Gaussian processes

March 19, 2018

This article is an export of the Gaussian processes (https://nbviewer.jupyter.org /github/krasserm/bayesian-machine-learning/blob/master /gaussian_processes.ipynb) notebook which is part of the bayesian-machine-learning (https://github.com/krasserm/bayesian-machine-learning) repo on Github.

Open in Colab
(https://colab.research.google.com/github/krasserm/bayesian-machine-learning/blob/master/gaussian_processes.ipynb)

Introduction

In supervised learning, we often use parametric models $p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta})$ to explain data and infer optimal values of parameter $\boldsymbol{\theta}$ via maximum likelihood (https://en.wikipedia.org/wiki/Maximum_likelihood_estimation) or maximum a posteriori (https://de.wikipedia.org/wiki/Maximum_a_posteriori) estimation. If needed we can also infer a full posterior distribution (https://en.wikipedia.org/wiki/Posterior_probability) $p(\boldsymbol{\theta}|\mathbf{X}, \mathbf{y})$ instead of a point estimate $\hat{\boldsymbol{\theta}}$. With increasing data complexity, models with a higher number of parameters are usually needed to explain data reasonably well. Methods that use models with a fixed number of parameters are called parametric methods.

In non-parametric methods, on the other hand, the number of parameters depend on the dataset size. For example, in Nadaraya-Watson kernel regression (https://en.wikipedia.org/wiki/Kernel_regression), a weight w_i is assigned to each observed target y_i and for predicting the target value at a new point $\mathbf{x}$ a weighted average is computed:

$$f(\mathbf{x}) = \sum_{i=1}^{N} w_i(\mathbf{x}) y_i$$

$$w_i(\mathbf{x}) = \frac{\kappa(\mathbf{x}, \mathbf{x}_i)}{\sum_{i'=1}^{N} \kappa(\mathbf{x}, \mathbf{x}_{i'})}$$

Observations that are closer to $\mathbf{x}$ have a higher weight than observations that are further away. Weights are computed from $\mathbf{x}$ and observed $\mathbf{x}_i$ with a kernel κ. A special case is k-nearest neighbors (KNN) where the k closest observations have a weight $1/k$, and all others have weight 0. Non-parametric methods often need to process all training data for prediction and are therefore slower at inference time than parametric methods. On the other hand, training is usually faster as non-parametric models only need to remember training data.

Another example of non-parametric methods are Gaussian processes (https://en.wikipedia.org/wiki/Gaussian_process) (GPs). Instead of inferring a distribution over the parameters of a parametric function Gaussian processes can be used to infer a distribution over functions directly. A Gaussian process defines a prior over functions. After having observed some function values it can be converted into a posterior over functions. Inference of continuous function values in this context is known as GP regression but GPs can also be used for classification.

A Gaussian process is a random process (https://en.wikipedia.org /wiki/Stochastic_process) where any point $\mathbf{x} \in \mathbb{R}^d$ is assigned a random variable $f(\mathbf{x})$ and where the joint distribution of a finite number of these variables $p(f(\mathbf{x}_1), \dots, f(\mathbf{x}_N))$ is itself Gaussian:

$$p(\mathbf{f}|\mathbf{X}) = \mathcal{N}(\mathbf{f}|\boldsymbol{\mu}, \mathbf{K}) \tag{1}$$

In Equation (1), $\mathbf{f} = (f(\mathbf{x}_1), \dots, f(\mathbf{x}_N))$, $\boldsymbol{\mu} = (m(\mathbf{x}_1), \dots, m(\mathbf{x}_N))$ and $K_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j)$. m is the mean function and it is common to use $m(\mathbf{x}) = 0$ as GPs are flexible enough to model the mean arbitrarily well. κ is a positive definite *kernel function* or *covariance function*. Thus, a Gaussian process is a distribution over functions whose shape (smoothness, ...) is defined by $\mathbf{K}$. If points $\mathbf{x}_i$ and $\mathbf{x}_j$ are considered to be similar by the kernel the function values at these points, $f(\mathbf{x}_i)$ and $f(\mathbf{x}_j)$, can be expected to be similar too.

