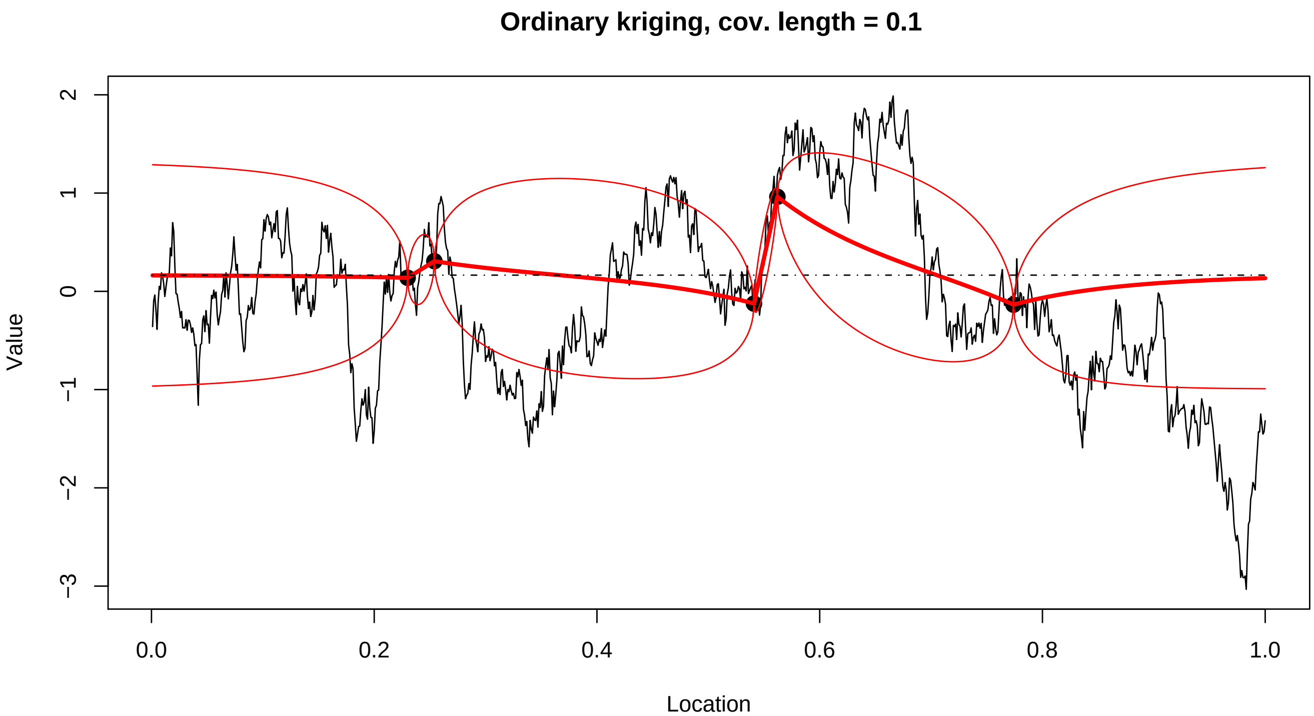
Lecture 10: Kriging Extensions

Math 586

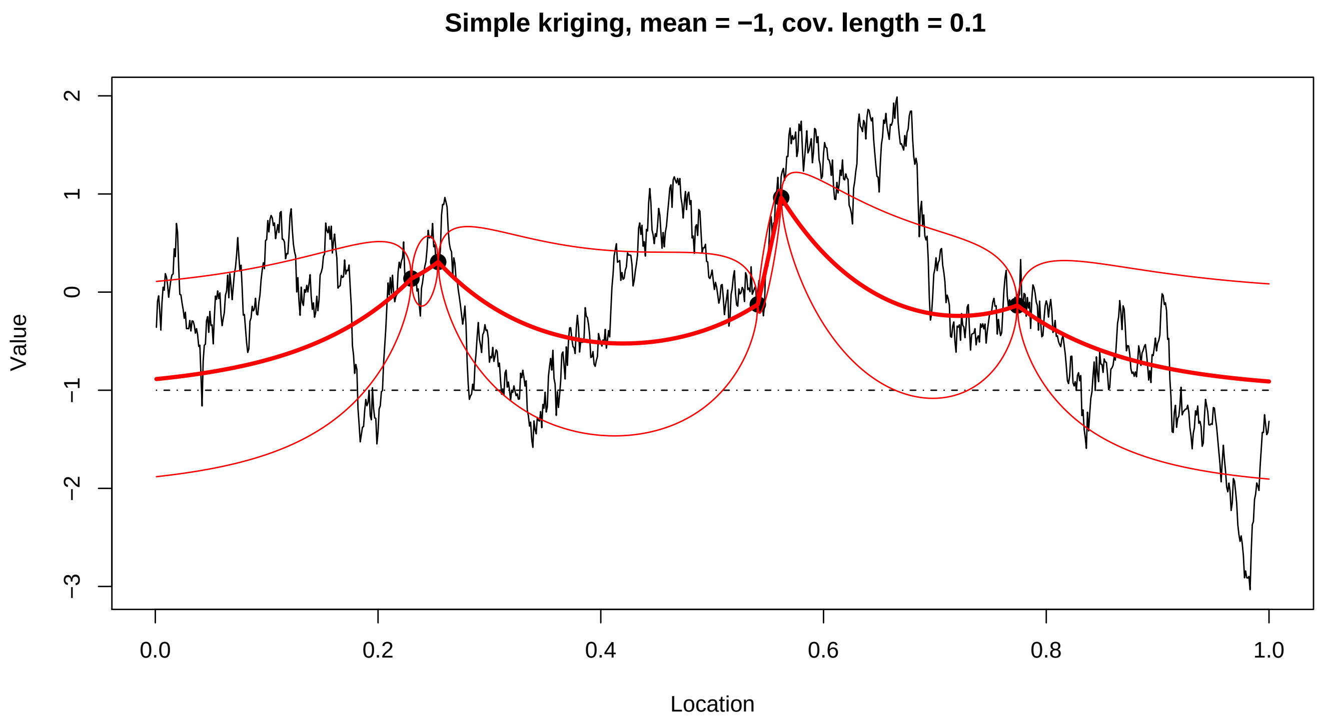
Example for Ordinary Kriging.

Consider 5 points sampled from a 1-d random field with known covariance function $C(h) = exp(-|h|/\ell)$, with scale parameter $\ell = 0.1$



Plot shows kriging mean $\pm$ one st.dev.; broken line = estimate of the mean; circles are observation points and the choppy line is the actual (unobserved) process.

However, if we knew the value of the mean, we could use simple kriging. This will decrease kriging variance σ_K^2, but what happens when the mean is incorrect? See the next Figure.



Other relevant data:						
	locations	0.230	0.254	0.541	0.562	0.774
	observations	0.138	0.307	-0.125	0.963	-0.136

C-matrix:

1.0000	0.7857	0.0439	0.0356	0.0042
0.7857	1.0000	0.0559	0.0453	0.0054
0.0439	0.0559	1.0000	0.8097	0.0962
0.0356	0.0453	0.8097	1.0000	0.1188
