Exponential Covariance Functions

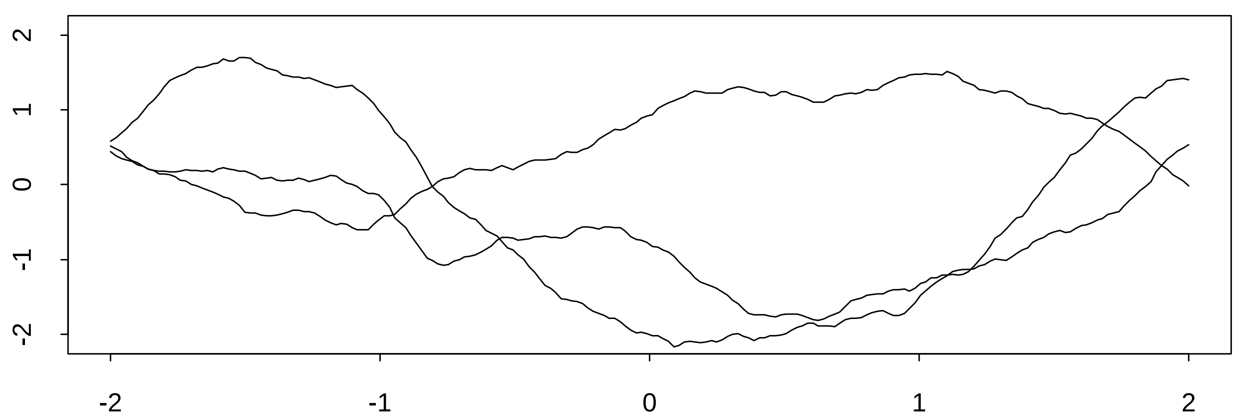
Other covariance functions produce functions that aren't linear. One useful class of valid covariances functions for a univariate x has the form

$$\mathrm{Cov}(y_{i_1}, y_{i_2}) \;\;=\;\; \eta^2 \exp\left(-\left(|x_{i_1} - x_{i_2}| \,/\, \rho\right)^R\right)$$

where $0 < R \leq 2$. Usually, we let the mean function be constant (eg, zero). The process is then stationary, with variance η^2, and a length scale determined by ρ.

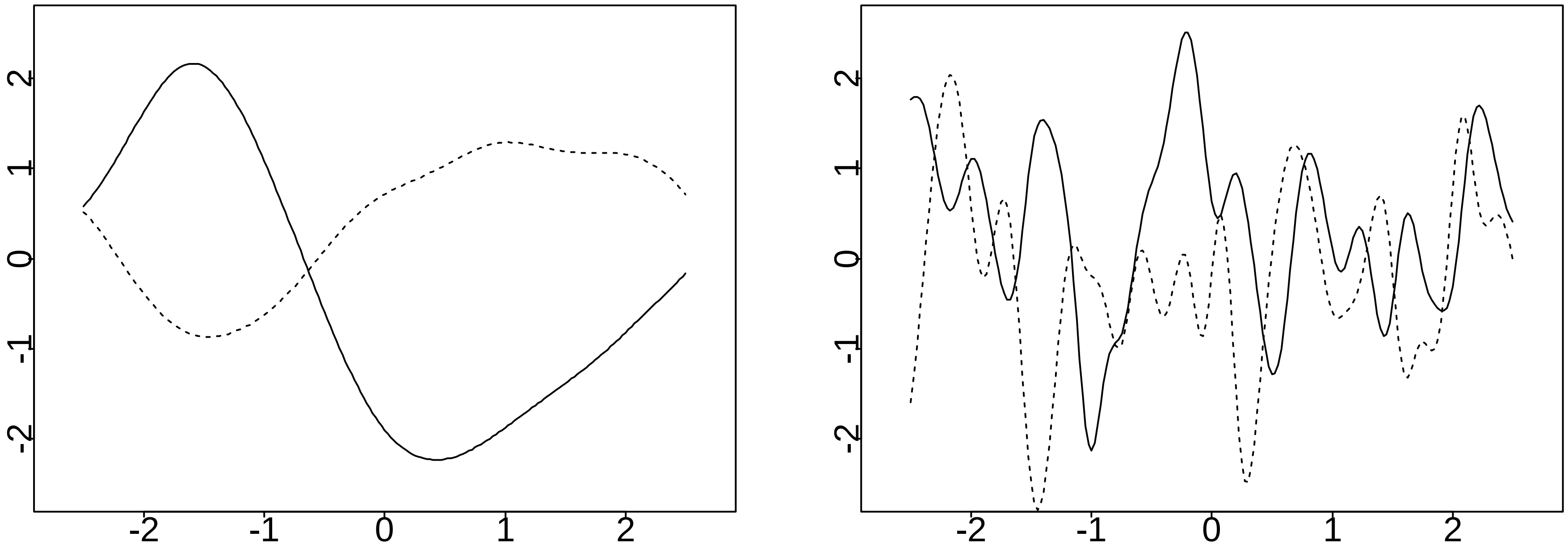
A prior using this covariance function says that nearby points are likely to have similar y values, but the responses may be much different for far-away points.

