

Derivatives of GPs

Two things need understanding:

- how the GP representation of a derivative of an unknown function represented by a GP is related to the GP representation of the function,
- how to compare the alignment of two contour plots.

1 How the GP representation of a derivative of an unknown function represented by a GP is related to the GP representation of the function

1.1 Fitting a GP in R

The following is taken from <https://www.r-bloggers.com/2012/04/gaussian-process-regression-with-r>, a demo of Gaussian process regression with R by James Keirstead (5 April 2012). He writes:

`\begin{tcolorbox}`

Chapter 2 of Rasmussen and Williams (2006) provides a detailed explanation of the math for Gaussian process regression. It doesn't provide much in the way of code though. This Gist is a brief demo of the basic elements of Gaussian process regression, as described on pages 13 to 16.

`\end{tcolorbox, cache=T}`

1.1.1 The GP prior

First for a (dense) set of 50 regularly-spaced input values (denoted x^*) we populate the covariance matrix using the chosen covariance function, or *kernel*, $k(\cdot, \cdot)$, in this case the squared exponential with length parameter $\Psi = 1$. One such covariance matrix $k(x^*, x^*)$ is printed below, but for only 10 points.

```
# Utility function to print matrices in proper LaTeX format
print_mat <- function(mat) {
  n <- nrow(mat)
  c('\begin{bmatrix}',
    paste0(sapply(seq_len(n - 1),
                  function(i) paste0(mat[i, ], collapse = ' & ')),
          ' \\\\''),
    paste0(mat[n, ], collapse = ' & '),
    '\end{bmatrix}'))
}
```

$$\begin{bmatrix} 1 & 0.784 & 0.377 & 0.112 & 0.02 & 0.002 & 0 & 0 & 0 & 0 \\ 0.784 & 1 & 0.784 & 0.377 & 0.112 & 0.02 & 0.002 & 0 & 0 & 0 \\ 0.377 & 0.784 & 1 & 0.784 & 0.377 & 0.112 & 0.02 & 0.002 & 0 & 0 \\ 0.112 & 0.377 & 0.784 & 1 & 0.784 & 0.377 & 0.112 & 0.02 & 0.002 & 0 \\ 0.02 & 0.112 & 0.377 & 0.784 & 1 & 0.784 & 0.377 & 0.112 & 0.02 & 0.002 \\ 0.002 & 0.02 & 0.112 & 0.377 & 0.784 & 1 & 0.784 & 0.377 & 0.112 & 0.02 \\ 0 & 0.002 & 0.02 & 0.112 & 0.377 & 0.784 & 1 & 0.784 & 0.377 & 0.112 \\ 0 & 0 & 0.002 & 0.02 & 0.112 & 0.377 & 0.784 & 1 & 0.784 & 0.377 \\ 0 & 0 & 0 & 0.002 & 0.02 & 0.112 & 0.377 & 0.784 & 1 & 0.784 \\ 0 & 0 & 0 & 0 & 0.002 & 0.02 & 0.112 & 0.377 & 0.784 & 1 \end{bmatrix}$$

Plotting some sample functions drawn from the the zero-mean Gaussian process prior with the aforementioned covariance matrix gives us an idea of the type of functions it specifies:

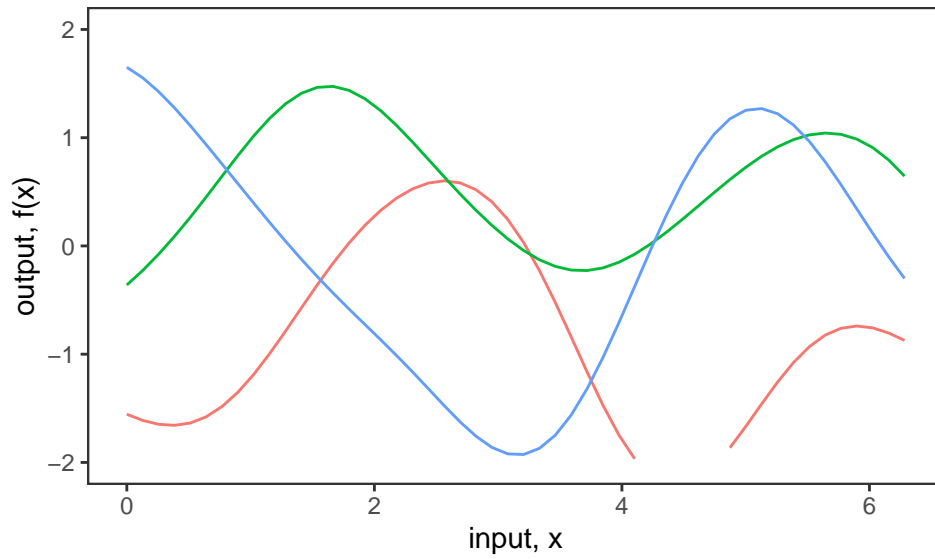


Figure 1: Three functions sampled from the GP prior distribution.