A GP prior $p(\mathbf{f}|\mathbf{X})$ can be converted into a GP posterior $p(\mathbf{f}|\mathbf{X}, \mathbf{y})$ after having observed some data $\mathbf{y}$. The posterior can then be used to make predictions $\mathbf{f}_*$ given new input $\mathbf{X}_*$:

$$\begin{aligned} p(\mathbf{f}_* | \mathbf{X}_*, \mathbf{X}, \mathbf{y}) &= \int p(\mathbf{f}_* | \mathbf{X}_*, \mathbf{f}) p(\mathbf{f} | \mathbf{X}, \mathbf{y})\, d\mathbf{f} \\ &= \mathcal{N}(\mathbf{f}_* | \boldsymbol{\mu}_*, \boldsymbol{\Sigma}_*) \end{aligned} \tag{2}$$

Equation (2) is the posterior predictive distribution which is also a Gaussian with mean $\boldsymbol{\mu}_*$ and $\boldsymbol{\Sigma}_*$. By definition of the GP, the joint distribution of observed data $\mathbf{y}$ and predictions $\mathbf{f}_*$ is

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N} \left(\mathbf{0}, \begin{pmatrix} \mathbf{K}_y & \mathbf{K}_* \\ \mathbf{K}_*^T & \mathbf{K}_{**} \end{pmatrix} \right) \tag{3}$$

With N training data and N_* new input data, $\mathbf{K}_y = \kappa(\mathbf{X}, \mathbf{X}) + \sigma_y^2 \mathbf{I} = \mathbf{K} + \sigma_y^2 \mathbf{I}$ is $N \times N$, $\mathbf{K}_* = \kappa(\mathbf{X}, \mathbf{X}_*)$ is $N \times N_*$ and $\mathbf{K}_{**} = \kappa(\mathbf{X}_*, \mathbf{X}_*)$ is $N_* \times N_*$. σ_y^2 is the noise term in the diagonal of $\mathbf{K_y}$. It is set to zero if training targets are noise-free and to a value greater than zero if observations are noisy. The mean is set to $\mathbf{0}$ for notational simplicity. The sufficient statistics of the posterior predictive distribution, $\boldsymbol{\mu}_*$ and $\boldsymbol{\Sigma}_*$, can be computed with[1][3]

$$\boldsymbol{\mu}_* = \mathbf{K}_*^T \mathbf{K}_y^{-1} \mathbf{y} \tag{4}$$

$$\boldsymbol{\Sigma}_* = \mathbf{K}_{**} - \mathbf{K}_*^T \mathbf{K}_y^{-1} \mathbf{K}_* \tag{5}$$

This is the minimum we need to know for implementing Gaussian processes and applying them to regression problems. For further details, please consult the literature in the References section. The next section shows how to implement GPs with plain NumPy from scratch, later sections demonstrate how to use GP implementations from scikit-learn (http://scikit-learn.org/stable/) and GPy (http://sheffieldml.github.io/GPy/).

Implementation with NumPy

Here, we will use the squared exponential kernel, also known as Gaussian kernel or RBF kernel:

$$\kappa(\mathbf{x}_i, \mathbf{x}_j) = \sigma_f^2 \exp(-\frac{1}{2l^2} (\mathbf{x}_i - \mathbf{x}_j)^T (\mathbf{x}_i - \mathbf{x}_j)) \tag{6}$$

The length parameter l controls the smoothness of the function and σ_f the vertical variation. For simplicity, we use the same length parameter l for all input dimensions (isotropic kernel).

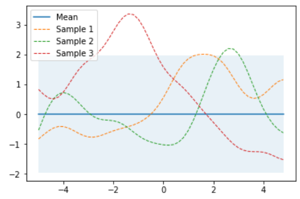
```
import numpy as np

def kernel(X1, X2, l=1.0, sigma_f=1.0):
    '''
    Isotropic squared exponential kernel. Computes
    a covariance matrix from points in X1 and X2.

    Args:
        X1: Array of m points (m x d).
        X2: Array of n points (n x d).

    Returns:
        Covariance matrix (m x n).
    '''
    sqdist = np.sum(X1**2, 1).reshape(-1, 1) + np.sum(X2**2, 1) - 2 * np.dot(X1, X2.T)
    return sigma_f**2 * np.exp(-0.5 / l**2 * sqdist)
```

There are many other kernels that can be used for Gaussian processes. See [3] for a detailed reference or the scikit-learn documentation for some examples (http://scikit-learn.org/stable/modules/gaussian_process.html#gp-kernels).