0.0042	0.0054	0.0962	0.1188	1.0000

Estimate of the mean: $\hat{m} = 0.1648$ with weights $\lambda_j = 0.1926,\ 0.1744,\ 0.1719,\ 0.1536,\ 0.3075$. Note the higher weight for the observation #5 that stands alone.

I. Extension to IRF-0

Covariance may not exist.
To the definition of IRF-0 add one more requirement:

$$\begin{array}{rll} (i) & \mathbb{E}\, V(\mathbf{x}) = const & \\ (ii) & \gamma(\mathbf{h}) = \frac{1}{2}\mathbb{E}\,[V(\mathbf{x}+\mathbf{h}) - V(\mathbf{x})]^2 & \text{is independent of } \mathbf{x} \\ (iii) & Var\,[\sum_{j=0}^{J} \alpha_j V(\mathbf{x}_j)] & \text{exists (is finite)} \end{array}$$

for every J, set of $\mathbf{x}_j$ and every set of α_j such that $\sum \alpha_j = 0$.

$\sum \alpha_j V(\mathbf{x}_j)$ represents "allowable" linear combinations. Even though $Var(V(\mathbf{x}))$ may not exist, $Var(\sum \alpha_j V(\mathbf{x}_j))$ does. For example, can you express $Var[V(\mathbf{x}) - V(\mathbf{y})]$?

