5. Effects of Parameters on Kernel Functions

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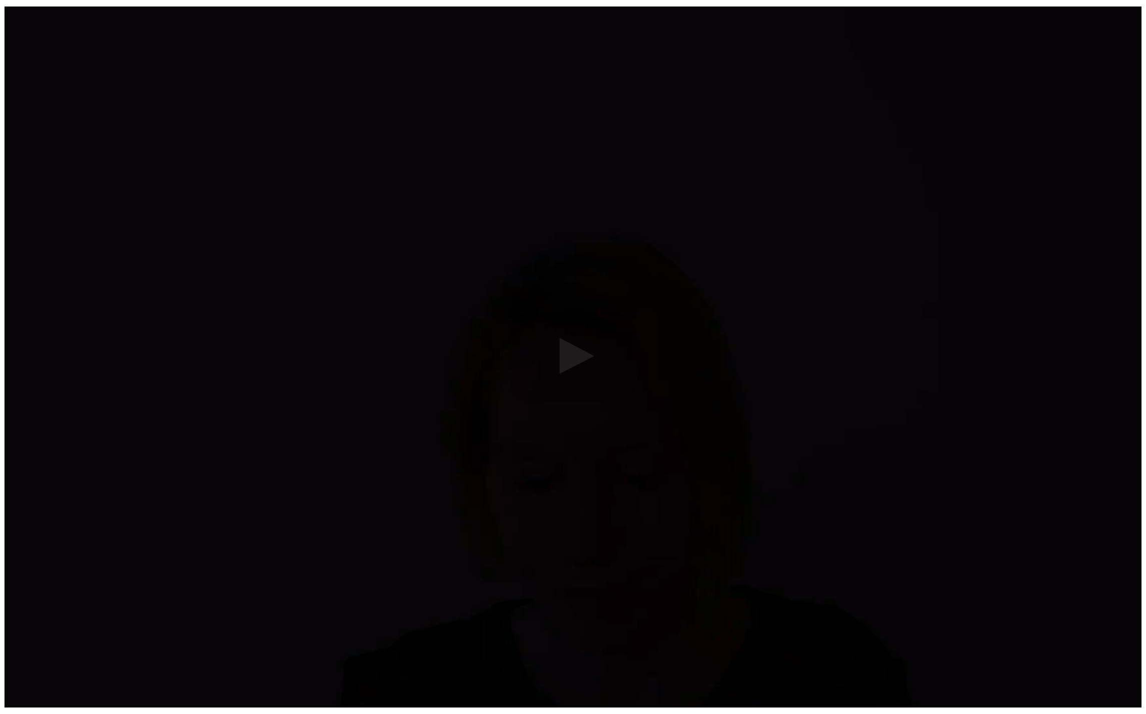
Exercises due May 21, 2021 19:59 EDT

Effects of Parameters on Kernel Functions



23:56 / 23:56 1.50x

take

a square distance between time and space together.

So you can do a product of these.

Now, so with this, we have a good set

of tools of different types of kernels we can use.

Next what I want to do is, I just

want to show you two other important questions

and this is, that of modeling measurement noise

and the effect of non-stationary in your kernel.

