Complementary mathematical topics

These topics will not be tested in STM5001 assignments. They are given for students interested in the mathematical background and justifications of models considered in this week lectures.

Simple Kriging.

We will derive formulae for the simple kriging.

Simple kriging assumes a known constant trend ($m(x) = 0$) and has the next properties of the kriging predictor:

1. It is a **linear combination** of the data values, i.e.,

$$\hat{X}(\mathbf{s}_0) = \sum_{i=1}^{n} \lambda_i X(\mathbf{s}_i).$$

2. It is **unbiased**, i.e., it satisfies

$$E[\hat{X}(\mathbf{s}_0)] = E[X(\mathbf{s}_0)].$$

3. Among all function of the data that satisfy the first 2 properties, it is the **best in the sense that minimizes the variance of prediction error,** $\mathrm{var}[\hat{X}(\mathbf{s}_0) - X(\mathbf{s}_0)]$.

The properties we have imposed on our predictor lead us to minimize

$$\boxed{\mathrm{var}[\hat{X}(\mathbf{s}_0) - X(\mathbf{s}_0)]}$$

subject to the restriction

$$\boxed{\sum_{i=1}^{n} \lambda_i = 1.}$$

Now we derive the kriging equations and the expression for the kriging variance:

$$
\begin{aligned}
\sigma^2 &= Var\left(\hat{X}(s_0) - X(s_0)\right) = E\left[\hat{X}(s_0) - X(s_0)\right]^2 - \left[E\left(\hat{X}(s_0) - X(s_0)\right)\right]^2 \\
&= |\text{for simple Kriging } m = 0| = E\left[\hat{X}^2(s_0) + X^2(s_0) - 2\hat{X}(s_0)X(s_0)\right] \\
&= \sum_{i,j=1}^{n} \lambda_i \lambda_j C(s_i - s_j) + C(s_0 - s_0) - 2\sum_{i=1}^{n} \lambda_i C(s_i - s_0) \\
&= 2\lambda_i \sum_{\substack{j=1 \\ j \neq i}}^{n} \lambda_j C(s_i - s_j) + \lambda_i^2 C(0) + \sum_{k,j \neq i} \lambda_k \lambda_j C(s_k - s_j) \\
&+ \quad C(0) - 2\sum_{k \neq i} \lambda_k C(s_k - s_0) - 2\lambda_i C(s_i - s_0).
\end{aligned}
$$

Then

$$
\frac{\partial \sigma^2}{\partial \lambda_i} = 0 \Rightarrow 2\sum_{\substack{j=1 \\ j \neq i}}^{n} \lambda_j C(s_i - s_j) + 2\lambda_i C(0) - 2C(s_i - s_0) = 0.
$$

Note that

$$\sum_{i=1}^{n} \lambda_i = 1 \Rightarrow \lambda_i = 1 - \sum_{\substack{j=1 \\ j \neq i}}^{n} \lambda_j.$$

Therefore

$$C(0) - C(s_i - s_0) = \sum_{\substack{j=1 \\ j \neq i}}^{n} \lambda_j [C(0) - C(s_i - s_j)] = \sum_{j=1}^{n} \lambda_j [C(0) - C(s_i - s_j)].$$

Finally, $\gamma(h) = C(0) - C(h)$ and we obtain the kriging equations

$$\boxed{\gamma(s_i - s_0) = \sum_{j=1}^{n} \lambda_j \gamma(s_i - s_j).}$$

Now, we can calculate σ^2:

$$\begin{aligned}
\sigma^2 &= E\left[\sum_{i=1}^{n}\lambda_i X(s_i) - X(s_0)\right]^2 = \sum_{i,j=1}^{n}\lambda_i\lambda_j C(s_i - s_j) + C(0) \\
&\quad -2\sum_{i=1}^{n}\lambda_i C(s_i - s_0) = \sum_{i,j=1}^{n}\lambda_i\lambda_j\left[C(s_i - s_j) - C(0)\right] + 2C(0) \\
&\quad -2\sum_{i=1}^{n}\lambda_i C(s_i - s_0) = -\sum_{i,j=1}^{n}\lambda_i\lambda_j\gamma(s_i - s_j) + 2\sum_{i=1}^{n}\lambda_i\gamma(s_i - s_0) \\
&= -\sum_{i=1}^{n}\lambda_i\gamma(s_i - s_0) + 2\sum_{i=1}^{n}\lambda_i\gamma(s_i - s_0) = \sum_{i=1}^{n}\lambda_i\gamma(s_i - s_0).
\end{aligned}$$

Thus,

$$\boxed{\sigma^2 = \sum_{i=1}^{n}\lambda_i\gamma(s_i - s_0).}$$