As another example, if $\sum_{j=1}^{n} \lambda_j = 1$ then we require

$$Var[V(\mathbf{x}_0) - \sum_{j=1}^{n} \lambda_j V(\mathbf{x}_j)] \text{ is finite.}$$

Lemma. (1)

$$Cov\,[V(\mathbf{x}_i) - V(\mathbf{x}_0), V(\mathbf{x}_j) - V(\mathbf{x}_0)] = \gamma(\mathbf{x}_i - \mathbf{x}_0) + \gamma(\mathbf{x}_j - \mathbf{x}_0) - \gamma(\mathbf{x}_i - \mathbf{x}_j)$$

Proof. Consider

$$Cov[V(\mathbf{x}_i) - V(\mathbf{x}_0), V(\mathbf{x}_j) - V(\mathbf{x}_0)] = \mathbb{E}\left\{[V(\mathbf{x}_i) - V(\mathbf{x}_0)][V(\mathbf{x}_j) - V(\mathbf{x}_0)]\right\}.$$

Then,

$$\gamma(\mathbf{x}_i - \mathbf{x}_j) = \frac{1}{2}\,\mathbb{E}\,[V(\mathbf{x}_i) - V(\mathbf{x}_j)]^2 = \frac{1}{2}\,\mathbb{E}\left\{[V(\mathbf{x}_i) - V(\mathbf{x}_0)] - [V(\mathbf{x}_j) - V(\mathbf{x}_0)]\right\}^2 =$$

$$= \frac{1}{2}\,\mathbb{E}\left\{[V(\mathbf{x}_i) - V(\mathbf{x}_0)]^2 + [V(\mathbf{x}_j) - V(\mathbf{x}_0)]^2 - 2[V(\mathbf{x}_i) - V(\mathbf{x}_0)][V(\mathbf{x}_j) - V(\mathbf{x}_0)]\right\} =$$

$$= \gamma(\mathbf{x}_i - \mathbf{x}_0) + \gamma(\mathbf{x}_j - \mathbf{x}_0) - \mathbb{E}\left\{[V(\mathbf{x}_i) - V(\mathbf{x}_0)][V(\mathbf{x}_j) - V(\mathbf{x}_0)]\right\}$$

□

Now consider kriging equations to find best linear unbiased predictor:

$$\texttt{Linear} \quad \hat{V} = \sum_{j=1}^{n} \lambda_j V(\mathbf{x}_j)$$

$$\texttt{Unbiased} \quad \mathbb{E}\,(\hat{V}) = m \quad \Rightarrow \quad \sum_{j=1}^{n} \lambda_j m = m \quad \text{or} \quad \sum_{j=1}^{n} \lambda_j = 1.$$

$$\texttt{MSE} = \mathbb{E}\,[\hat{V} - V(\mathbf{x}_0)]^2 = \mathbb{E}\left\{\sum_{j=1}^{n} \lambda_j [V(\mathbf{x}_j) - V(\mathbf{x}_0)]\right\}^2 =$$

$$= \sum_{k=1}^{n}\sum_{j=1}^{n} \lambda_k \, \mathbb{E} \left\{ [V(\mathbf{x}_k) - V(\mathbf{x}_0)][V(\mathbf{x}_j) - V(\mathbf{x}_0)] \right\} \lambda_j = \quad \text{using (1)}$$

$$= \sum_{k=1}^{n}\sum_{j=1}^{n} \lambda_k [\gamma(\mathbf{x}_k - \mathbf{x}_0)]\lambda_j + \sum_{k=1}^{n}\sum_{j=1}^{n} \lambda_k [\gamma(\mathbf{x}_j - \mathbf{x}_0)]\lambda_j - \sum_{k=1}^{n}\sum_{j=1}^{n} \lambda_k [\gamma(\mathbf{x}_k - \mathbf{x}_j)]\lambda_j$$

Finally (argh), we obtain

$$\texttt{MSE} = 2\sum_{j=1}^{n} \lambda_j \gamma(\mathbf{x}_j - \mathbf{x}_0) - \sum_{j=1}^{n}\sum_{i=1}^{n} \lambda_i \lambda_j \gamma(\mathbf{x}_i - \mathbf{x}_j) \tag{2}$$

Again, minimize with the constraint that $\sum_{j=1}^{n} \lambda_j = 1$. Using Lagrange multiplier μ, minimize

$$H(\lambda_1, ..., \lambda_n; \mu) = \texttt{MSE} - 2\mu \left[\sum_{j=1}^{n} \lambda_j - 1 \right],$$

take partials with respect to λ_i, μ and equate to 0:

$$2\gamma(\mathbf{x}_i - \mathbf{x}_0) - 2\sum_{j=1}^{n} \lambda_j \gamma(\mathbf{x}_i - \mathbf{x}_j) - 2\mu = 0, \quad \text{therefore}$$

$$\boxed{\begin{array}{l} \displaystyle\sum_{j=1}^{n} \lambda_j \gamma(\mathbf{x}_j - \mathbf{x}_i) = \gamma(\mathbf{x}_i - \mathbf{x}_0) - \mu, \quad i = 1, ..., n \quad \text{and} \\ \displaystyle\qquad\qquad \sum_{j=1}^{n} \lambda_j = 1 \end{array}}$$

Kriging error, using (2), is $\boxed{\sigma^2_{\texttt{OK}} = \sum_{j=1}^{n} \lambda_j \gamma(\mathbf{x}_j - \mathbf{x}_0) + \mu}$

Note: If we use $\gamma(\mathbf{x}_i - \mathbf{x}_j) = C(0,0) - C(i,j)$ in stationary case, then get back to ordinary kriging equations from last Lecture.