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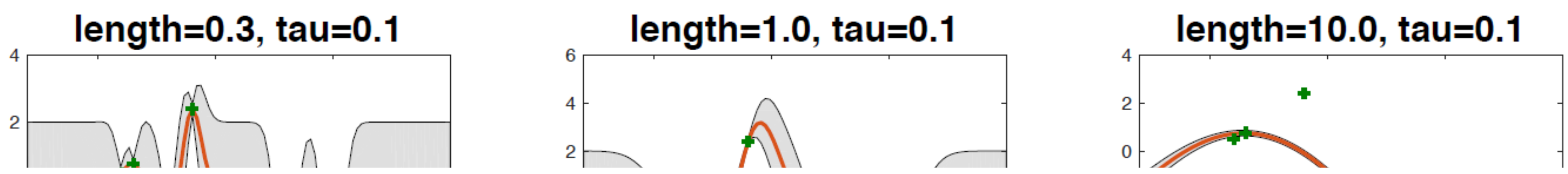
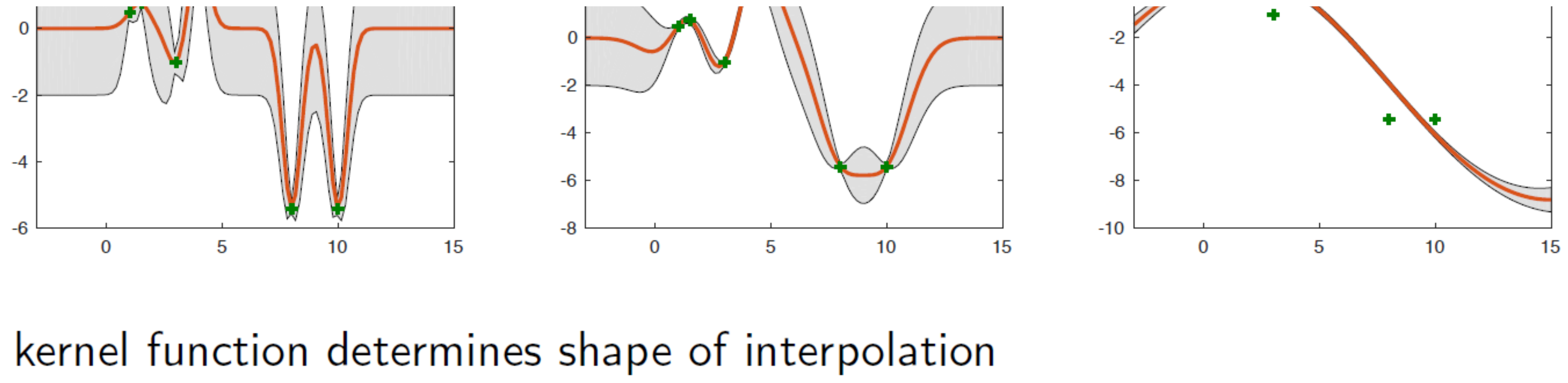
The below figure shows the effects of selecting different values of ℓ in the selected kernel function. In the figure, we observe the curve estimation, as shown in the previous example, with six observations. We see the effects of different values of the selected parameter ℓ: as one selects a larger ℓ the interpolations become smoother.

Note that higher values do not necessarily mean better estimates. This is a parameter that needs to be selected carefully. For example, in the left-most image, a value that is too small introduces artifacts in the estimates that might not exist in reality, see, for instance, the region between the right-most two points, where the predicted mean departs sharply back to zero. A value that is too large is shown in the right-most image; this ignores, or deletes, some of the changes observed in the data leading to a prediction that is too smooth.

$$k(x_i, x_j) = \exp\left(-\frac{||x_i - x_j||^2}{2\ell^2}\right)$$





36: Effects of the parametrization of a kernel function

Note also that the same ℓ parameter does not need to be used for each coordinate of the observations, one can have kernel functions with different parameters for each coordinate.

The below table shows other examples of possible forms for kernel functions. Assume here that x is a difference between points, eg: $x = Z_1 - Z_2$, and r is a distance, eg: $r = \|Z_1 - Z_2\|$.

constant	σ_0^2
linear	$\sum_{d=1}^{D} \sigma_d^2 x_d x'_d$
polynomial	$\left(x \cdot x' + \sigma_0^2\right)^p$
squared exponential	$\exp\left(-\frac{r^2}{2\ell^2}\right)$
Matérn	$\frac{1}{2^{\nu-1}\Gamma(\nu)}\left(\frac{\sqrt{2\nu}}{\ell}r\right)^{\nu} K_\nu\left(\frac{\sqrt{2\nu}}{\ell}r\right)$
exponential	$\exp\left(-\frac{r}{\ell}\right)$
γ-exponential	$\exp\left(-\left[\frac{r}{\ell}\right]^{\gamma}\right)$
rational quadratic	$\left(1 + \frac{r^2}{2\alpha\ell^2}\right)^{-\alpha}$
neural network	$\sin^{-1}\left(\frac{2x^{\mathsf{T}}\Sigma x}{\sqrt{(1+2x^{\mathsf{T}}\Sigma x)(1+2x'^{\mathsf{T}}\Sigma x')}}\right)$

