

Bayesian smoothing with extended second order random walk model: An detailed overview and comparison

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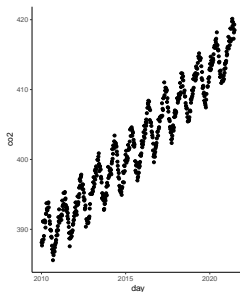
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 - RW2 Prior
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Consider the atmospheric Carbon Dioxide (CO₂) concentrations data from an observatory in Hawaii. This dataset contains the observation of CO₂ concentrations from 1960 to 2021, with unequally spaced observation times.





Model:

$$y_i = f_p(t_i) + f_{np}(t_i) + \epsilon_i$$

- $\epsilon_i \stackrel{iid}{\sim} N(0, \sigma_\epsilon^2)$
- $f_p(t_i)$ is defined as
$$\beta_0 + \beta_1 \cos(2\pi t) + \beta_2 \sin(2\pi t) + \beta_3 \cos(4\pi t) + \beta_4 \sin(4\pi t).$$
- $f_{np}(t_i)$ is the non-parametric part.

Question of interest: A smooth function $f_{np}(t)$ as well as its derivative for $t \geq 2020$.



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Fitting Smoothing Spline

Consider $y_i = g(x_i) + \epsilon_i$ where $\epsilon_i \stackrel{iid}{\sim} N(0, \sigma_\epsilon^2)$ and $x_i \in [a, b]$, then the (traditional) smoothing spline aims to solve:

$$\arg \min_{g \in \mathbb{C}^2} \left\{ \sum_i \left(\frac{y_i - g(x_i)}{\sigma_\epsilon} \right)^2 + \lambda \int_a^b g''(x)^2 dx \right\} \quad (1)$$

The sum of square term on the left can be replaced by negative log likelihood, which is also called *penalized likelihood* method.

Problem: The parameters σ_ϵ and λ are unknown.

One Solution: Bayesian hierarchical model.

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Vectorize the equation 1 into the following:

$$\frac{1}{\sigma_\epsilon^2}(\mathbf{y}-\mathbf{g})^T(\mathbf{y}-\mathbf{g})+\lambda\mathbf{g}^TK\mathbf{g}, \quad (2)$$

This can be interpreted as:

$$\text{log-likelihood} + \text{prior for } \mathbf{g}. \quad (3)$$

The matrix K can be factorized as the following:

$$K = D^TR^{-1}D. \quad (4)$$

The $(n-2) \times n$ matrix D is a second-order differencing matrix. The $(n-2) \times (n-2)$ matrix R^{-1} corresponds to the precision matrix of a MA(1) process ([Brown and De Jong, 2001](#)).

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When covariates are unit spaced, we have the following expressions for D and R :

$$D = \begin{bmatrix} 1 & -2 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & \vdots & & & \ddots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \end{bmatrix}, \quad R = \begin{bmatrix} \frac{2}{3} & \frac{1}{6} & 0 & 0 & 0 & \cdots & 0 \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 & 0 & \cdots & 0 \\ \frac{1}{6} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & 0 & \cdots & 0 \\ 0 & \frac{1}{6} & \frac{1}{6} & \frac{2}{3} & 0 & \cdots & 0 \\ & & & & \ddots & \ddots & \\ 0 & 0 & 0 & \cdots & 0 & \frac{1}{6} & \frac{2}{3} \end{bmatrix} \quad (5)$$

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- **Problem 1** : This ARIMA(0,2,1) interpretation requires covariate values to be equally spaced. Not directly applicable to irregular spaced locations.
- **Problem 2** : R^{-1} is a dense matrix, and hence the precision matrix of \mathbf{g} is dense as well. Computation will be hard and not compatible with inference method such as Integrated Nested Laplace Approximation(INLA) ([Rue et al., 2009](#)).

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From result of [Wahba \(1978\)](#), there is a well known connection between smoothing spline and folded Wiener process prior:

- 1 Let $W(t)$ denote the standard Wiener's process (Brownian motion), a SDE based prior is assigned to $g(t)$ in the following way ($\sigma_s = 1/\sqrt{\lambda}$):

$$\frac{d^2 g(t)}{dt^2} = \sigma_s \frac{dW(t)}{dt}.$$

- 2 The derivative of $W(t)$ does not exist in ordinary definition, but can be defined as a generalized function, the *white noise* process.
- 3 If $g(0)$ and $g'(0)$ are given diffuse Gaussian prior, the limiting posterior mean of \mathbf{g} will be the minimizer of the smoothing spline problem ([Wahba, 1978](#)).

