Prediction in regression models with continuous observations

Andrey Pepelyshev

joint with Holger Dette and Anatoly Zhigljavsky

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The model

Consider the common linear regression model

$$y(t) = \theta_1 f_1(t) + \ldots + \theta_m f_m(t) + \varepsilon(t)\ , \ \ t \in \mathcal{T} \subset \mathbb{R}^d$$

- functions $f_1(t), \ldots, f_m(t)$ are linearly independent and continuous,
- a random error field $\varepsilon(t)$ has the zero mean and the covariance kernel $K(t,s) = \mathrm{E}[\varepsilon(t)\varepsilon(s)]$,
- parameters $\theta_1, \ldots, \theta_m$ are unknown and have to be estimated.

Suppose that we observe one realization of a random field.

Prediction with discrete observation

The best linear unbiased predictor (BLUP) of $y(t_0)$ is

$$\hat{y}(t_0) = f^\top(t_0)\hat{\theta}_{\mathrm{BLUE}} + K_{t_0}^\top \Sigma^{-1}(Y - X\hat{\theta}_{\mathrm{BLUE}}),$$

where $\Sigma = \big(K(t_i, t_j)\big)_{i,j=1}^N$, $K_{t_0} = \big(K(t_0, t_1), \ldots, K(t_0, t_N)\big)^\top$, $X = (f(t_1), \ldots, f(t_N))^\top$, $Y = (y(t_1), \ldots, y(t_N))^\top \in \mathbb{R}^N$ and

$$\hat{\theta}_{\mathrm{BLUE}} = (X^\top\Sigma^{-1}X)^{-1}X^\top\Sigma^{-1}Y.$$

The BLUP satisfies the unbiased condition $\mathbb{E}[\hat{y}(t_0)] = \mathbb{E}[y(t_0)]$ and minimizes the mean squared error $\mathrm{MSE}(\tilde{y}(t_0)) = \mathbb{E}\left(y(t_0) - \tilde{y}(t_0)\right)^2$ in the class of all linear unbiased predictors $\tilde{y}(t_0)$; its mean squared error is

$$\mathrm{MSE}(\hat{y}(t_0)) = K(t_0, t_0) - \begin{bmatrix} f(t_0) \\ K_{t_0} \end{bmatrix}^\top \begin{bmatrix} 0 & X^\top \\ X & \Sigma \end{bmatrix}^{-1} \begin{bmatrix} f(t_0) \\ K_{t_0} \end{bmatrix}.$$

Gradient-enhanced kriging is possible.

BLUE for discrete observation

A general estimator

$$\hat{\theta} = G^T Y, \quad Y = (y(t_1), \dots, y(t_N))^T,$$

where G is a $N \times m$-matrix.
The condition of unbiasedness $\mathbb{E}[\hat{\theta}] = \theta$ means

$$G^T X = \mathbf{1}_{m \times m},$$

where $X = (f(t_1), \dots, f(t_N))^T$ is a $N \times m$-matrix.

$$\mathrm{Var}(\hat{\theta}) = G^T \Sigma G \to \min_{unbiased \;\; G}$$

By Gauss-Markov theorem, the best linear unbiased estimator (BLUE) is

$$G_*^T = (X^T \Sigma^{-1} X)^{-1} X^T \Sigma^{-1},$$

where $\Sigma = (K(t_i, t_j))_{i,j=1}^N$.

BLUE for discrete observation with derivatives

A general estimator

$$\hat{\theta} = G_0^T Y_0 + G_1^T Y_1, \quad Y_0 = (y(t_1), \ldots, y(t_N))^T,$$

$$Y_1 = (y'(t_1), \ldots, y'(t_N))^T,$$

where G_0 and G_1 are $N \times m$-matrices.
The covariance matrix is

$$\mathrm{Var}(\hat{\theta}) = G^T \Sigma G,$$

where $G = \begin{pmatrix} G_0 \\ G_1 \end{pmatrix}$, $\Sigma = \begin{pmatrix} \Sigma_{00} & \Sigma_{10}^\top \\ \Sigma_{10} & \Sigma_{11} \end{pmatrix}$ is a block matrix,
$\Sigma_{00} = \big(K(t_i, t_j)\big)_{i,j=1}^N$, $\Sigma_{10} = \big(\frac{\partial}{\partial t_i} K(t_i, t_j)\big)_{i,j=1}^N$,
$\Sigma_{11} = \big(\frac{\partial^2}{\partial t_i \partial t_j} K(t_i, t_j)\big)_{i,j=1}^N$.

