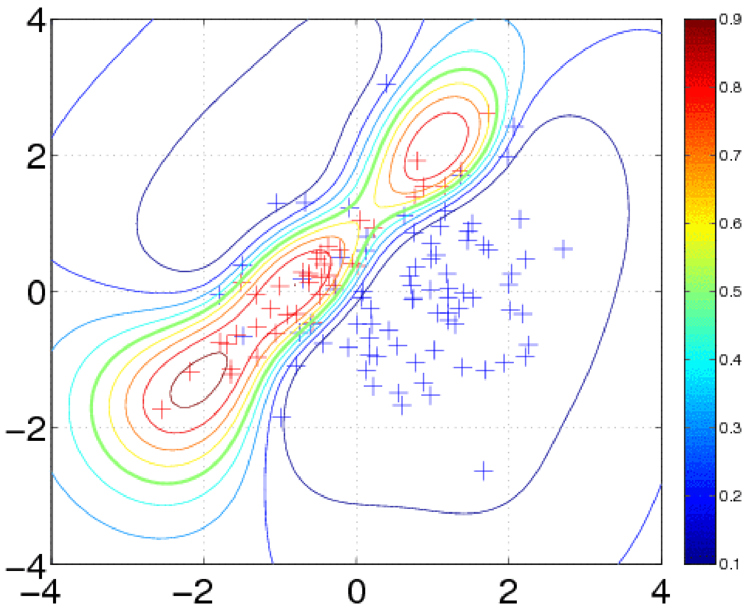
```
  p2 = n2*exp(-sum(tmm*inv(S2).*tmm/2,2))/sqrt(det(S2));
  contour(t1, t2, reshape(p2./(p1+p2), size(t1)), [0.1:0.1:0.9]);
```



We specify a Gaussian process model as follows: a constant mean function, with initial parameter set to 0, a squared exponential with automatic relevance determination (ARD) covariance function covSEard. This covariance function has one characteristic length-scale parameter for each dimension of the input space, and a signal magnitude parameter, for a total of 3 parameters (as the input dimension is `D=2`). ARD with separate length-scales for each input dimension is a very powerful tool to learn which inputs are important for predictions: if length-scales are short, inputs are very important, and when they grow very long (compared to the spread of the data), the corresponding inputs will be largely ignored. Both length-scales and the signal magnitude are initialized to 1 (and represented in the log space). Finally, the likelihood function likErf has the shape of the error-function (or cumulative Gaussian), which doesn't take any hyperparameters (so `hyp.lik` does not exist).

```
  meanfunc = @meanConst; hyp.mean = 0;
  covfunc = @covSEard; ell = 1.0; sf = 1.0; hyp.cov = log([ell ell sf]);
  likfunc = @likErf;

  hyp = minimize(hyp, @gp, -40, @infEP, meanfunc, covfunc, likfunc, x, y);
  [a b c d lp] = gp(hyp, @infEP, meanfunc, covfunc, likfunc, x, y, t, ones(n, 1));

  plot(x1(1,:), x1(2,:), 'b+'); hold on; plot(x2(1,:), x2(2,:), 'r+')
  contour(t1, t2, reshape(exp(lp), size(t1)), [0.1:0.1:0.9]);
```

We train the hyperparameters using minimize, to minimize the negative log marginal likelihood. We allow for `40` function evaluations, and specify that inference should be done with the Expectation Propagation (EP) inference method @infEP, and pass the usual parameters. Training is done using algorithm 3.5 and 5.2 from the gpml book. When computing test probabilities, we call `gp` with additional test inputs, and as the last argument a vector of targets for which the log probabilities `lp` should be computed. The fist four output arguments of the function are mean and variance for the targets and corresponding latent variables respectively. The test set predictions are computed using algorithm 3.6 from the GPML book. The contour plot for the predictive distribution is shown below. Note, that the predictive probability is fairly close to the probabilities of the generating process in regions of high data density. Note also, that as you move away from the data, the probability approaches 1/3, the overall class probability.



Examining the two ARD characteristic length-scale parameters after learning, you will find that they are fairly similar, reflecting the fact that for this data set, both inputs important.

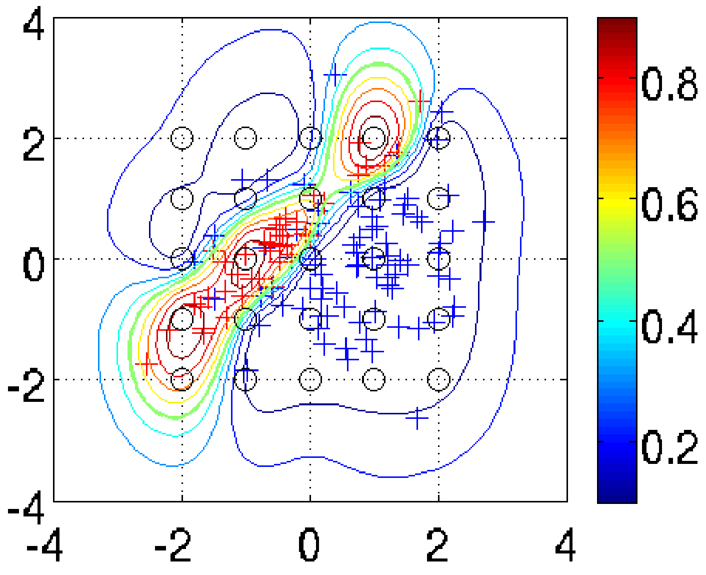
Large scale classification using the FITC approximation

In case the number of training inputs x exceeds a few hundreds, approximate inference using infLaplace.m, infEP.m and infVB.m takes too long. As in regression, we offer the FITC approximation based on a low-rank plus diagonal approximation to the exact covariance to deal with these cases. The general idea is to use inducing points u and to base the computations on cross-covariances between training, test and inducing points only.

Using the FITC approximation is very simple, we just have to wrap the covariance function `covfunc` into apxSparse.m and call gp.m with the inference methods infLaplace.m or infVB.m as demonstrated by the following lines of code.

```
[u1,u2] = meshgrid(linspace(-2,2,5)); u = [u1(:),u2(:)]; clear u1; clear u2
nu = size(u,1);
covfuncF = {@apxSparse, {covfunc}, u};
inffunc = @infLaplace;                                       % or infEP
hyp = minimize(hyp, @gp, -40, inffunc, meanfunc, covfuncF, likfunc, x, y);
[a b c d lp] = gp(hyp, inffunc, meanfunc, covfuncF, likfunc, x, y, t, ones(n,1));
```

We define equispaced inducing points u that are shown in the figure as black circles. Alternatively, a random subset of the training points can be used as inducing points.



Large scale classification exploiting the grid structure

Similar to regression using `infGaussLik`, we can perform approximate inference using `infLaplace` to scale GPs beyond the O(n³) limit. Please visit the website by Seth Flaxman for an extended example and related datasets.

Exercise for the reader

Inference Methods
: Use the Laplace Approximation for inference `@infLaplace`, and compare the approximate marginal likelihood for the two methods. Which approximation is best?

Covariance Function
: Try using the squared exponential with isotropic distance measure `covSEiso` instead of ARD distance measure `covSEard`. Which is best?

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