Model Selection for Gaussian Process Regression

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Table of Contents

Preliminary

In a regression setting, we are interested in finding an optimal map $f(x)$ between data points and labels/ function values.

$$f : X \to Y$$

#Gaussian-Process can be used to represent a prior distribution over a space of functions. Gaussian Process can be written as,

$$y = f(x) \sim GP\Big(m(x),\ k(x, x')\Big)$$

Note

This Note contains the following:

(1) Compute the marginal likelihood for Gaussian Process Model

(2) Compute the gradients of (1) w.r.t the hyper-parameters of kernel

(3) Check (2) using Standard Finite Difference

(4) Evaluate (1) and (2) to scipy's 'SLSQP' to maximize log marginal likelihood

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Model Selection for GP Regression

Although Gaussian Process is a non-parametric model, the so called 'hyper-parameters' in the kernel heavily influence the inference process. It is therefore essential to select the best possible parameters for the kernel. For example in the R.B.F-kernel; the *length* (l) and *scale* (σ) are the hyper-parameters.

$$k(x, x') = \sigma^2 \exp\left(\frac{|x - x'|^2}{2l^2}\right)$$

where, l controls the 'reach of influence on neighbors' and σ dictates the average amplitude from the mean of the function.

Marginal Likelihood

Bayes' Rule

$$\text{Posterior} = \frac{\text{Likelihood} \times \text{ Prior}}{\text{Marginal Likelihood}}$$

$$\mathbb{P}(\theta|y, X) = \frac{\mathbb{P}(y|X, \theta) \times \mathbb{P}(\theta)}{\mathbb{P}(y|X)}$$

A #Marginal-Likelihood is a likelihood function that has been integrated over the parameter space. It represents the probability of generating the observed sample from a #prior and is often referred to as the #model-evidence or #evidence.

Let θ represent the parameters of the model. We now formulate a #prior over the output of the function as a #Gaussian-Process.

$$\mathbb{P}(f|X, \theta) = \mathcal{N}\Big(0, k(x, x')\Big) \tag{1}$$

We can always transform the data to have zero mean and (1) can be viewed as a general case. Assume that the #likelihood takes the following form

$$\mathbb{P}(Y|f) \sim \mathcal{N}(f, \sigma_n^2 I) \tag{2}$$

(2) tells that the observations y are subject to additive Gaussian noise. Now, the joint distribution is given by;

$$\mathbb{P}(Y, f|X, \theta) = \mathbb{P}(Y|f)\ \mathbb{P}(f|X, \theta) \tag{3}$$

It is worth noting that we would eventually like to optimize the hyper-parameters θ for the kernel function. However, the #prior here is over the mapping f and not any parameters directly. In the ***evidence-based*** framework, which approximates Bayesian averaging by optimizing the #Marginal-Likelihood we can make use of the denominator part in the ***Bayes' Rule*** as an objective function for optimization. For this we take the joint distribution (3) and marginalize over f since we are not directly interested in optimizing it. This can be done in the following way:

$$\begin{aligned}\mathbb{P}(Y|X, \theta) &= \int \mathbb{P}(Y, f|X, \theta)\ df \\ &= \int \mathbb{P}(Y|f)\ \mathbb{P}(f|X, \theta)\ df \\ &= \int \mathcal{N}(y; f, \sigma_n^2 I)\ \ \mathcal{N}(f; 0, K)\end{aligned} \tag{4}$$

(4) is an integration performed all possible spaces of f and it aims to remove f
from the distribution of Y. After marginalization Y is no longer dependent on f but it depends on the hyper-parameters θ.

As per Rasmussen & Williams, the log marginal likelihood is given by;

$$\log \mathbb{P}(y|X, \theta) = -\frac{1}{2} y^T K_y^{-1} y - \frac{1}{2} \log |K_y| - \frac{n}{2} \log (2\pi) \tag{5}$$

Derivation

Let $\Sigma = \sigma_n^2 I$. Now, (4) can be fleshed out as follows;

$$\begin{aligned}\mathbb{P}(y|X, \theta) &= \int \frac{1}{(2\pi)^{n/2}} |\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(f-y)^T \Sigma^{-1}(f-y)\right) \times \frac{1}{(2\pi)^{n/2}} |K|^{-1/2} \exp\left(-\frac{1}{2}(f)^T K^{-1}(f)\right) df \\ &= \frac{1}{(2\pi)^n} \frac{1}{\sqrt{|\Sigma||K|}} \int \exp\left(-\frac{1}{2}\left[(f-y)^T \Sigma^{-1}(f-y) + f^T K^{-1} f\right]\right) df\end{aligned} \tag{6}$$