Continuous observation without derivatives

A general estimator

$$\hat{\theta}_G = \int_{\mathcal{T}} G_0(dt) y(t),$$

where $G_0(dt)$ is a signed vector-measure.
The condition of unbiasedness $\mathbb{E}[\hat{\theta}] = \theta$ means

$$\int_{\mathcal{T}} f(t) G_0^T(dt) = \mathbf{1}_{m \times m}.$$

The covariance matrix of any unbiased estimator $\hat{\theta}_G$ is

$$\mathrm{Var}(\hat{\theta}_G) = \int_{\mathcal{T}} \int_{\mathcal{T}} K(t,s) G_0(dt) G_0^T(ds).$$

The continuous BLUE minimizes this matrix and may not exist.

Continuous observation with derivatives

A general estimator

$$\hat{\theta}_G = \int_{\mathcal{T}} G_0(dt)y(t) + \ldots + \int_{\mathcal{T}} G_q(dt)y^{(q)}(t),$$

where $G_0(dt), \ldots, G_q(dt)$ are signed vector-measures.
The condition of unbiasedness $\mathbb{E}[\hat{\theta}] = \theta$ means

$$\int_{\mathcal{T}} f(t)G_0^T(dt) + \ldots + \int_{\mathcal{T}} f^{(q)}(t)G_q^T(dt) = \mathbf{1}_{m\times m}.$$

The covariance matrix of any unbiased estimator $\hat{\theta}_G$ is

$$\mathrm{Var}(\hat{\theta}_G) = \sum_{i=0}^{q}\sum_{j=0}^{q}\int_{\mathcal{T}}\int_{\mathcal{T}} \frac{\partial^{i+j}K(t,s)}{\partial t^i \partial s^j} G_i(dt)G_j^T(ds).$$

The continuous BLUE minimizes this matrix and may not exist.

Representation of continuous BLUE

Let $\zeta_0, \dots, \zeta_q$ be some signed vector-measures defined on $\mathcal{T}$ such that the $m \times m$ matrix

$$C = \sum_{i=0}^{q} \int_{\mathcal{T}} \zeta_i(dt) \left(f^{(i)}(t) \right)^T$$

is non-degenerate. Define $G = (G_0, \dots, G_q)$, where G_i are the signed vector-measures and $G_i(dt) = C^{-1}\zeta_i(dt)$ for $i = 0, \dots, q$.

Then the estimator $\hat{\theta}_G$ is unbiased.

Solution for continuous BLUE

Let $K(\cdot,\cdot) \in C^q([A,B]\times[A,B])$ for some $q \geq 0$. Suppose that the process $\{y(t)|t \in [A,B]\}$ along with its q derivatives can be observed at all $t \in \mathcal{T} \subseteq [A,B]$. Assume also that all components of $f(\cdot)$ are q times differentiable. Let $\zeta_0, \ldots, \zeta_q$ be signed vector-measures defined on $\mathcal{T}$ such that the matrix C is non-degenerate. Define $G = (G_0, \ldots, G_q)$, $G_i(dt) = C^{-1}\zeta_i(dt)$ for $i = 0, \ldots, q$.

The estimator $\hat{\theta}_G = \int_{\mathcal{T}} G(dt)Y(t)$ is the BLUE if and only if

$$\sum_{i=0}^{q} \int_{\mathcal{T}} K^{(i)}(t,s)\zeta_i(dt) = f(s) \quad \forall s \in \mathcal{T}.$$

In this case, the covariance matrix of $\hat{\theta}_G$ is $\mathrm{Var}(\hat{\theta}_G) = C^{-1}$.

Properties

To construct the BLUE, we have to solve

$$\sum_{i=0}^{q} \int_{\mathcal{T}} K^{(i)}(t,s)\zeta_i(dt) = f(s) \quad \forall s \in \mathcal{T}.$$

- For $q = 0$ the BLUE measure is a solution of Fredholm integral equation of the first kind.
- We can solve the equation individually for each component of the vector of regression functions $f(t)$.
- The BLUE measure may not exist.
- For $q > 0$ the BLUE measure is not unique [due to possibility of integration by parts].