1.1.2 GP posteriors

1.1.2.1 Noisy-observations but a noise-free GP posterior Next, we'll generate 5 data points using the $\sin(x)$ function in the range $x \in [0.2, 2\pi]$, imagining that that is the underlying real-like function we're interested in learning about. Some observation error is included too. The observations are denoted z and the associated input values x . The $\sin(x)$ function is thus acting as the underlying real-life process. The observations produced are shown in Figure 2.

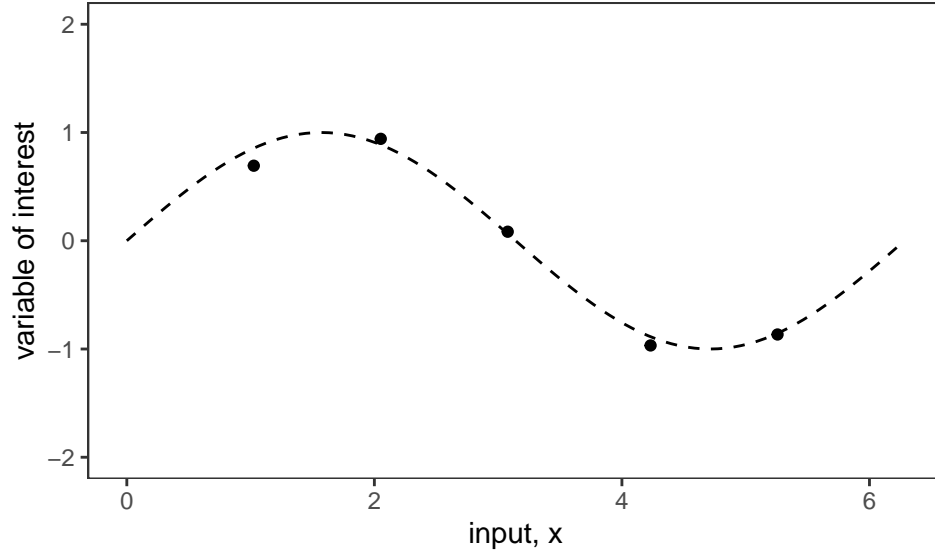


Figure 2: The true process, $\zeta(x)$, is indicated with the line, and five observations, z , by the points.

To specify the posterior GP distribution, we need three further covariance matrices: $k(x, x)$, $k(x, x^*)$ and $k(x^*, x)$. These are calculated as per Equation (2.19) in Rasmussen and Williams (2006).

Next, we'll generate and plot 20 functions from the posterior distribution, along with the mean function and 95% confidence interval. Outside of the interval on which we have data, the mean function returns towards zero.