Looking at the exponent term in (6):

$$\begin{aligned}&= f^T(\Sigma^{-1} + K^{-1})f - 2f^T\Sigma^{-1}y + y^T\Sigma^{-1}y \\ &= f^T\Pi^{-1}f - 2f^T\Pi^{-1}\nu + y^T\Sigma^{-1}y \\ &= (f-\nu)^T\Pi^{-1}(f-\nu) - \nu^T\Pi^{-1}\nu + y^T\Sigma^{-1}y\end{aligned}$$

where $\Pi = (\Sigma^{-1} + K^{-1})^{-1}$ and $\nu = \Pi\Sigma^{-1}y$.
By definition we have;

$$\frac{1}{\sqrt{2\pi\Pi}} \int \exp\left[-\frac{1}{2}(f-\nu)^T\Pi^{-1}(f-\nu)\right] df = 1$$

Plugging this back to (6) gives the following expression;

$$\frac{\sqrt{(2\pi)^n|\Pi|}}{(2\pi)^n\sqrt{|\Sigma||K|}} \exp\left[\frac{1}{2}(\nu^T\Pi^{-1}\nu - y^T\Sigma^{-1}y)\right]$$

Substitute values for Π and ν we get;

$$\begin{aligned}\mathbb{P}(y|X, \theta) &= \frac{1}{(2\pi)^{n/2}} \left(|\Sigma||K||\Sigma^{-1} + K^{-1}|\right)^{-1/2} \exp\left[-\frac{1}{2}\left(y^T\Sigma^{-1}(\Sigma^{-1} + K^{-1})^{-1}K^{-1}y\right)\right] \\ &= \frac{1}{(2\pi)^{n/2}} \left(|\Sigma||K||\frac{\Sigma + K}{\Sigma K}|\right)^{-1/2} \exp\left[-\frac{1}{2}\left(y^T\Sigma^{-1}(\frac{K+\Sigma}{\Sigma K})^{-1}K^{-1}y\right)\right] \\ &= \frac{1}{(2\pi)^{n/2}} \left(|\Sigma + K|\right)^{-1/2} \exp\left[-\frac{1}{2}\left(y^T(K+\Sigma)^{-1}y\right)\right] \\ &= \frac{1}{(2\pi)^{n/2}} \left(|\sigma_n^2 I + K|\right)^{-1/2} \exp\left[-\frac{1}{2}\left(y^T(K+\sigma_n^2 I)^{-1}y\right)\right] \\ &= \frac{1}{(2\pi)^{n/2}} |K_y|^{-1/2} \exp\left[-\frac{1}{2} y^T K_y^{-1} y\right]\end{aligned}$$

Taking log on both sides yields (5)

Note that this expression depends on the hyperparameters θ of the kernel function through the kernel matrix K, which depends on the input values x_i and the values of the hyperparameters. Therefore, the log marginal likelihood can be used to optimize the hyperparameters of the kernel function using numerical optimization techniques such as gradient descent or L-BFGS.

Gradients of Marginal Likelihood

Recall

$\frac{\partial}{\partial\theta} K^{-1} = -K^{-1}\frac{\partial K}{\partial\theta}K^{-1}$

$\frac{\partial}{\partial\theta} \log|K| = \text{trace}\left(K^{-1}\frac{\partial K}{\partial\theta}\right)$

Now, the partial derivatives w.r.t. the hyper-parameters is given by;

$$\begin{aligned}\frac{\partial}{\partial\theta_j}\log\mathbb{P}(y|X,\theta) &= \frac{1}{2}y^TK^{-1}\frac{\partial K}{\partial\theta_j}K^{-1}y - \frac{1}{2}\text{trace}\left(K^{-1}\frac{\partial K}{\partial\theta_j}\right) \\ &= \frac{1}{2}\text{trace}\left((\alpha\alpha^T - K^{-1})\frac{\partial K}{\partial\theta_j}\right) \end{aligned} \tag{6}$$

where, $\alpha = K^{-1}y$

Warning

In general, computing the inverse of a matrix directly (e.g: np.linalg.inv()) is not stable and there is a loss of precision. In the case when the matrix is positive definite, Cholesky decompostion can be used to compute inverse.