BLUP without derivatives

Assume that (1) the best linear unbiased estimator (BLUE) $\hat{\theta}_{\mathrm{BLUE}} = \int_{\mathcal{T}} y(t)G(dt)$ exists,
(2) there exists a signed measure $\zeta_{t_0}(dt)$ which satisfies

$$\int_{\mathcal{T}} K(t,s)\zeta_{t_0}(dt) = K(t_0,s), \;\; \forall s \in \mathcal{T}.$$

Then the BLUP measure Q_* exists and is given by

$$Q_*(dt) = \zeta_{t_0}(dt) + c^\top G(dt),$$

where $c = f(t_0) - \int_{\mathcal{T}} f(t)\zeta_{t_0}(dt)$. The MSE of the BLUP $\hat{y}_{Q_*}(t_0) = \int_{\mathcal{T}} y(t)Q_*(dt)$ is given by

$$\mathrm{MSE}(\hat{y}_{Q_*}(t_0)) = K(t_0,t_0) + c^\top Df(t_0) - \int_{\mathcal{T}} K(t,t_0)Q_*(dt)\,,$$

where $D = \int_{\mathcal{T}}\int_{\mathcal{T}} K(t,s)G(dt)G^\top(ds)$ is the covariance matrix of $\hat{\theta}_{\mathrm{BLUE}} = \int_{\mathcal{T}} y(t)G(dt)$.

BLUP with derivatives 1

Consider the problem of prediction of $y^{(p)}(t_0)$, the p-th derivative of y at a point $t_0 \notin \mathrm{T}_p$, where $0 \le p \le q$.
A general linear predictor of the p-th derivative $y^{(p)}(t_0)$ can be defined as

$$\hat{y}_{p,Q}(t_0) = \int \mathbf{Y}^\top(t)\mathbf{Q}(dt) = \sum_{i=0}^{q} \int_{\mathrm{T}_i} y^{(i)}(t) Q_i(dt).$$

The estimator $\hat{y}_{p,Q}(t_0)$ is unbiased if $\mathbb{E}[\hat{y}_{p,Q}(t_0)] = \mathbb{E}[y^{(p)}(t_0)]$, which is equivalent to

$$\int \mathbf{F}(t)\mathbf{Q}(dt) = f^{(p)}(t_0),$$

where $\mathbf{F}(t) = \big(f(t), f^{(1)}(t), \dots, f^{(q)}(t)\big)$ is a $m \times (q+1)$-matrix.

BLUP with derivatives 2

Assume that

(1) The best linear unbiased estimator (BLUE) $\hat{\theta}_{\mathrm{BLUE}} = \int \mathbf{G}(dt)\mathbf{Y}(t)$ exists, where $\mathbf{G}(dt)$ is some signed $m \times (q+1)$-matrix measure (that is, the j-th column of $\mathbf{G}(dt)$ is a signed vector measure defined on $\mathcal{T}_j$);

(2) There exists a signed vector-measure $\zeta_{p,t_0}(dt)$ (of size $q+1$) which satisfies the equation

$$\int \mathbf{K}^\top(t,s)\zeta_{p,t_0}(dt) = \frac{\partial^p K(s,t_0)}{\partial t_0^p}, \;\; \forall s \in \mathrm{T}_i \, ,$$

where $\mathbf{K}(t,s) = \left(\frac{\partial^j K(t,s)}{\partial s^j}\right)_{j=0}^{q}$ is a $(q+1)$-dimensional vector.

BLUP with derivatives 3

Under above assumptions,
the BLUP measure $\mathbf{Q}_*$ exists and is given by

$$\mathbf{Q}_*(dt) = \zeta_{p,t_0}(dt) + \mathbf{G}^\top(dt)c_p,$$

where

$$c_p = f^{(p)}(t_0) - \int \mathbf{F}(t)\zeta_{p,t_0}(dt).$$

The MSE of the BLUP $\hat{y}_{p,Q_*}(t_0)$ is given by

$$\mathrm{MSE}(\hat{y}_{p,Q_*}(t_0)) = \left.\frac{\partial^{2p}K(t,s)}{\partial t^p \partial s^p}\right|_{\substack{t=t_0\\ s=t_0}} + c_p^\top D f^{(p)}(t_0) - \int \mathbf{K}^\top(t,t_0)\mathbf{Q}_*(dt),$$

where

$$D = \int\int \mathbf{G}(dt)\mathbb{K}(t,s)\mathbf{G}^\top(ds)$$

is the covariance matrix of $\hat{\theta}_{\mathrm{BLUE}} = \int \mathbf{G}(dt)\mathbf{Y}(t)$.