When $R = 2$, the functions are infinitely differentiable; when $R < 2$, they are not differentiable. Here are 3 random functions from a GP with $R = 1.8$, $\eta = 1$, $\rho = 1$:



More Functions from Exponential Covariance Functions

These Gaussian processes use the exponential covariance function with $R = 2$ and $\eta = 1$, but one has $\rho = 1$, the other $\rho = 1/5$. Two random functions are shown for each process.



$$\mathrm{Cov}(y_{i_1}, y_{i_2}) \;=\; \exp(-(x_{i_1} - x_{i_2})^2) \qquad \mathrm{Cov}(y_{i_1}, y_{i_2}) \;=\; \exp(-((x_{i_1} - x_{i_2})\,/\,(1/5))^2)$$

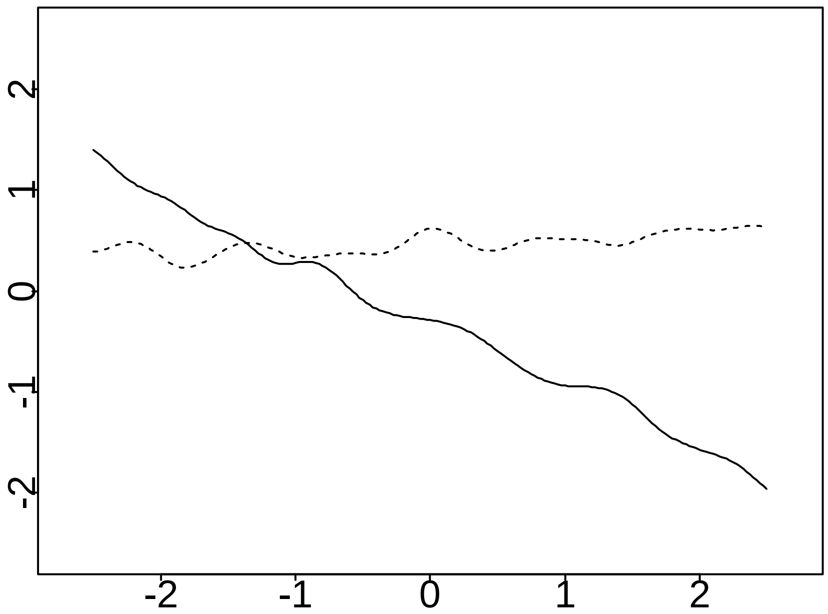
Combining Covariance Functions

If $C_1(x)$ and $C_2(x)$ are valid covariance functions, then $C_1(x) + C_2(x)$ and $C_1(x)C_2(x)$ are also valid covariance functions.

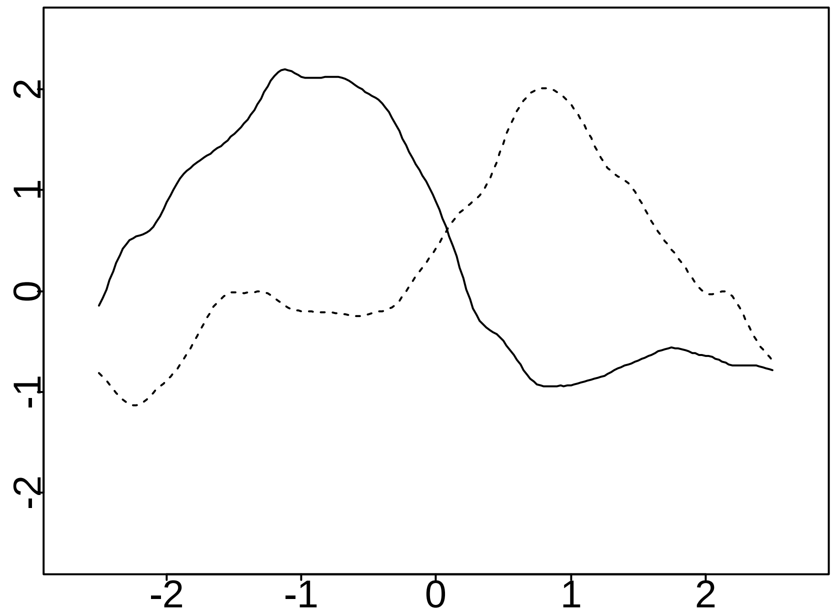
So we can build new covariance functions from old by taking sums and products. Some uses:

- The sum of a covariance function from a linear model and an exponential covariance function with small η yields an "almost linear" model.
- Sums of covariance functions with different length scales yield functions with both "large scale" and "small scale" variation.
- Sums of univariate covariance functions, each looking at a different input variable, describe additive models.
- Products of univariate covariance functions for different inputs yield multivariate covariance functions that allow for interactions.

