# Algorithm

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**Algorithm 1:** Sequential updating and sampling for time points $\boldsymbol{t} = (t_1, \ldots, t_w)^{\mathrm{T}}$ of the joint Gaussian process for the derivative and solution for the $s$ system states for initial values $\boldsymbol{u}_0$, treatment vector $\boldsymbol{x}$, physical parameters $\boldsymbol{\theta}$ and evaluation grid $\boldsymbol{\tau} = (\tau_1, \ldots, \tau_N)^{\mathrm{T}}$, with $\tau_1 = T_0$. (Adapted from Chkrebtii et al. 2016).

1 Set $\boldsymbol{\Lambda}_1 = 0$ and $\boldsymbol{f}_1 = \boldsymbol{f}(\boldsymbol{u}_0, T_0, \boldsymbol{x}; \boldsymbol{\theta})$

2 **for** $r = 1, \ldots, N-1$ **do**

(a) Set $\boldsymbol{\tau}_r = (\tau_1, \ldots, \tau_r)^{\mathrm{T}}$

(b) Compute

$\boldsymbol{B}_r = (\dot{C}_0(\boldsymbol{\tau}_r, \boldsymbol{\tau}_r) + \boldsymbol{\Lambda}_r)^{-1}$

$\boldsymbol{a}_r = \boldsymbol{B}_r \bar{C}_0(\boldsymbol{\tau}_r, \tau_{r+1})$

$C_r = C_0(\tau_r, \tau_r) - \bar{C}_0(\tau_{r+1}, \boldsymbol{\tau}_r)\boldsymbol{B}_r\bar{C}_0(\boldsymbol{\tau}_r, \tau_{r+1})$

$\dot{C}_{r+1} = \dot{C}_0(\tau_{r+1}, \tau_{r+1}) - \dot{C}_0(\tau_{r+1}, \boldsymbol{\tau}_r)\boldsymbol{B}_r\dot{C}_0(\boldsymbol{\tau}_r, \tau_{r+1})$

$\boldsymbol{\Lambda}_{r+1} = \mathrm{diag}\{\boldsymbol{\Lambda}_r, \dot{C}_{r+1}\}$

(c) Compute

$\boldsymbol{m}_r = \boldsymbol{u}_0 + \boldsymbol{F}_r^{\mathrm{T}}\boldsymbol{a}_r$, where $\boldsymbol{F}_r$ is the $r \times s$ matrix with $k$th row $\boldsymbol{f}_k$ $(k = 1, \ldots, N-1)$

(d) Sample

$\boldsymbol{u}(\tau_{r+1}) \sim N(\boldsymbol{m}_r, C_r \boldsymbol{I}_S)$

and compute

$\boldsymbol{f}_{r+1} = \boldsymbol{f}(\boldsymbol{u}(\tau_{r+1}), \tau_{r+1}, \boldsymbol{x}; \boldsymbol{\theta})$

3 Compute

$\boldsymbol{B}_N = (\dot{C}_0(\boldsymbol{\tau}_N, \boldsymbol{\tau}_N) + \boldsymbol{\Lambda}_N)^{-1}$

$\boldsymbol{A}_N(\boldsymbol{t}) = \boldsymbol{B}_N \bar{C}_0(\boldsymbol{\tau}, \boldsymbol{t})$

$\boldsymbol{M}_N(\boldsymbol{t}) = \boldsymbol{1}_n \otimes \boldsymbol{u}_0^{\mathrm{T}} + \boldsymbol{A}_N^{\mathrm{T}}(\boldsymbol{t})\boldsymbol{F}_N$, with $\boldsymbol{1}_n$ the $n$-vector with all entries equal to one and $\boldsymbol{F}_N$ the $N \times s$ matrix with $k$th row $\boldsymbol{f}_k$ $(k = 1, \ldots, N)$

$\boldsymbol{C}_N(\boldsymbol{t}, \boldsymbol{t}) = \boldsymbol{C}_0(\boldsymbol{t}) - \bar{C}_0(\boldsymbol{t}, \boldsymbol{\tau})\boldsymbol{B}_N\bar{C}_0(\boldsymbol{\tau}, \boldsymbol{t})$

4 For $h = 1, \ldots, s$, sample

$u_h(t_1), \ldots, u_h(t_n) \sim N(\boldsymbol{M}_N(\boldsymbol{t})\boldsymbol{e}_h, \boldsymbol{C}_N(\boldsymbol{t}, \boldsymbol{t}))$, where $\boldsymbol{e}_h$ is the $h$th unit vector

**Algorithm 3:** Precomputation of variances $C_r, \dot{C}_{r+1}, \boldsymbol{B}_r$ and covariances $\boldsymbol{a}_r$ for evaluation grid $\boldsymbol{\tau} = (\tau_1, \ldots, \tau_N)^{\mathrm{T}}$

1 Set $\boldsymbol{\Lambda}_1 = 0$

2 **for** $r = 1, \ldots, N-1$ **do**

(a) Set $\boldsymbol{\tau}_r = (\tau_1, \ldots, \tau_r)^{\mathrm{T}}$

(b) Compute

$\boldsymbol{B}_r = (\dot{C}_0(\boldsymbol{\tau}_r, \boldsymbol{\tau}_r) + \boldsymbol{\Lambda}_r)^{-1}$

$\boldsymbol{a}_r = \boldsymbol{B}_r \bar{C}_0(\boldsymbol{\tau}_r, \tau_{r+1})$

$C_r = C_0(\tau_r, \tau_r) - \bar{C}_0(\tau_{r+1}, \boldsymbol{\tau})\boldsymbol{B}_r\bar{C}_0(\boldsymbol{\tau}_r, \tau_{r+1})$