Example:

Let K be a symmetric positive definite matrix. Now, if we want to calculate $\alpha = K^{-1}y$, we can do the following:

$$K = \text{Cholesky } \rightarrow LL^T$$

$$K^{-1} = (L^T)^{-1}L^{-1}$$

$$\alpha = \text{np.linalg.solve(L.T, np.linalg.solve(L, y))}$$

Implementation

```
def kernel(x, xp, σ, l):
        '''k(x,x') = sigma^2 exp(-0.5*length^2*|x-x'|^2)'''
        length = l
        sq_norm = (scipy.spatial.distance.cdist(x, xp))**2
        return σ**2 * np.exp(-0.5*sq_norm/(length**2))


def dKdL(x1, x2, σ, l):
        '''
        computes partial derivative of K w.r.t length (l)
        arg: x1 = (N1, D), x2 = (N2, D)
        return: (N1, N2)
        '''
        sq_norm = (scipy.spatial.distance.cdist(x1, x2))**2
        return (σ**2) * np.exp(-sq_norm/(2*l**2)) * (sq_norm) / (l**3)

def dKdσ(x1, x2, σ, l):
        '''
        computes partal derivatice of K w.r.t sigma (std not variance)
        arg: x1 = (N1, D), x2 = (N2, D)
        return: (N1, N2)
        '''
        sq_norm = (scipy.spatial.distance.cdist(x1, x2))**2
        return 2*σ*np.exp(-sq_norm/(2*l**2))


def dLdt(a, iKxx, dKdt):
        '''
        computes gradient of log marginal likelihood w.r.t. a hyper-parameter
        i.e. either sigma or length
        '''
        return 0.5**np.trace(np.dot(a @ a.T - iKxx), dKdt)


def f_opt(kernel, X, y, σ, l):
        '''
        Evalaute Negative-Log Marginal Likelihood
        '''
        σ_n = 0.1 # std of noise hard-coded for now
        K = kernel(X,X, σ = σ, l = l) + (σ_n**2)*np.eye(X.shape[0])
        L = np.linalg.cholesky(K) + 1e-12 # Cholesky decomposition
        a = np.linalg.solve(L.T, np.linalg.solve(L, y)) # compute alpha

        #log_likelihood = -0.5 * y.T @ a - 0.5 * np.trace(np.log(L)) - 0.5 * X.shape[0] * np.log(2*np.pi)
        log_likelihood = -0.5 * y.T @ a - 0.5 * np.log(np.linalg.det(K)) - 0.5 * X.shape[0] * np.log(2*np.pi)

        return -log_likelihood


def grad_f(kernel, X, y, l, σ):
        '''
        Compute gradient of objective function w.r.t. two parameters
        '''
```

```
        l, σ = params
        σ_n = 0.1 # std of noise hard-coded for now
        K = kernel(X,X, σ = σ, l = l) + (σ_n**2)*np.eye(X.shape[0])
        L = np.linalg.cholesky(K) # Cholesky decomposition
        a = np.linalg.solve(L.T, np.linalg.solve(L, y)) # compute alpha

        inv_k = np.linalg.inv(K)
        grad = np.empty([2,])
        grad[0] = dLdt(a = a, iKxx = inv_k, dKdt = dKdσ(X, X, σ, l)) # gradient w.r.t sigma
        grad[1] = dLdt(a = a, iKxx = inv_k, dKdt = dKdL(X, X, σ, l)) # gradient w.r.t length

        return grad



def marginal(params, X, y):
        '''
        Evalaute Negative-Log Marginal Likelihood -- for scipy optimization
        '''
        #print (params)
        l, σ = params
        σ_n = 0.1 # std of noise hard-coded for now
        K = kernel(X, X, σ = σ, l = l) + (σ_n**2)*np.eye(X.shape[0])
        L = np.linalg.cholesky(K) + 1e-12 # Cholesky decomposition
        a = np.linalg.solve(L.T, np.linalg.solve(L, y)) # compute alpha

        #log_likelihood = -0.5 * y.T @ a - 0.5 * np.trace(np.log(L)) - 0.5 * X.shape[0] * np.log(2*np.pi)

        log_likelihood = -0.5 * y.T @ a - 0.5 * np.log(np.linalg.det(K)) - 0.5 * X.shape[0] * np.log(2*np.pi)

        return -log_likelihood
```

```
'''
True function f(x) = sin(x) & X ~ Unif(-4,4) with 10 samples
'''
f_sin = lambda x: (np.sin(x)).flatten()
X = np.random.uniform(-4, 4, size = (10, 1))
y = f_sin(X)

# Scipy-optimization via SLSQP

lim = [10**-3, 10**3]
bound = [lim, lim]
start = [0.3, 0.1] # initial hyper-parameters
result = scipy.optimize.minimize(fun = marginal, x0 = start, args = (X, y), method = 'SLSQP', options = {'disp':True},
bounds = bound, tol = 0.0001)
```