Prior

Let's first define a prior over functions with mean zero and a covariance matrix computed with kernel parameters $l = 1$ and $\sigma_f = 1$. To draw random functions from that GP we draw random samples from the corresponding multivariate normal. The following example draws three random samples and plots it together with the zero mean and the 95% confidence interval (computed from the diagonal of the covariance matrix).

```
%matplotlib inline

from gaussian_processes_util import plot_gp

# Finite number of points
X = np.arange(-5, 5, 0.2).reshape(-1, 1)

# Mean and covariance of the prior
mu = np.zeros(X.shape)
cov = kernel(X, X)

# Draw three samples from the prior
samples = np.random.multivariate_normal(mu.ravel(), cov, 3)

# Plot GP mean, confidence interval and samples
plot_gp(mu, cov, X, samples=samples)
```



The `plot_gp` function is defined here (https://github.com/krasserm/bayesian-machine-learning/blob/af6882305d9d65dbbf60fd29b117697ef250d4aa/gaussian_processes_util.py#L7).

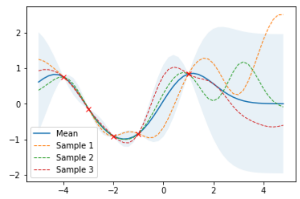
Prediction from noise-free training data

To compute the sufficient statistics i.e. mean and covariance of the posterior predictive distribution we implement Equations (4) and (5)

```
from numpy.linalg import inv

def posterior_predictive(X_s, X_train, Y_train, l=1.0, sigma_f=1.0, sigma_y=1e-8):
    '''
    Computes the suffifient statistics of the GP posterior predictive distribution
    from m training data X_train and Y_train and n new inputs X_s.

    Args:
        X_s: New input locations (n x d).
        X_train: Training locations (m x d).
        Y_train: Training targets (m x 1).
        l: Kernel length parameter.
        sigma_f: Kernel vertical variation parameter.
        sigma_y: Noise parameter.

    Returns:
        Posterior mean vector (n x d) and covariance matrix (n x n).
    '''
    K = kernel(X_train, X_train, l, sigma_f) + sigma_y**2 * np.eye(len(X_train))
    K_s = kernel(X_train, X_s, l, sigma_f)
    K_ss = kernel(X_s, X_s, l, sigma_f) + 1e-8 * np.eye(len(X_s))
    K_inv = inv(K)

    # Equation (4)
    mu_s = K_s.T.dot(K_inv).dot(Y_train)

    # Equation (5)
    cov_s = K_ss - K_s.T.dot(K_inv).dot(K_s)

    return mu_s, cov_s
```

and apply them to noise-free training data `X_train` and `Y_train`. The following example draws three samples from the posterior predictive and plots them along with the mean, confidence interval and training data. In a noise-free model, variance at the training points is zero and all random functions drawn from the posterior go through the trainig points.

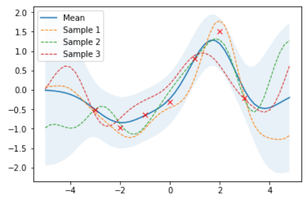
```
# Noise free training data
X_train = np.array([-4, -3, -2, -1, 1]).reshape(-1, 1)
Y_train = np.sin(X_train)

# Compute mean and covariance of the posterior predictive distribution
mu_s, cov_s = posterior_predictive(X, X_train, Y_train)

samples = np.random.multivariate_normal(mu_s.ravel(), cov_s, 3)
plot_gp(mu_s, cov_s, X, X_train=X_train, Y_train=Y_train, samples=samples)
```



Prediction from noisy training data

If some noise is included in the model, training points are only approximated and the variance at the training points is non-zero.