$\dot{C}_{r+1} = \dot{C}_0(\tau_{r+1}, \tau_{r+1}) - \dot{C}_0(\tau_{r+1}, \boldsymbol{\tau})\boldsymbol{B}_r\dot{C}_0(\boldsymbol{\tau}_r, \tau_{r+1})$

$\boldsymbol{\Lambda}_{r+1} = \mathrm{diag}\{\boldsymbol{\Lambda}_r, \dot{C}_{r+1}\}$

3 Compute $\boldsymbol{B}_N = (\dot{C}_0(\boldsymbol{\tau}_N, \boldsymbol{\tau}_N) + \boldsymbol{\Lambda}_N)^{-1}$

$$\left.\begin{aligned} \dot{u}_1(t) &= \tfrac{x_1(u_2(t)+\theta_2\theta_4)-u_1(t)(x_2+\theta_2\theta_3)}{u^\star(\boldsymbol{u}(t),t,\theta,x)},\\ \dot{u}_2(t) &= \tfrac{x_2(u_1(t)+\theta_2\theta_4)-u_2(t)(x_1+\theta_2\theta_3)}{u^\star(\boldsymbol{u}(t),t,\theta,x)},\\ u_1(0) &= u_{01},\\ u_2(0) &= u_{02}, \end{aligned}\right\} t \in [0, 600], \quad (2)$$

$\exp^{t_1+t_2} \rightarrow$ valor

$(\text{Valor} + 0)^{-1}$ $\quad \frac{1}{\text{valor}}$ Valor

• Vectores ( ) ( )

$\begin{pmatrix} x & x \\ x & x \end{pmatrix}\begin{pmatrix} \ \end{pmatrix} = \begin{pmatrix} \cdot \\ \cdot \end{pmatrix}$ 2x2 2x1 2x1

① Si $r=1$,

$\tau_1 = (\tau_1)$ Matriz

Vector parado.

$B_1 = [\dot{C}_0(\tau_1, \tau_1) + \Lambda_1]^{-1}$

$a_1 = B_1 \bar{C}_0(\tau_1, \tau_2)$ $\begin{bmatrix} x \\ x \end{bmatrix} \tau_2$

Valor [.]

La matriz $B_1$ tiene que tener las mismas columnas que la matriz $\bar{C}_0$

filas

Valor

$C_1 = C_0(\tau_1, \tau_1) - \bar{C}_0(\tau_2, \tau_1) B_r \bar{C}_0(\tau_1, \tau_2)^{T}$

Valor

$C_1 = \boxed{*} - \boxed{a_1 \ a_2} \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$

1x2 2x2

$(a_1 b_{11} + a_2 b_{21}, a_1 b_{12} + a_2 b_{22})$ 1x2

Valor exp( ) valor

$\dot{C}_2 = \dot{C}_0(\tau_2, \tau_2) - \dot{C}_0(\tau_2, \tau_1) B_r \dot{C}_0(\tau_1, \tau_2)$

Valor

Vector $+ \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

Valor

$\Lambda_2 = \mathrm{diag}\{\Lambda_1, \dot{C}_2\}$ → Tamaño

$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ $\dot{C}_2 = *$ $\begin{pmatrix} \Lambda_1 & 0 \\ 0 & \dot{C}_2 \end{pmatrix}$

$\Lambda_1$ $\cancel{\begin{pmatrix} \dot{C}_2 & 0 \\ 0 & \dot{C}_2 \end{pmatrix}}$

$r = 2$

$\tau_2 = (\tau_1, \tau_2)^T$ 2x2

$B_2 = (\dot{C}_0(\tau_2, \tau_2) + \Lambda_2)^{-1}$ $\quad \int \dot{C}_0$ $\quad \bar{C}_0$ ?

$\dot{C}_0\left(\begin{bmatrix} \tau_1 \\ \tau_2 \end{bmatrix}, \begin{bmatrix} \tau_1 \\ \tau_2 \end{bmatrix}\right)$

function $\begin{bmatrix} x & x \\ x & x \end{bmatrix} = \begin{pmatrix} \cdot & \cdot \end{pmatrix}$

function $\begin{bmatrix} x & x \\ x & x \end{bmatrix} = \begin{pmatrix} \cdot & \cdot \\ \cdot & \cdot \end{pmatrix}$

$a_2 = B_2 \bar{C}_0(\tau_2, \tau_3)$

$\bar{C}_0\left(\begin{bmatrix} \tau_1 \\ \tau_2 \end{bmatrix}, \tau_3\right)$

Vector Valor

$(\tau_1, \tau_2)$

$\tau_2 \rightarrow \cancel{x}$

$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} \bar{C}_{01} \\ \bar{C}_{02} \end{pmatrix} = \begin{pmatrix} \cdot \\ x \end{pmatrix}$

Valor $\rightarrow C_2 = C_0(\tau_2, \tau_2)$ – de arriba

Valor Valor

Valor $\rightarrow \dot{C}_3 = \dot{C}_0(\tau_3, \tau_3)$ – más lógica

Valor Valor Valor

$A_3 = \mathrm{diag}\{A_2, \dot{C}_3\}$

$\begin{pmatrix} A_2 & 0 \\ 0 & \dot{C}_3 \end{pmatrix}$

$\begin{pmatrix} A_r & 0 \\ 0 & \dot{C}_{r+1} \end{pmatrix}$