In matrix form: let $\mathbf{\Gamma}$ be a matrix with entries $\gamma_{ij} = \gamma(\mathbf{x}_i - \mathbf{x}_j)$. Let also $\mathbf{1} = (1, 1, ..., 1)'$ an n-vector of ones, $\mathbf{U}$ is the $n \times n$ matrix of ones, and $\mathbf{a}$ = vector of $\gamma(\mathbf{x}_i - \mathbf{x}_0)$.
Then

OK using variogram

$$\begin{bmatrix} \mathbf{\Gamma} & \mathbf{1} \\ \mathbf{1}' & 0 \end{bmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \mu \end{pmatrix} = \begin{pmatrix} \mathbf{a} \\ 1 \end{pmatrix}$$

OK using covariance

$$\begin{bmatrix} \mathbf{C} & -\mathbf{1} \\ \mathbf{1}' & 0 \end{bmatrix} \begin{pmatrix} \boldsymbol{\lambda} \\ \mu \end{pmatrix} = \begin{pmatrix} \mathbf{b} \\ 1 \end{pmatrix},$$

keeping in mind $\mathbf{\Gamma} = \sigma^2\mathbf{U} - \mathbf{C}$ and $\mathbf{a} = \sigma^2\mathbf{1} - \mathbf{b}$.

II. Nugget effect

Now: allow for measurement error.
First, let $V(\mathbf{x}_j)$ be WSS stationary, $Cov[V(\mathbf{x}+\mathbf{h}), V(\mathbf{x})] = C_V(\mathbf{h})$.

$$\text{Measurements: } \tilde{V}_j := V(\mathbf{x}_j) + W_j, \quad j = 1, ..., n$$

where W_j represent measurement errors (think residuals for regression) and

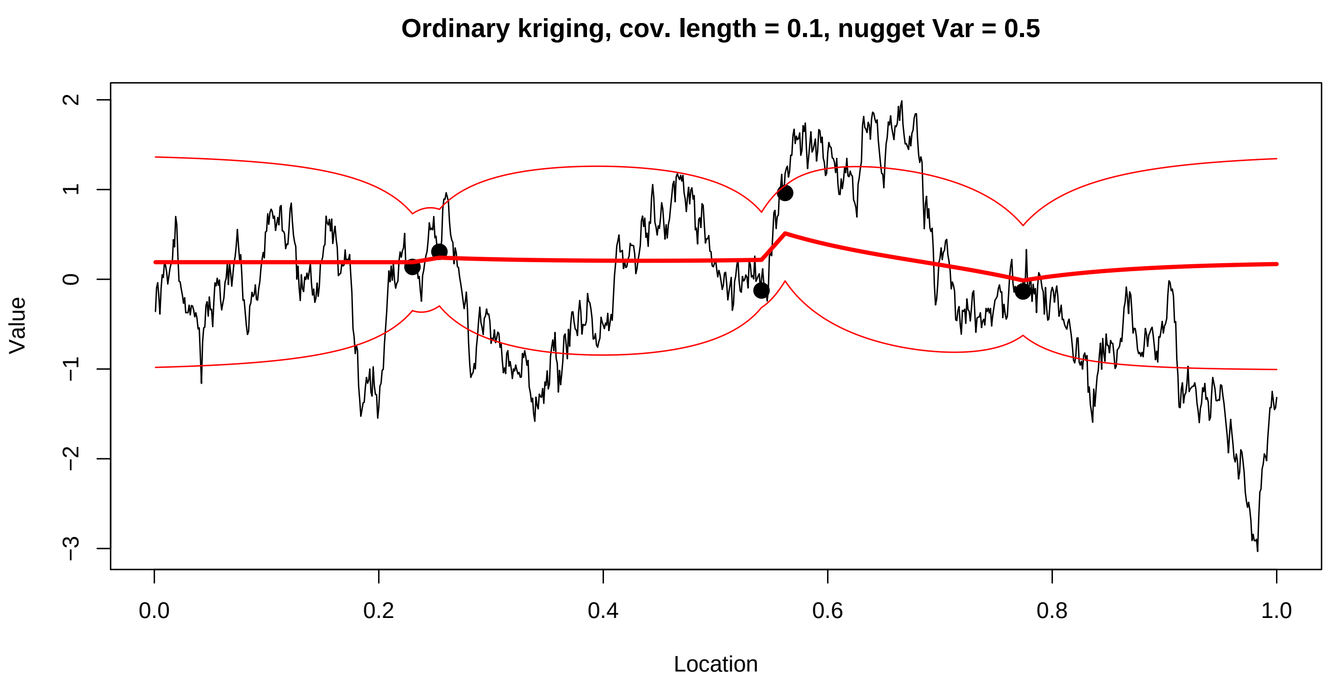
$$\mathbb{E}(W_j) = 0, \quad Var(W_j) = \sigma_W^2,$$