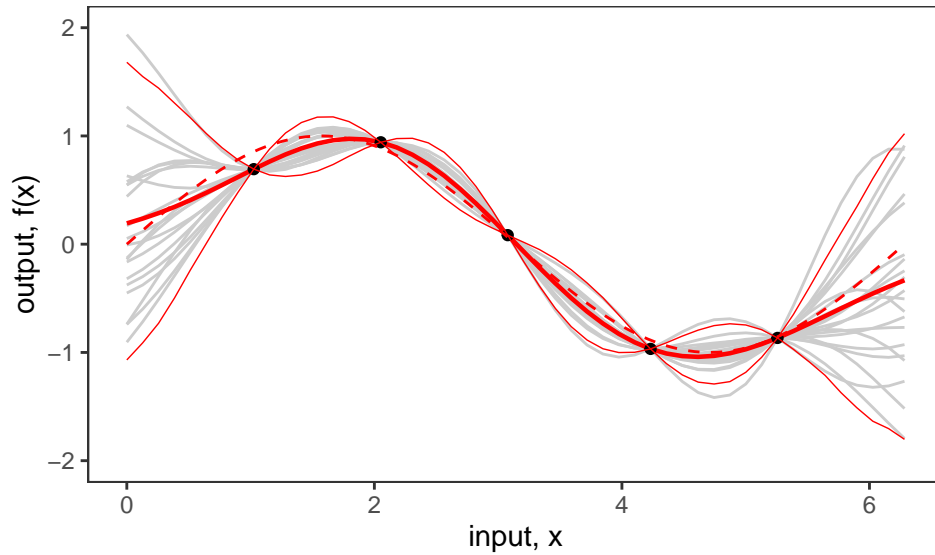


Figure 3: The posterior mean function (red solid line) along with 20 functions sampled from the posterior (grey) and 95% confidence intervals (red dashed line). The underlying real-life function is again a dashed black line.

1.1.2.2 Noisy-observations and a GP posterior with noise Since there is observation error, it might make more sense for the posterior draws *not* to pass through the observed points. This can be achieved by

adding a constant (observation noise) term onto the diagonal of the covariance matrix. Normally distributed measurement errors sampled from $N(0, 0.01)$ were added to the simulated values. We'll add 0.1 to the diagonal of the covariance matrix as observation noise.

Figure 4 replicates Figure 3 to incorporate this added noise, and now the mean function doesn't pass through the data points:

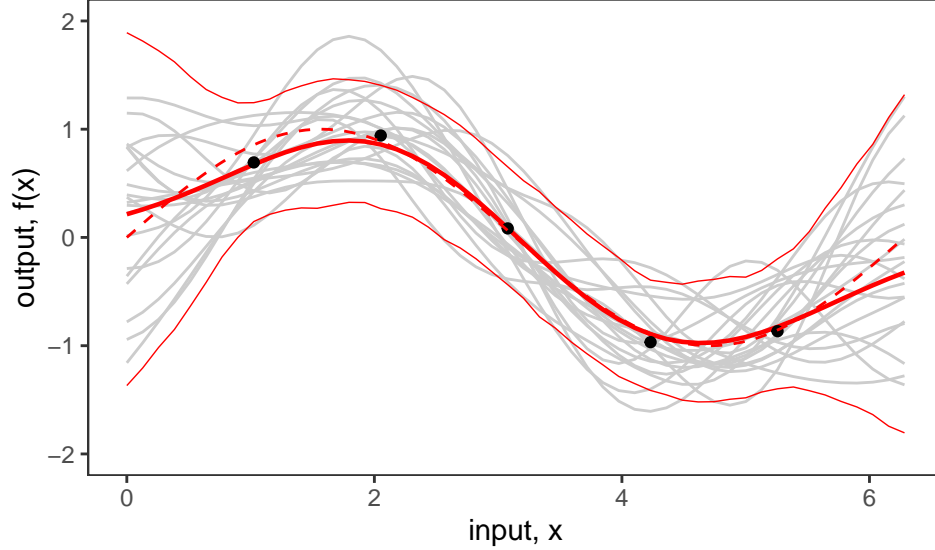


Figure 4: The posterior mean function (red solid line) along with 20 functions sampled from the posterior (grey) and 95% confidence intervals (red dashed line). The underlying real-life function is again a dashed black line.

1.2 The GP representation of a derivative of an unknown function represented by a GP

The GP posterior with noise built in Section (2.2.2) will be used. To obtain the derivative of the posterior mean function, we first need an expression for the posterior mean function. Viewing the posterior mean function, $\bar{f}(x^*)$, as a linear combination of 5 kernel functions, each centered at one of the 5 training points, Equation (2.27) in Rasmussen and Williams (2006), states that, for any particular input value x^* ,

$$\bar{f}(x^*) = \sum_{i=1}^5 a_i k(x_i, x^*)$$

where $\boldsymbol{\alpha} = (k(x, x) + 0.1I_5)^{-1}\mathbf{y}$. As such, the posterior mean function here will be

$$\begin{aligned} \bar{f}(x^*) = & \alpha_1 \exp\left(-\frac{1}{2}\left(\frac{x_1 - x^*}{l}\right)^2\right) + \alpha_2 \exp\left(-\frac{1}{2}\left(\frac{x_2 - x^*}{l}\right)^2\right) \\ & + \alpha_3 \exp\left(-\frac{1}{2}\left(\frac{x_3 - x^*}{l}\right)^2\right) + \alpha_4 \exp\left(-\frac{1}{2}\left(\frac{x_4 - x^*}{l}\right)^2\right) + \alpha_5 \exp\left(-\frac{1}{2}\left(\frac{x_5 - x^*}{l}\right)^2\right), \end{aligned} \quad (1)$$

which is plotted as the solid red line in Figure 5.

