Chapter 1

Gaussian Conditionals

A standard result shows how to condition on knowing a subset of the dimensions $\mathbf{y}_B$ of a vector $\mathbf{y}$ having a multivariate Gaussian distribution. If

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}_A \\ \mathbf{y}_B \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_A \\ \boldsymbol{\mu}_B \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{AA} & \boldsymbol{\Sigma}_{AB} \\ \boldsymbol{\Sigma}_{BA} & \boldsymbol{\Sigma}_{BB} \end{bmatrix} \right) \tag{1.1}$$

then

$$\mathbf{y}_A | \mathbf{y}_B \sim \mathcal{N}(\boldsymbol{\mu}_A + \boldsymbol{\Sigma}_{AB}\boldsymbol{\Sigma}_{BB}^{-1}\left(\mathbf{x}_B - \boldsymbol{\mu}_B\right), \boldsymbol{\Sigma}_{AA} - \boldsymbol{\Sigma}_{AB}\boldsymbol{\Sigma}_{BB}^{-1}\boldsymbol{\Sigma}_{BA}). \tag{1.2}$$

This result can be used in the context of Gaussian process regression, where $\mathbf{y}_B = [f(\mathbf{x}_1), f(\mathbf{x}_2), \ldots, f(\mathbf{x}_N)]$ represents a set of function values observed at some subset of locations $[\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N]$, while $\mathbf{y}_A = [f(\mathbf{x}_1\star), f(\mathbf{x}_2\star), \ldots, f(\mathbf{x}_N\star)]$ represents test points whose predictive distribution we'd like to know. In this case, the necessary covariance matrices are given by:

$$\boldsymbol{\Sigma}_{AA} = k(\mathbf{X}, \mathbf{X}) \tag{1.3}$$

$$\boldsymbol{\Sigma}_{AB} = k(\mathbf{X}, \mathbf{X}^\star) \tag{1.4}$$

$$\boldsymbol{\Sigma}_{BA} = k(\mathbf{X}^\star, \mathbf{X}) \tag{1.5}$$

$$\boldsymbol{\Sigma}_{BB} = k(\mathbf{X}^\star, \mathbf{X}^\star) \tag{1.6}$$

and similarily for the mean vectors.

Chapter 2

Kernel Definitions

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

$$\mathrm{C}(x, x') = 1 \tag{2.1}$$

$$\mathrm{WN}(x, x') = \delta(x - x') \tag{2.2}$$

$$\mathrm{Lin}(x, x') = (x - c)(x' - c) \tag{2.3}$$

$$\mathrm{SE}(x, x') = \exp\left(-\frac{(x - x')^2}{2\ell^2}\right) \tag{2.4}$$

$$\mathrm{RQ}(x, x') = \left(1 + \frac{(x - x')^2}{2\alpha\ell^2}\right)^{-\alpha} \tag{2.5}$$

$$\mathrm{Per}(x, x') = \sigma_f^2 \frac{\exp\left(\frac{1}{\ell^2}\cos 2\pi\frac{(x-x')}{p}\right) - I_0\left(\frac{1}{\ell^2}\right)}{\exp\left(\frac{1}{\ell^2}\right) - I_0\left(\frac{1}{\ell^2}\right)} \tag{2.6}$$

$$\cos(x, x') = \cos\left(\frac{2\pi(x - x')}{p}\right) \tag{2.7}$$

$$\mathrm{CP}(k_1, k_2)(x, x') = \sigma(x)k_1(x, x')\sigma(x') + (1 - \sigma(x))k_2(x, x')(1 - \sigma(x')) \tag{2.8}$$

$$\boldsymbol{\sigma} = \sigma(x)\sigma(x') \tag{2.9}$$

$$\bar{\boldsymbol{\sigma}} = (1 - \sigma(x))(1 - \sigma(x')) \tag{2.10}$$

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 kernel parameters. Equations (2.3), (2.4) and (2.6) are plotted in **??**, and equations (2.2), (2.5) and (2.7) are plotted in **??**. Draws from GP priors with changepoint kernels are shown in **??**.

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 the equivalent periodic kernel without any constant component, shown in equation (2.6). He further showed that its limit as the lengthscale grows is the cosine kernel:

$$\lim_{\ell \to \infty} \mathrm{Per}(x, x') = \cos\left(\frac{2\pi(x - x')}{p}\right). \tag{2.11}$$

Separating out the constant component allows us to express negative prior covariance, as well as increasing the interpretability of the resulting models.

Chapter 3

Search Operators

The model construction phase of ABCD starts with 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.

The search used in the multidimensional regression experiments in **????** used only the following search operators:

$$\mathcal{S} \rightarrow \mathcal{S} + \mathcal{B} \tag{3.1}$$

$$\mathcal{S} \rightarrow \mathcal{S} \times \mathcal{B} \tag{3.2}$$

$$\mathcal{B} \rightarrow \mathcal{B}' \tag{3.3}$$

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 (3.2) is applied to the subexpression $k_1 + k_2$, the resulting expression is $(k_1 + k_2) \times \mathcal{B}$.

Afterwards, we added several more search operators in order to speed up the search. These new operators do not change the set of possible models.

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

$$\mathcal{S} \rightarrow \mathrm{CP}(\mathcal{S}, \mathcal{S}) \tag{3.4}$$

$$\mathcal{S} \rightarrow \mathrm{CW}(\mathcal{S}, \mathcal{S}) \tag{3.5}$$

$$\mathcal{S} \rightarrow \mathrm{CW}(\mathcal{S}, \mathrm{C}) \tag{3.6}$$

$$\mathcal{S} \rightarrow \mathrm{CW}(\mathrm{C}, \mathcal{S}) \tag{3.7}$$

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:

$$\mathcal{S} \rightarrow \mathcal{B} \tag{3.8}$$

$$\mathcal{S} + \mathcal{S}' \rightarrow \mathcal{S} \tag{3.9}$$

$$\mathcal{S} \times \mathcal{S}' \rightarrow \mathcal{S} \tag{3.10}$$

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

$$\mathcal{S} \rightarrow \mathcal{S} \times (\mathcal{B} + \mathrm{C}) \tag{3.11}$$

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. (page 3)

Nutonian. Eureqa, 2011. URL http://www.nutonian.com/.