and W_j are independent of each other and everything else.
Goal: predict $V(\mathbf{x}_0)$ (and not $V(\mathbf{x}_0) + W_0$). Now

$$\tilde{C}(i,j) \equiv C_{\tilde{V}}(i,j) = Cov[V(\mathbf{x}_i) + W_i, V(\mathbf{x}_j) + W_j] = \begin{cases} C_V(\mathbf{x}_i - \mathbf{x}_j) & \text{if} \quad i \neq j \\ C_V(\mathbf{0}) + \sigma_W^2 & \text{if} \quad i = j \end{cases}$$

Ordinary kriging equations apply, but the $\mathbf{C}$-matrix changes.

Not an exact interpolator, smoothing effect. Also note the increase in kriging variance.



The result for IRF-0 is similar. The effect of adding noise on (semi)variogram is

$$\tilde{\gamma}(\mathbf{h}) = \gamma(\mathbf{h}) + \sigma_W^2, \quad \mathbf{h} \neq \mathbf{0}$$

III. Block kriging

Sometimes we get weighted averages of the data:

$$V_{ave}(x) = \int_a^b g(x-y)V(y)\,dy$$

(say in 1-d), g is some averaging function.
E.g. pump test, ore grade data averaged over some volume etc.

Say, observations are

$$W_j = \int_{a_j}^{b_j} V(y)\,dy, \quad j = 1, ..., n$$

and we need to predict

$$W_0 = \int_{a_0}^{b_0} V(y)\,dy$$

Let $\mathbb{E}\left[V(x)\right] = const = m$ and $Cov[V(x+\xi), V(x)] = C_V(\xi)$.

Consider $C_W(i,k) = Cov(W_i, W_k)$ - will depend on C_V, and

$$\mathbb{E}\left(W_j\right) = \int_{a_j}^{b_j} \mathbb{E}\left[V(y)\right] dy = m[b_j - a_j]$$

Consider predictor

$$\hat{W}_0 = \sum_{j=1}^{n} \lambda_j W_j,$$

unbiasedness condition is

$$\mathbb{E}\left(W_0\right) = m(b_0 - a_0) = \mathbb{E}\left(\hat{W}_0\right) \quad \text{hence} \quad \sum_{j=1}^{n} \lambda_j [b_j - a_j] = b_0 - a_0.$$

Kriging equations are simple, constraint differs:

$$\boxed{\begin{aligned} &\sum_{j=1}^{n} \lambda_j C_W(j,k) - \mu[b_k - a_k] = C_W(0,k), \quad k = 1, ..., n \\ &\qquad \sum_{j=1}^{n} \lambda_j [b_j - a_j] = b_0 - a_0. \end{aligned}}$$

To compute C_W, use double integral

$$Cov[W_j, W_k] = \int_{a_j}^{b_j} \int_{a_k}^{b_k} C_V(x,y)\,dx\,dy$$

may be messy to find.

In higher dimensions: $\mathbf{x}$ is l-dim. vector, B_j is a region in l-space ($l = 1, 2, 3$).

$$W_j = \iint_{B_j} V(\mathbf{y})\, d\mathbf{y},$$

$$Cov[W_j, W_k] = \iint_{B_j} \iint_{B_k} C_V(\mathbf{x} - \mathbf{y})\, d\mathbf{x}\, d\mathbf{y}$$

Now the kriging equations become

$$\begin{cases} \sum_{j=1}^n \lambda_j C_W(j,k) - \mu |B_k| = C_W(0,k), \quad k = 1, ..., n \\ \sum_{j=1}^n \lambda_j |B_j| = |B_0|, \end{cases}$$

where $|B_k|$ is the size of region k.
Also, kriging variance

$$\sigma^2_{\mathtt{BK}} = C_W(0,0) - \sum_{j=1}^n \lambda_j C_W(j,0) + \mu |B_0|$$

Can also krige $V(\mathbf{x}_0)$ based on W_j's: consider later under co-kriging.