From O'Hagan (1992), the derivatives of functions modelled by a Gaussian process with

$$\begin{aligned} E\{\eta(x)\} &= \mathbf{h}^T(x)\boldsymbol{\beta} \\ Cov\{\eta(x), \eta(\mathbf{x}')\} &= k(x, x) \end{aligned}$$

can also be modelled by a Gaussian process, with

$$\begin{aligned} E \left\{ \frac{\partial}{\partial x} \eta(x) \right\} &= \frac{\partial}{\partial x} \mathbf{h}^T(x) \boldsymbol{\beta} \\ Cov \left\{ \frac{\partial}{\partial x} \eta(x), \frac{\partial}{\partial x} \eta(x') \right\} &= \frac{\partial^2}{\partial x \partial x'} k(x, x'). \end{aligned} \quad (2)$$

Led by Equation (2), differentiating the posterior mean function in Equation (1) gives

$$\frac{\partial}{\partial x^*} \bar{f}(x^*) = \frac{1}{l^2} \left[\alpha_1 (x_1 - x^*) \exp \left(-\frac{1}{2} \left(\frac{x_1 - x^*}{l} \right)^2 \right) + \dots + \alpha_5 (x_5 - x^*) \exp \left(-\frac{1}{2} \left(\frac{x_5 - x^*}{l} \right)^2 \right) \right],$$

which is also plotted in Figure 5. Since the real, underlying function is $\sin(x)$, whose derivative is $\cos(x)$, these functions are included in Figure 5 too, for comparison.

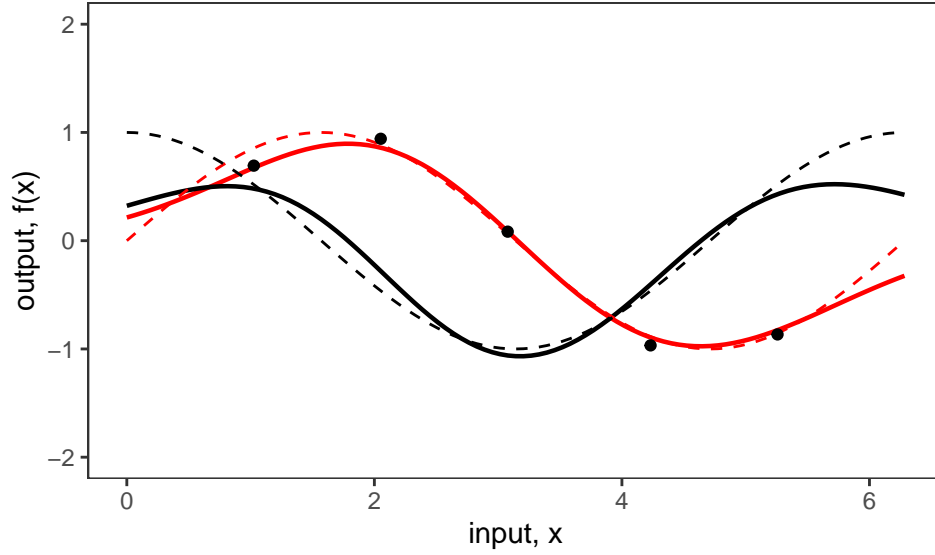


Figure 5: The posterior mean function (red solid line) and the true real-life process function, $\sin(x)$ (red dashed line). Also shown is the derivative of the posterior mean function (black solid line) and the derivative of the true real-life process function, $\cos(x)$ (black dashed line). Observations are shown as black dots.

2 How to compare the alignment of two contour plots

Citations

- O'Hagan, A. 1992. "Some Bayesian Numerical Analysis." In *Bayesian Statistics 4: Proceedings of the Fourth Valencia International Meeting*. Oxford University Press. <https://doi.org/10.1093/oso/9780198522669.003.0019>.
- Rasmussen, C. E., and C. K. I. Williams. 2006. *Gaussian Processes for Machine Learning*. Cambridge, MA: MIT Press.