Examples of continuous BLUP 1

Consider the model

$$y(t) = \theta + \varepsilon(t), \;\; t = (t_1, t_2) \in \mathcal{T} = [0, 1]^2,$$

$$\mathrm{K}(t, t') = \mathbb{E}[\varepsilon(t)\varepsilon(t')] = \exp\left\{-\lambda\left[|t_1 - t_1'| + |t_2 - t_2'|\right]\right\},$$

where $\lambda > 0$ and $t = (t_1, t_2), t' = (t_1', t_2') \in [0, 1]^2$.
The BLUP at the point $T = (T_1, T_2)$ is $\int_{\mathcal{T}} y(t)\mathrm{Q}_*(dt)$, where

$$\mathrm{Q}_*(dt) = \zeta_T(dt) + c\,\mathrm{G}(dt) \;\; \text{with} \;\; c = 1 - \int_{\mathcal{T}} \zeta_T(dt),$$

where $\mathrm{G}(dt)$ is the BLUE measure and does not depend on $T = (T_1, T_2)$.

Examples of continuous BLUP 2

Define

$$G(dt_i) = \frac{1}{2+\lambda}\left[\delta_0(dt_i) + \delta_1(dt_i) + \lambda dt_i\right], \quad t_i \in [0,1].$$

Define

$$\zeta_{T_i}(dt_i) = \begin{cases} e^{-\lambda|T_i|}\delta_0(dt_i), & \text{if} \quad T_i \le 0, \\ \delta_{T_i}(dt_i), & \text{if} \quad 0 \le T_i \le 1, \\ e^{-\lambda(T_i-1)}\delta_1(dt_i), & \text{if} \quad T_i \ge 1. \end{cases}$$

Then we have $\mathrm{Q}_*(dt) = \zeta_T(dt) + c\,\mathrm{G}(dt)$ with

$$\zeta_T(dt) = \zeta_{T_1}(dt_1)\zeta_{T_2}(dt_2), \quad \mathrm{G}(dt) = G(dt_1)G(dt_2).$$

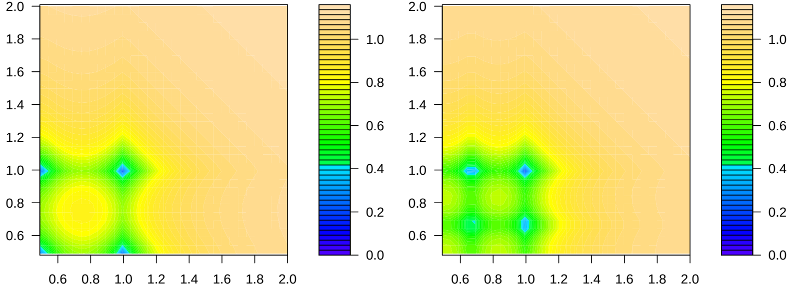
Examples of continuous BLUP 3

For $T_1 \leq 0$ we obtain

$$Q_*(dt) = \begin{cases} e^{-\lambda|T_1|}\delta_0(dt_1)\delta_{T_2}(dt_2) + \left(1 - e^{-\lambda|T_1|}\right) G(dt), & \text{if } 0 \leq T_2 \leq 1, \\ e^{-\lambda|T_1|-\lambda|T_2|}\delta_0(dt_1)\delta_0(dt_2) + \left(1 - e^{-\lambda|T_1|-\lambda|T_2|}\right) G(dt), & \\ \qquad \text{if } \; T_2 \leq 0, & \\ e^{-\lambda|T_1|-\lambda(T_2-1)}\delta_0(dt_1)\delta_1(dt_2) + \left(1 - e^{-\lambda|T_1|-\lambda|T_2-1|}\right) G(dt), & \\ \qquad \text{if } \; T_2 \geq 1. & \end{cases}$$

Similar formulas can be obtained for $0 < T_1 < 1$ and $T_1 \geq 1$.

Examples of continuous BLUP 4



The square root of the MSE of the BLUP for the $N \times N$-point equidistant design at points $(i/(N-1), j/(N-1))$ with $N = 3$ (left) and $N = 4$ (right) and the exponential kernel with $\lambda = 2$.