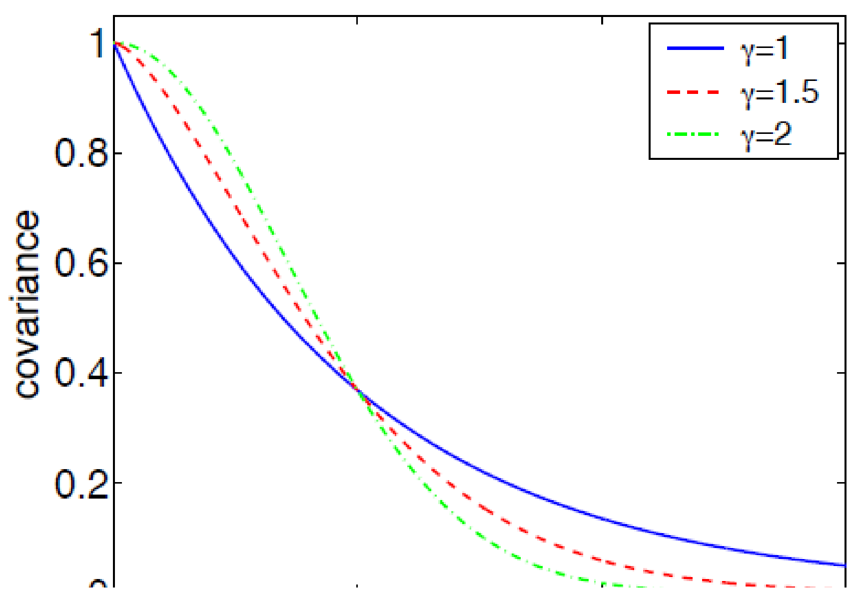
Note, for example, that the last kernel in this table is stationary, but it is not isotropic as the matrix $\mathbf{\Sigma}$ means that the kernel is no longer a function of purely distance. Rather, the distance between two points is scaled depending on the direction of the vector between them; hence, the kernel is not isotropic.

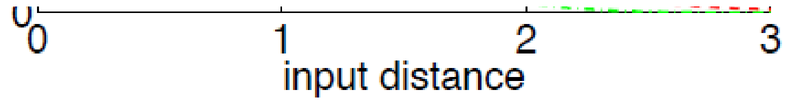
For example, consider the following covariance function:

$$k(Z_1, Z_2) = \exp\left(-\left[\frac{\|Z_1 - Z_2\|}{\ell}\right]^{\gamma}\right).$$

This is the γ-exponential shown in table above.

Examples of this function are shown below for various choices of γ.





37: The effects of the parameter γ on the covariance function.

When $\gamma = 1$, the peak of the function is sharp, and the function is heavy tailed. For $\gamma = 2$ the function is smooth around the peak, but falls off sharply at large distance. Although $\gamma = 2$ is a common choice, we can make other choices if we have reason to suspect that the observations are heavily correlated at large distance.

We can also combine kernel functions to form new kernel functions.

If k_1 is a kernel function, and k_2 is also a kernel function, then

$$k(Z_1, Z_2) = k_1(Z_1, Z_2) + k_2(Z_1, Z_2)$$

is also a kernel function.

Similarly,

$$k(Z_1, Z_2) = k_1(Z_1, Z_2) \times k_2(Z_1, Z_2)$$

is also a kernel function.

Combinations of kernel functions 1

1 point possible (graded)

Suppose that k_1 and k_2 are both isotropic kernel functions.

Is the linear combination

$$k(Z_1, Z_2) = 2k_1(Z_1, Z_2) + k_2(Z_1, Z_2)$$

also an isotropic kernel function?

- ◯ Yes
- ◯ No

Submit

You have used 0 of 1 attempt

Combinations of kernel functions 2

1 point possible (graded)

Suppose that k_1 is an isotropic kernel function, but k_2 is a stationary kernel function.

What can we say about the product

$$k(Z_1, Z_2) = 2k_1(Z_1, Z_2) + k_2(Z_1, Z_2)$$

It is

- ☐ Stationary
- ☐ Isotropic
- ☐ None of the above

Submit You have used 0 of 2 attempts

For a comprehensive study of covariance functions and kernels, the reader should check Chapter 4 in Williams, Christopher KI, and Carl Edward Rasmussen. Gaussian processes for machine learning. Vol. 2. No. 3. Cambridge, MA: MIT Press, 2006.

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Link to the reference
https://www.cs.toronto.edu/~duvenaud/cookbook/ 2

[Staff] Combinations of kernel functions 2
The question asks about the product but shows a sum. Please correct. 2

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