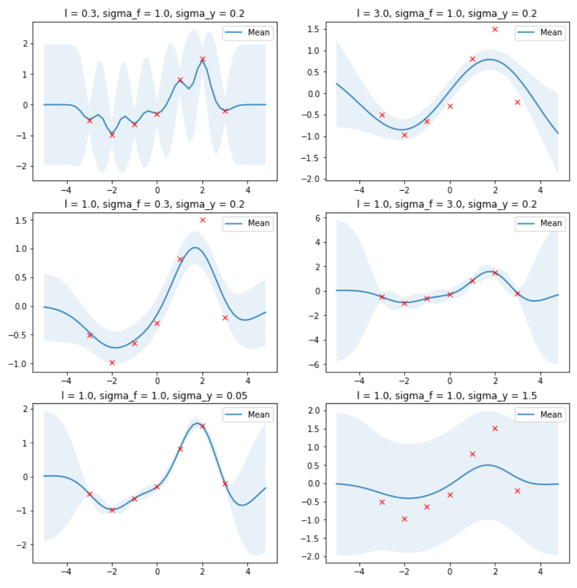
```
noise = 0.4

# Noisy training data
X_train = np.arange(-3, 4, 1).reshape(-1, 1)
Y_train = np.sin(X_train) + noise * np.random.randn(*X_train.shape)

# Compute mean and covariance of the posterior predictive distribution
mu_s, cov_s = posterior_predictive(X, X_train, Y_train, sigma_y=noise)

samples = np.random.multivariate_normal(mu_s.ravel(), cov_s, 3)
plot_gp(mu_s, cov_s, X, X_train=X_train, Y_train=Y_train, samples=samples)
```



Effect of kernel parameters and noise parameter

The following example shows the effect of kernel parameters l and σ_f as well as the noise parameter σ_y. Higher l values lead to smoother functions and therefore to coarser approximations of the training data. Lower l values make functions more wiggly with wide confidence intervals between training data points. σ_f controls the vertical variation of functions drawn from the GP. This can be seen by the wide confidence intervals outside the training data region in the right figure of the second row. σ_y represents the amount of noise in the training data. Higher σ_y values make more coarse approximations which avoids overfitting to noisy data.

```
import matplotlib.pyplot as plt

params = [
    (0.3, 1.0, 0.2),
    (3.0, 1.0, 0.2),
    (1.0, 0.3, 0.2),
    (1.0, 3.0, 0.2),
    (1.0, 1.0, 0.05),
    (1.0, 1.0, 1.5),
]

plt.figure(figsize=(12, 5))

for i, (l, sigma_f, sigma_y) in enumerate(params):
    mu_s, cov_s = posterior_predictive(X, X_train, Y_train, l=l,
                                       sigma_f=sigma_f,
                                       sigma_y=sigma_y)
    plt.subplot(3, 2, i + 1)
    plt.subplots_adjust(top=2)
    plt.title(f'l = {l}, sigma_f = {sigma_f}, sigma_y = {sigma_y}')
    plot_gp(mu_s, cov_s, X, X_train=X_train, Y_train=Y_train)
```

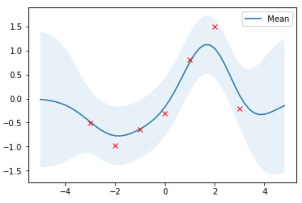


Optimal values for these parameters can be estimated by maximizing the log marginal likelihood which is given by[1][3]

$$\log p(\mathbf{y}|\mathbf{X}) = \log \mathcal{N}(\mathbf{y}|\mathbf{0}, \mathbf{K}_y) = -\frac{1}{2}\mathbf{y}^T\mathbf{K}_y^{-1}\mathbf{y} - \frac{1}{2}\log|\mathbf{K}_y| - \frac{N}{2}\log(2\pi) \quad (7)$$