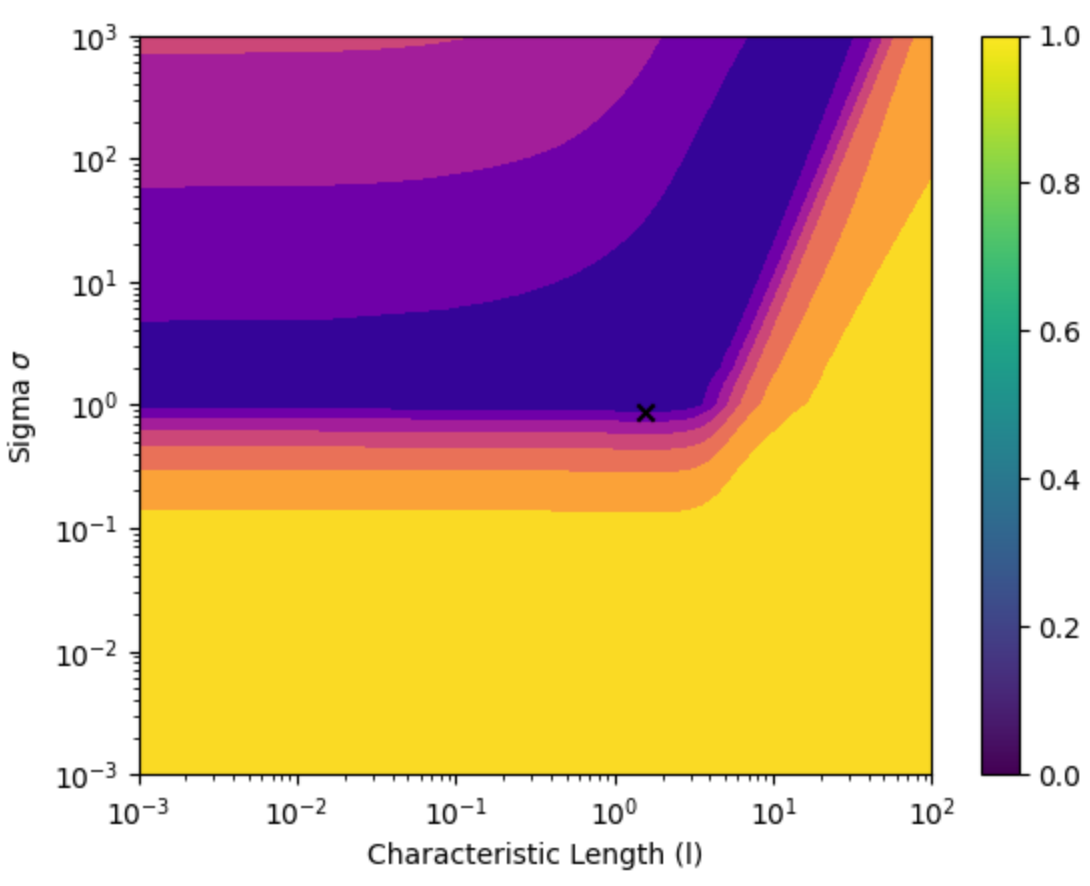
```
'''
Contour Plot
'''

L = np.linspace(10**-3, 10**2, 1000)
S = np.linspace(10**-3, 10**3, 1000)
σ, l = np.meshgrid(L, S)

func_val = np.zeros_like(σ)

for i in range(σ.shape[0]):
        for j in range(l.shape[0]):
                func_val[i, j] = f_opt(kernel = kernel, X = X.reshape(-1,1), y = y.reshape(-1,1), σ = S[i], l = L[j])

plt.contourf(σ, l, func_val, cmap = 'plasma')
plt.xscale('log')
plt.yscale('log')
plt.scatter(result.x[0], result.x[1], color = 'black', marker = 'x')
plt.colorbar()
plt.show()
```


Sigma σ
Characteristic Length (l)
10^{3}
10^{2}
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
10^{2}
1.0
0.8
0.6
0.4
0.2
0.0