Univariate Functions with Combined Covariance Functions



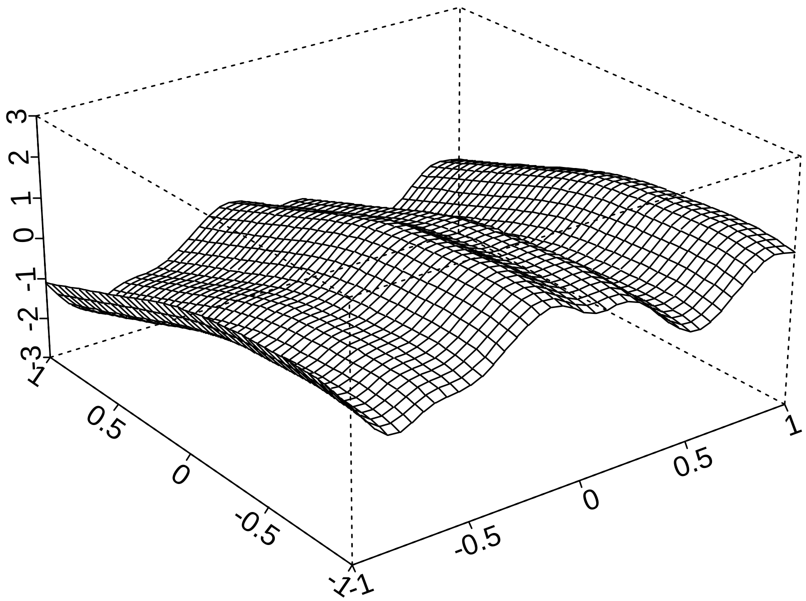
$$\mathrm{Cov}(y_{i_1}, y_{i_2}) \;=\; 1 + x_{i_1} x_{i_2} \\ + \; 0.1^2 \exp(-((x_{i_1} - x_{i_2}) \,/\, (1/3))^2)$$

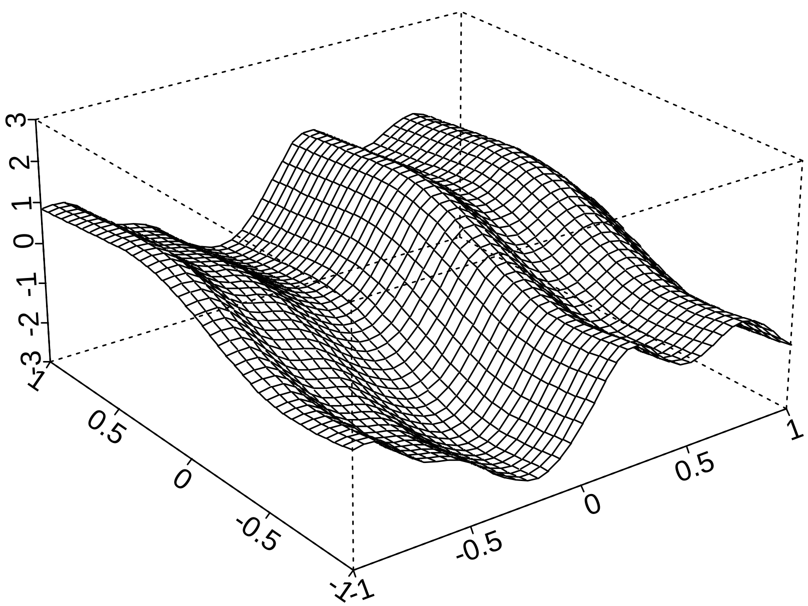


$$\mathrm{Cov}(y_{i_1}, y_{i_2}) \;=\; \exp(-(x_{i_1} - x_{i_2})^2) \\ + \; 0.1^2 \exp(-((x_{i_1} - x_{i_2}) \,/\, (1/5))^2)$$

Bivariate Functions Using an Additive Covariance Function

Here are two functions drawn from a Gaussian process whose covariance function is the sum of a funtion of x_1 and a function of x_2.