In the following we will minimize the negative log marginal likelihood w.r.t. parameters l and σ_f, σ_y is set to the known noise level of the data. If the noise level is unknown, σ_y can be estimated as well along with the other parameters.

```
from numpy.linalg import cholesky, det, lstsq
from scipy.optimize import minimize

def nll_fn(X_train, Y_train, noise, naive=True):
    '''
    Returns a function that computes the negative log marginal
    likelihood for training data X_train and Y_train and given
    noise level.

    Args:
        X_train: training locations (m x d).
        Y_train: training targets (m x 1).
        noise: known noise level of Y_train.
        naive: if True use a naive implementation of Eq. (7), if
               False use a numerically more stable implementation.

    Returns:
        Minimization objective.
    '''
    def nll_naive(theta):
        # Naive implementation of Eq. (7). Works well for the examples
        # in this article but is numerically less stable compared to
        # the implementation in nll_stable below.
        K = kernel(X_train, X_train, l=theta[0], sigma_f=theta[1]) + \
            noise**2 * np.eye(len(X_train))
        return 0.5 * np.log(det(K)) + \
               0.5 * Y_train.T.dot(inv(K).dot(Y_train)) + \
               0.5 * len(X_train) * np.log(2*np.pi)

    def nll_stable(theta):
        # Numerically more stable implementation of Eq. (7) as described
        # in http://www.gaussianprocess.org/gpml/chapters/RW2.pdf, Section
        # 2.2, Algorithm 2.1.
        K = kernel(X_train, X_train, l=theta[0], sigma_f=theta[1]) + \
            noise**2 * np.eye(len(X_train))
        L = cholesky(K)
        return np.sum(np.log(np.diagonal(L))) + \
               0.5 * Y_train.T.dot(lstsq(L.T, lstsq(L, Y_train)[0])[0]) + \
               0.5 * len(X_train) * np.log(2*np.pi)

    if naive:
        return nll_naive
    else:
        return nll_stable

# Minimize the negative log-likelihood w.r.t. parameters l and sigma_f.
# We should actually run the minimization several times with different
# initializations to avoid local minima but this is skipped here for
# simplicity.
res = minimize(nll_fn(X_train, Y_train, noise), [1, 1],
               bounds=((1e-5, None), (1e-5, None)),
               method='L-BFGS-B')

# Store the optimization results in global variables so that we can
# compare it later with the results from other implementations.
l_opt, sigma_f_opt = res.x
l_opt, sigma_f_opt

# Compute the prosterior predictive statistics with optimized kernel parameters and plot th
mu_s, cov_s = posterior_predictive(X, X_train, Y_train, l=l_opt, sigma_f=sigma_f_opt, sig
plot_gp(mu_s, cov_s, X, X_train=X_train, Y_train=Y_train)
```

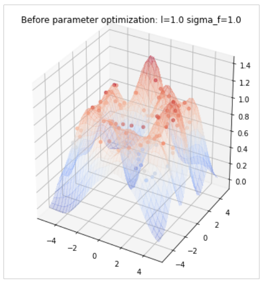


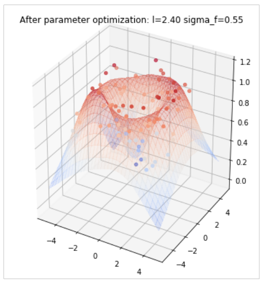
With optimized kernel parameters, training data are reasonably covered by the 95% confidence interval and the mean of the posterior predictive is a good approximation.

Higher dimensions

The above implementation can also be used for higher input data dimensions. Here, a GP is used to fit noisy samples from a sine wave originating at $\mathbf{0}$ and expanding in the x-y plane. The following plots show the noisy samples and the posterior predictive mean before and after kernel parameter optimization.

```
from gaussian_processes_util import plot_gp_2D

noise_2D = 0.1

rx, ry = np.arange(-5, 5, 0.3), np.arange(-5, 5, 0.3)
gx, gy = np.meshgrid(rx, rx)

X_2D = np.c_[gx.ravel(), gy.ravel()]

X_2D_train = np.random.uniform(-4, 4, (100, 2))
Y_2D_train = np.sin(0.5 * np.linalg.norm(X_2D_train, axis=1)) + \
             noise_2D * np.random.randn(len(X_2D_train))

plt.figure(figsize=(14,7))

mu_s, _ = posterior_predictive(X_2D, X_2D_train, Y_2D_train, sigma_y=noise_2D)
plot_gp_2D(gx, gy, mu_s, X_2D_train, Y_2D_train,
           f'Before parameter optimization: l={1.00} sigma_f={1.00}', 1)

res = minimize(nll_fn(X_2D_train, Y_2D_train, noise_2D), [1, 1],
               bounds=((1e-5, None), (1e-5, None)),
               method='L-BFGS-B')

mu_s, _ = posterior_predictive(X_2D, X_2D_train, Y_2D_train, *res.x, sigma_y=noise_2D)
plot_gp_2D(gx, gy, mu_s, X_2D_train, Y_2D_train,
           f'After parameter optimization: l={res.x[0]:.2f} sigma_f={res.x[1]:.2f}', 2)
```





Note how the true sine wave is approximated much better after parameter optimization.

