

Appendix

0.1 Kernels

0.1.1 Base kernels

Here we give the formulas for all one-dimensional base kernels mentioned in the thesis. Each of these formulas includes a scale factor, σ_f^2 , which we omit for clarity.

$$C(x, x') = 1 \tag{1}$$

$$WN(x, x') = \delta(x - x') \tag{2}$$

$$Lin(x, x') = (x - c)(x' - c) \tag{3}$$

$$SE(x, x') = \exp\left(-\frac{(x - x')^2}{2\ell^2}\right) \tag{4}$$

$$RQ(x, x') = \left(1 + \frac{(x - x')^2}{2\alpha\ell^2}\right)^{-\alpha} \tag{5}$$

$$Per(x, x') = \sigma_f^2 \frac{\exp\left(\frac{1}{\ell^2} \cos 2\pi \frac{(x-x')}{p}\right) - I_0\left(\frac{1}{\ell^2}\right)}{\exp\left(\frac{1}{\ell^2}\right) - I_0\left(\frac{1}{\ell^2}\right)} \tag{6}$$

$$\cos(x, x') = \cos\left(\frac{2\pi(x - x')}{p}\right) \tag{7}$$

$$CP(k_1, k_2)(x, x') = \sigma(x)k_1(x, x')\sigma(x') + (1 - \sigma(x))k_2(x, x')(1 - \sigma(x')) \tag{8}$$

$$\sigma = \sigma(x)\sigma(x') \tag{9}$$

$$\bar{\sigma} = (1 - \sigma(x))(1 - \sigma(x')) \tag{10}$$

where $\delta_{x,x'}$ is the Kronecker delta function, I_0 is the modified Bessel function of the first kind of order zero, and other symbols are parameters of the kernel functions. Equations (3), (4) and (6) are plotted in ??, and equations (2), (5) and (7) are plotted in ??. Draws from GP priors with changepoint kernels are shown in ??.

0.2 Formula for Gaussian Conditionals

A standard result of multivariate Gaussians states shows how to condition on a knowing a subset of the dimensions of a Gaussian vector. If

$$\begin{bmatrix} \mathbf{x}_A \\ \mathbf{x}_B \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_A \\ \boldsymbol{\mu}_B \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{AA} & \boldsymbol{\Sigma}_{AB} \\ \boldsymbol{\Sigma}_{BA} & \boldsymbol{\Sigma}_{BB} \end{bmatrix}\right) \quad (11)$$

then

$$\mathbf{x}_A | \mathbf{x}_B \sim \mathcal{N}(\boldsymbol{\mu}_A + \boldsymbol{\Sigma}_{AB} \boldsymbol{\Sigma}_{BB}^{-1} (\mathbf{x}_B - \boldsymbol{\mu}_B), \boldsymbol{\Sigma}_{AA} - \boldsymbol{\Sigma}_{AB} \boldsymbol{\Sigma}_{BB}^{-1} \boldsymbol{\Sigma}_{BA}) \quad (12)$$

In the case of Gaussian processes, this result tells us how to condition on knowing the function values $[f(\mathbf{x}_1), f(\mathbf{x}_2), \dots, f(\mathbf{x}_N)]$ at some subset of locations along the real line, indexed by $[\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N]$.

0.2.1 The Generalized Periodic Kernel

Lloyd (2013) showed that the standard periodic kernel due to ? can be decomposed into a periodic and a constant component. He derived a more general form of periodic kernel, shown in equation (6), without a constant component. He further showed that its limit as the lengthscale grows is the cosine kernel:

$$\lim_{\ell \rightarrow \infty} \text{Per}(x, x') = \cos\left(\frac{2\pi(x - x')}{p}\right). \quad (13)$$

0.3 Details of Model Search

The model construction phase of ABCD starts with the kernel equal to the noise kernel, WN. New kernel expressions are generated by applying search operators to the current kernel, which replace some part of the existing kernel expression with a new kernel expression.

0.3.1 Search operators

ABCD is based on a search algorithm which used the following search operators

$$\mathcal{S} \rightarrow \mathcal{S} + \mathcal{B} \quad (14)$$

$$\mathcal{S} \rightarrow \mathcal{S} \times \mathcal{B} \quad (15)$$

$$\mathcal{B} \rightarrow \mathcal{B}' \quad (16)$$

where \mathcal{S} represents any kernel subexpression and \mathcal{B} is any base kernel within a kernel expression. These search operators represent addition, multiplication and replacement. When the multiplication operator is applied to a subexpression which includes a sum of subexpressions, parentheses () are introduced. For instance, if rule (15) is applied to the subexpression $k_1 + k_2$, the resulting expression is $(k_1 + k_2) \times \mathcal{B}$.

To accommodate changepoints and changewindows, we introduced the following additional operators to our search:

$$\mathcal{S} \rightarrow \text{CP}(\mathcal{S}, \mathcal{S}) \quad (17)$$

$$\mathcal{S} \rightarrow \text{CW}(\mathcal{S}, \mathcal{S}) \quad (18)$$

$$\mathcal{S} \rightarrow \text{CW}(\mathcal{S}, \text{C}) \quad (19)$$

$$\mathcal{S} \rightarrow \text{CW}(\text{C}, \mathcal{S}) \quad (20)$$

where C is the constant kernel. The last two operators result in a kernel only applying outside, or within, a certain region.

To allow the search to simplify existing expressions, we introduced the following operators:

$$\mathcal{S} \rightarrow \mathcal{B} \quad (21)$$

$$\mathcal{S} + \mathcal{S}' \rightarrow \mathcal{S} \quad (22)$$

$$\mathcal{S} \times \mathcal{S}' \rightarrow \mathcal{S} \quad (23)$$

where \mathcal{S}' represents any other kernel expression. We also introduced the operator

$$\mathcal{S} \rightarrow \mathcal{S} \times (\mathcal{B} + \text{C}) \quad (24)$$

Which allows a new base kernel to be added along with the constant kernel, for cases when multiplying by a base kernel by itself would restrict the model too much.

References

James Robert Lloyd. personal communication, 2013.

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Nutonian. Eureka, 2011. URL <http://www.nutonian.com/>.