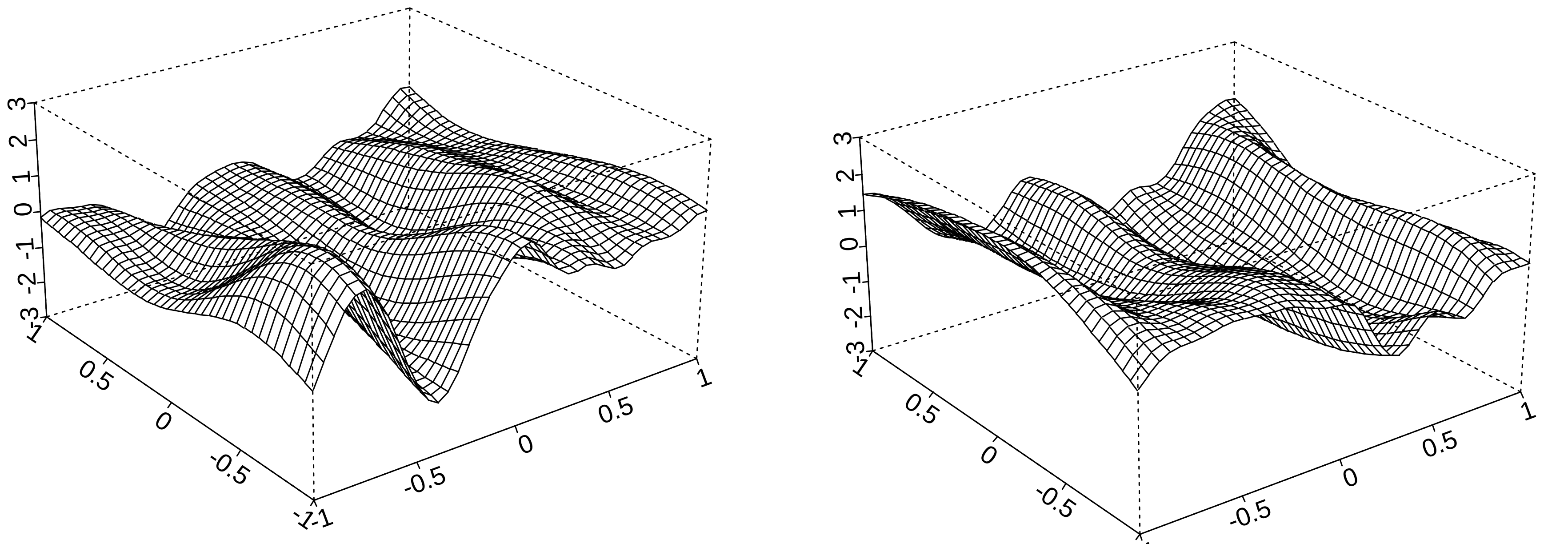




$$\text{Cov}(y_{i_1}, y_{i_2}) \;=\; \exp\left(-\,((x_{i_1,1} - x_{i_2,1})\,/\,0.88)^2\right) + \exp\left(-\,((x_{i_1,2} - x_{i_2,2})\,/\,0.24)^2\right)$$

Bivariate Functions Using a Product Covariance Function

Here are two functions drawn from a Gaussian process whose covariance function is the product of a funtion of x_1 and a function of x_2.



$$\mathrm{Cov}(y_{i_1}, y_{i_2}) \;=\; \exp\Big(-\,((x_{i_1,1}-x_{i_2,1})\,/\,0.88)^2 \;-\; ((x_{i_1,2}-x_{i_2,2})\,/\,0.24)^2\Big)$$

How Were These Plots Generated?

To produce these plots of functions drawn from a Gaussian process, I first defined a fine grid of x values, $x_1, \ldots, x_n$. For the 1D plots, the grid might have values of -2.00, -1.99, -1.98, $\ldots$, 1.98, 1.99, 2.00.

For the processes shown, the mean function is zero.

I computed the covariance matrix, $\mathbf{C}$, of the y_i values that go with each of the x_i. The elements are $C_{i_1,i_2} = \mathrm{Cov}(y_{i_1}, y_{i_2})$.

I found the Cholesky decomposition of $\mathbf{C}$, which is the lower-triangular matrix $\mathbf{L}$ such that $\mathbf{C} = \mathbf{L}\mathbf{L}^T$.

I drew a random vector $\mathbf{n}$ of length n, in which the components are drawn independently from the normal distribution with mean 0 and variance 1.

I set the vector of y_i values, $\mathbf{y} = [y_1 \ldots y_n]^T$, to $\mathbf{Ln}$.

Clearly, $E(\mathbf{y}) = E(\mathbf{Ln}) = \mathbf{L}E(\mathbf{n}) = \mathbf{0}$. The covariance matrix of $\mathbf{y}$ is

$$E(\mathbf{y}\mathbf{y}^T) \;=\; E(\mathbf{L}\mathbf{n}\mathbf{n}^T\mathbf{L}^T) \;=\; \mathbf{L}E(\mathbf{n}\mathbf{n}^T)\mathbf{L}^T \;=\; \mathbf{L}\mathbf{L}^T \;=\; \mathbf{C}$$