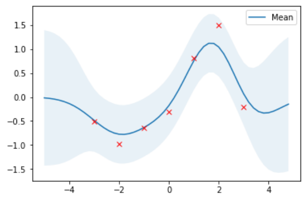
Libraries that implement GPs

This section shows two examples of libraries that provide implementations of GPs. I'll provide only a minimal setup here, just enough for reproducing the above results. For further details please consult the documentation of these libraries.

Scikit-learn

Scikit-learn provides a `GaussianProcessRegressor` for implementing GP regression models (http://scikit-learn.org/stable/modules/gaussian_process.html#gaussian-process-regression-gpr). It can be configured with pre-defined kernels and user-defined kernels (http://scikit-learn.org/stable/modules/gaussian_process.html#gp-kernels). Kernels can also be composed. The squared exponential kernel is the `RBF` kernel in scikit-learn. The `RBF` kernel only has a `length_scale` parameter which corresponds to the l parameter above. To have a σ_f parameter as well, we have to compose the `RBF` kernel with a `ConstantKernel`.

```
from sklearn.gaussian_process import GaussianProcessRegressor
from sklearn.gaussian_process.kernels import ConstantKernel, RBF

rbf = ConstantKernel(1.0) * RBF(length_scale=1.0)
gpr = GaussianProcessRegressor(kernel=rbf, alpha=noise**2)

# Reuse training data from previous 1D example
gpr.fit(X_train, Y_train)

# Compute posterior predictive mean and covariance
mu_s, cov_s = gpr.predict(X, return_cov=True)

# Obtain optimized kernel parameters
l = gpr.kernel_.k2.get_params()['length_scale']
sigma_f = np.sqrt(gpr.kernel_.k1.get_params()['constant_value'])

# Compare with previous results
assert(np.isclose(l_opt, l))
assert(np.isclose(sigma_f_opt, sigma_f))

# Plot the results
plot_gp(mu_s, cov_s, X, X_train=X_train, Y_train=Y_train)
```

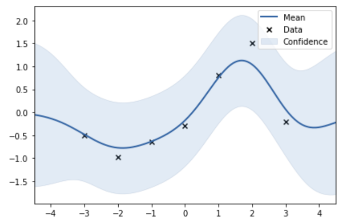


GPy

GPy (http://sheffieldml.github.io/GPy/) is a Gaussian processes framework from the Sheffield machine learning group. It provides a `GPRegression` class for implementing GP regression models. By default, `GPRegression` also estimates the noise parameter σ_y from data, so we have to `fix()` this parameter to be able to reproduce the above results.

```
import GPy

rbf = GPy.kern.RBF(input_dim=1, variance=1.0, lengthscale=1.0)
gpr = GPy.models.GPRegression(X_train, Y_train, rbf)

# Fix the noise variance to known value
gpr.Gaussian_noise.variance = noise**2
gpr.Gaussian_noise.variance.fix()

# Run optimization
gpr.optimize();

# Obtain optimized kernel parameters
l = gpr.rbf.lengthscale.values[0]
sigma_f = np.sqrt(gpr.rbf.variance.values[0])

# Compare with previous results
assert(np.isclose(l_opt, l))
assert(np.isclose(sigma_f_opt, sigma_f))

# Plot the results with the built-in plot function
gpr.plot();
```

```
 UserWarning:This figure includes Axes that are not compatible with tight_layout, so resu
```



Thanks for reading up to here :-) In another article, I'll show how Gaussian processes can be used for black-box optimization.

