

Details on kriging predictions

Spatial Statistics

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1 Prediction problem formulation

Observations $\mathbf{y}^T = (y_1, \dots, y_n)$ available for a set of n locations $\mathbf{x}_i$

Consider $\mathbf{y}$ as a realization of the random variable $\mathbf{Y}^T = (Y_1, \dots, Y_n)$

Model: $Y_i = S(\mathbf{x}_i) + Z_i$ with:

- Y_i : the i^{th} datum
- $S(\mathbf{x}_i)$: “signal” (the true quantity) at location $\mathbf{x}_i$
- $\{S(\mathbf{x}_i)\}$: Gaussian process, parametrized by:
 - Trend: $\mu(\mathbf{x}_i) = \sum_k d_k(\mathbf{x}_i)\beta_k = \mathbf{d}(\mathbf{x}_i)^T \boldsymbol{\beta}$
 - Covariance function $\gamma(\mathbf{h}; \theta)$ or variogram $V(\mathbf{h}; \theta)$
- Z_i : independent, identically distributed (iid) Gaussian measurement error with variance τ^2

Predictions: Let's say $\hat{\mathbf{S}}$ is the prediction of $\mathbf{S}^T = (S(\mathbf{x}'_1), \dots, S(\mathbf{x}'_m))$ for a set of m locations $\mathbf{x}'_j$ without data.

$\hat{\mathbf{S}}$ is computed from $\mathbf{Y}$, therefore $\hat{\mathbf{S}} = \hat{\mathbf{S}}(\mathbf{Y})$.

2 Kriging prediction at new point location

Ordinary punctual kriging

For same spatial *support* – prediction entities are assumed to have same extension as observations (i.e. sampling area, sensor size)

Prediction of signal $S(\mathbf{x}_0)$ at location $\mathbf{x}_0$ without measurement

$$\hat{S}(\mathbf{x}_0) = \sum_{i=1}^n \kappa_i(\mathbf{x}_0) y(\mathbf{x}_i)$$

with kriging weights $\kappa_i(\mathbf{x}_0)$. To ensure unbiased estimates, weights are made to sum to 1:

$$\sum_{i=1}^N \kappa_i(x_0) = 1$$

Expected difference $\mathbb{E}[S(\mathbf{x}_0) - \hat{S}(\mathbf{x}_0)] = 0$.

Estimate of kriging variances

Estimate of the variance of the prediction error:

$$\begin{aligned} \text{var}[\hat{S}(\mathbf{x}_0)] &= \mathbb{E} \left[\left\{ S(\mathbf{x}_0) - \hat{S}(\mathbf{x}_0) \right\}^2 \right] \\ &= 2 \sum_{i=1}^N \kappa_i(\mathbf{x}_0) V(\mathbf{x}_i, \mathbf{x}_0) - \sum_{i=1}^N \sum_{j=1}^N \kappa_i(\mathbf{x}_0) \kappa_j(\mathbf{x}_0) V(\mathbf{x}_i, \mathbf{x}_j) \end{aligned}$$

with $V(\mathbf{x}_i, \mathbf{x}_0)$ being the semivariance of S between sampling point x_i and the target prediction point $\mathbf{x}_0$ and $V(\mathbf{x}_i, \mathbf{x}_j)$ the semivariance between the i th and the j th sampling points.

Find kriging weights

Kriging weights are calculated by solving the system of equations that minimizes the prediction error variance subject to the constraints of the variogram model.

Find weights $\kappa_i(\mathbf{x}_0)$ that minimize kriging variances and sum to 1 by solving $N + 1$ equations:

$$\sum_{i=1}^N \kappa_i(\mathbf{x}_0) V(\mathbf{x}_i, \mathbf{x}_j) + \psi(\mathbf{x}_0) = V(\mathbf{x}_j, \mathbf{x}_0) \quad \text{for all } j$$

$$\sum_{i=1}^N \kappa_i(x_0) = 1$$

The quantity $\psi(\mathbf{x}_0)$ is a Lagrange multiplier introduced to achieve minimization. Computed as the inverse of the semivariance matrix multiplied by the vector of semivariances to the target point.

3 Universal/external drift kriging predictions

Universal kriging: often referred if trend is modelled by coordinates

External-drift kriging: trend is modelled by spatial covariates

Evaluating $\hat{\mathbf{S}}_{\text{opt}}$ requires a fully specified weakly stationary model:

1. Structure of trend function is known
2. Regression coefficients β are known
3. Type of parametric covariance (variogram) function is known
4. Parameters θ and τ^2 of the covariance function are known

Relaxed assumptions: Only 1, 3, and 4 are assumed to be known, while β is implicitly estimated from the data using generalized least squares (GLS).

UK/EDK predictions

Therefore, we use the **universal kriging (UK) or external drift kriging (EDK) plug-in predictor**:

$$\hat{\mathbf{S}}_k = \mathbf{X}_S \hat{\beta}_{\text{GLS}} + \mathbf{\Lambda} \left(\mathbf{y} - \mathbf{X}_Y \hat{\beta}_{\text{GLS}} \right)$$

with:

$$\mathbf{\Lambda} = \mathbf{\Sigma}_{SY} \mathbf{\Gamma}_{YY}^{-1}$$

Computing universal kriging predictor requires:

1. known structure of trend function
2. known structure and parameters of variogram

“Plug-in” predictor: uncertainty of variogram is ignored when computing predictions



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