Examples of continuous BLUP for Matern 3/2

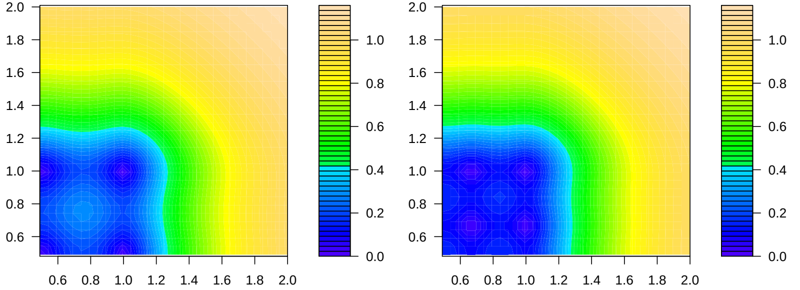
Consider the model $y(t) = \theta + \varepsilon(t)$, $t \in [A, B]$ with Matérn 3/2 covariance kernel $K(t,s) = (1 + \lambda|t - s|)e^{-\lambda|t-s|}$.
Let $t_0 > B$ and we want to predict $\hat{y}_{0,Q_*}(t_0)$. Define
$z_{t_0,B} = (1 + \lambda(t_0 - B))e^{-\lambda(t_0-B)}$, $\quad z_{t_0,1,B} = (t_0 - B)e^{-\lambda(t_0-B)}$,
$C = 1 + \lambda(B - A)/4$, $c_0 = 1 - z_{t_0,B}$). The BLUP measure is

$$\begin{aligned}\mathbf{Q}_*(dt) \;=\; & 0.5c_0\delta_A(dt)/C + (0.5c_0/C + z_{t_0,B})\delta_B(dt) + 0.25c_0\lambda dt/C \\ & -0.25c_0/(C\lambda)\delta_{A,y'}(dt) + (z_{t_0,1,B} + 0.25c_0/(C\lambda))\delta_{B,y'}(dt)\end{aligned}$$

The corresponding BLUP is

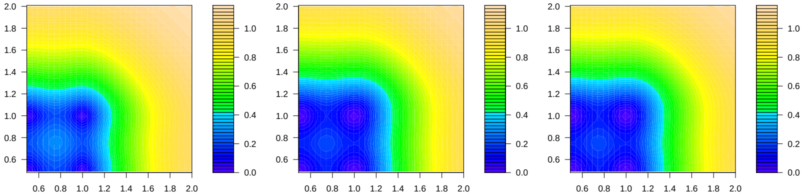
$$\begin{aligned}\hat{y}_{0,Q_*}(t_0) \;=\; & 0.5c_0 y(A)/C + (0.5c_0/C + z_{t_0,B})y(B) + 0.25c_0\lambda\int_A^B y(t)dt/C \\ & -0.25c_0/(C\lambda)y'(A) + (z_{t_0,1,B} + 0.25c_0/(C\lambda))y'(B).\end{aligned}$$

Examples of continuous BLUP for Matern 3/2



Square root of the MSE of the BLUP for the design $\xi_{N^2,0,0,0}$ with $N = 3$ (left) and $N = 4$ (right), and the Matérn 3/2 product-kernel with $\lambda = 2$.

Examples of continuous BLUP for Matern 3/2



Square root of the MSE of the BLUP for the design $\xi_{N^2,0,0,0}$ (left), $\xi_{N^2,4N-4,4N-4,4N-4}$ (center) and ξ_{N^2,N^2,N^2,N^2} (right) with $N = 3$ and the Matérn 3/2 product-kernel with $\lambda = 2$.

The MSE is the same for $\xi_{N^2,4N-4,4N-4,4N-4}$ and ξ_{N^2,N^2,N^2,N^2}.

References

- Dette, H., Pepelyshev, A. and Zhigljavsky, A. (2023). Prediction in regression models with continuous observations. Stat papers. accepted.
- Dette, H., Pepelyshev, A. and Zhigljavsky, A. (2019). The BLUE in continuous-time regression models with correlated errors. Annals of Statistics, 47, 1928-1959.
- Parzen, E. (1961). An approach to time series analysis. The Annals of Mathematical Statistics, 32(4):951–989.
- Näther, W. (1985). Effective observation of random fields. Teubner Verlagsgesellschaft, Leipzig.