References

[1] Kevin P. Murphy. Machine Learning, A Probabilistic Perspective (https://mitpress.mit.edu/books/machine-learning-0), Chapters 4, 14 and 15.
[2] Christopher M. Bishop. Pattern Recognition and Machine Learning (http://www.springer.com/de/book/9780387310732), Chapter 6.
[3] Carl Edward Rasmussen and Christopher K. I. Williams. Gaussian Processes for Machine Learning (http://www.gaussianprocess.org/gpml/).

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Name

Sourab Mangrulkar • 5 months ago
Thank you for this great post! Helped me a lot in clarifying my understanding of Gaussian Processes.
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Martin Krasser Mod Sourab Mangrulkar • 5 months ago
Thanks Sourab, glad it was helpful!
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Max Wilson • a year ago
Hey, great work. V readable and understandable.

Just checking - in the line starting 'a Gaussian process is a random process' you refer to the distribution over the random variable f(x). The notation indicates the distribution is over a set of the same function applied to many examples of x e.g. f(x1) f(x2), but am I right in saying its a distribution over different functions of the same input e.g. f1(x) f2(x).

Thanks!
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Martin Krasser Mod Max Wilson • a year ago • edited
The paragraph actually refers to the **joint** distribution of a finite number of random variables f(xi) and not to the distribution of a single random variable. A GP is a collection of these random variables and their joint distribution is a (multivariate) Gaussian distribution. A single sample drawn from a GP i.e. from the collection of random variables is therefore a function f. This sample can be interpreted as the same function f applied to multiple locations xi. Drawing several samples from a GP would give rise to functions f1, f2, ...
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Max Wilson Martin Krasser • a year ago
I get it! Thanks. I'm working on computing the derivatives of a gp distribution http://mlg.eng.cam.ac.uk/mc..., it isn't clear to me what the resulting covariance matrix is, do you know good resources in this direction?
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Anna Sot • a year ago
Thanks a lot for the detailed explanation! Helped me a lot.
1 • Reply • Share ›

Martin Krasser Mod Anna Sot • a year ago
Thank you Anna, glad it was helpful!
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Jia • a year ago
very nice explanation.
while, equation 4 and 5, K_*^{-1} should be K_y^{-1} ?
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Martin Krasser Mod Jia • a year ago • edited
You're right, thanks for the hint. Just fixed it. This was a typo in equations 4 and 5 only, the implementation is correct.
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ken henry • 2 years ago
Hi Martin, thank you for the terrific explanation. I have taken a class on Gaussian processes and your post really helped to refresh my understanding. I was wondering if you could elaborate a bit more about the mean function. You stated that "it is common to use m(x)=0 as GPs are flexible enough to model the mean arbitrarily well." From my understanding, we can always de-mean the data (subtract the sample mean) before fitting the GPs. This is one of the reasons why the mean function is often set to 0. I was wondering if that would be the case if we don't de-mean the data prior to fitting? I vaguely remember my lecturer explaining it before but can't recall the details. Do you mind explaining a bit more about the 'flexibility'? Thank you!!
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Martin Krasser Mod ken henry • 2 years ago • edited
The flexibility comes from the fact that the posterior predictive mean is not confined to be zero as it is a linear combination of the observations (see eq. 4). If the observation mean is not too distant from zero then a zero mean function is not a drastic limitation. In other situations, as you correctly pointed out, you need to shift observation by their mean and shift predictions accordingly. Eq. 3 uses a zero mean only for notational simplicity which simplifies eq. 4. A more general version of eq. 4 would include these shift operations explicitly. A fixed, non-zero mean function is therefore trivial to add. However, in some cases a fixed mean function is too restrictive and a linear model of the mean can be used (see section 2.7 in this chapter for details). I omitted these details here to keep the introduction simple but will try to make these things more explicit in a later version of this post.
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Joerg Martin Krasser • a year ago
Thanks for the explanations Martin. I had the same question as Ken. Coming from time series analysis, it really seems odd at first to assume a zero-mean and hope for the GP to automagically find the correct posterior predictive mean.

I have the following two additional question on the issue:

1.) How do I decide where to incroporate my a-priori knowledge into the model? For example, I could model periodicity/seasonality as a sinus-function either into the mean
function m(x) or into the covariance function k(x1,x2) with similar effects (I guess) on