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The extended RW2 method of [Lindgren and Rue \(2008\)](#) can be derived from the following procedures:

- 1 Assign the SDE based prior on g .
- 2 Discretize the SDE into a finite dimensional problem using finite element method. Resulting in precision matrix being:

$$H^T B^{-1} H.$$

- 3 Apply a diagonal approximation to the tri-diagonal matrix B . Resulting in precision matrix being:

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When covariates are unit spaced, we have the following expressions for H , B and A :

$$H = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & \vdots & & & \ddots & & \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}, B = \begin{bmatrix} \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{6} & \frac{1}{6} & \cdots & 0 & 0 \\ & & & & \ddots & & & \\ 0 & 0 & 0 & \cdots & \frac{1}{6} & \frac{1}{6} & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \frac{1}{6} & \frac{1}{6} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \frac{1}{6} & \frac{1}{3} \end{bmatrix}, \quad (6)$$

$$A = \begin{bmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cdots & 0 & 0 \\ & & & & \ddots & & & \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}. \quad (7)$$

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$$H = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & \vdots & & & \ddots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix}, B = \begin{bmatrix} \frac{1}{3} & \frac{1}{6} & 0 & 0 & 0 & \cdots & 0 & 0 \\ \frac{1}{6} & \frac{1}{3} & \frac{1}{6} & 0 & 0 & \cdots & 0 & 0 \\ 0 & \frac{1}{6} & \frac{1}{3} & \frac{1}{6} & 0 & \cdots & 0 & 0 \\ 0 & 0 & \frac{1}{6} & \frac{1}{3} & \frac{1}{6} & \cdots & 0 & 0 \\ & & & & \ddots & \ddots & & \\ 0 & 0 & 0 & \cdots & \frac{1}{6} & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \frac{1}{6} & \frac{2}{3} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & \frac{1}{6} & \frac{1}{3} \end{bmatrix}, \quad (6)$$

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However, INLA software does not accommodate prior with dense precision matrix such as $\text{ARIMA}(0,2,1)$.

- Re-parametrizing the smoothing parameter σ_s^2 as $\theta = -2 \log \sigma_s$, and let Q_θ denotes the precision matrix corresponding to the evaluation vector \mathbf{g} .
- Gaussian approximation:

$$\tilde{\pi}_G(\mathbf{g}|\mathbf{y}, \theta) \propto \exp \left\{ -\frac{1}{2} \left(\mathbf{g} - \hat{\mathbf{g}}_\theta \right)^T H_\theta(\hat{\mathbf{g}}_\theta) \left(\mathbf{g} - \hat{\mathbf{g}}_\theta \right) \right\}, \quad (8)$$

the quantity $\hat{\mathbf{g}}_\theta$ denotes $\operatorname{argmax}_{\mathbf{g}} \log \pi(\mathbf{g}|\theta, \mathbf{y})$ and $H_\theta(\mathbf{g})$ denotes $-\frac{d^2}{d\mathbf{g}d\mathbf{g}^T} \log \pi(\mathbf{g}|\theta, \mathbf{y})$.

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- Obtain the Laplace approximation as Tierney and Kadane (1986):

$$\tilde{\pi}_{\text{LA}}(\theta|\mathbf{y}) \propto \pi(\theta) \left\{ \frac{|Q_\theta|}{|H_\theta(\hat{\mathbf{g}}_\theta)|} \right\}^{1/2} \exp \left\{ -\frac{1}{2} \hat{\mathbf{g}}_\theta^T Q_\theta \hat{\mathbf{g}}_\theta + l(\mathbf{y}; \hat{\mathbf{g}}_\theta) \right\}. \quad (9)$$

- Numerical Integration:

$$\tilde{\pi}(\mathbf{g}|\mathbf{y}) = \sum_{k=1}^K \tilde{\pi}_G(\mathbf{g}|\mathbf{y}, \theta_k) \tilde{\pi}_{\text{LA}}(\theta_k|\mathbf{y}) \delta_k, \quad (10)$$

where $\{\theta_k, \delta_k\}_{k=1}^K$ is a set of K nodes and weights selected using Adaptive Gauss-Hermite Quadrature (AGHQ) rule (Stringer, 2021).

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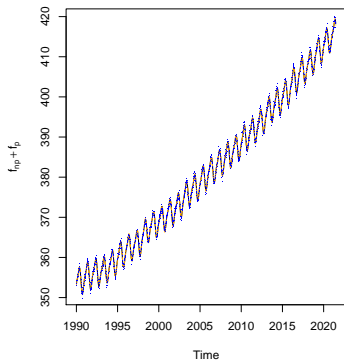
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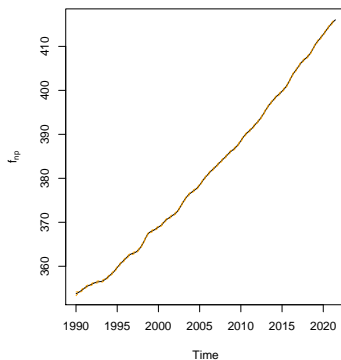
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Going back to the CO2 Example with RW2 method:



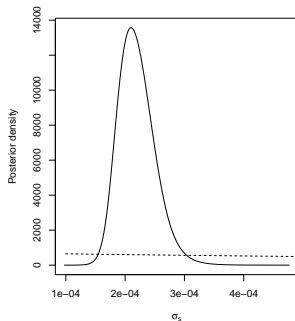
(a) Overall effect f



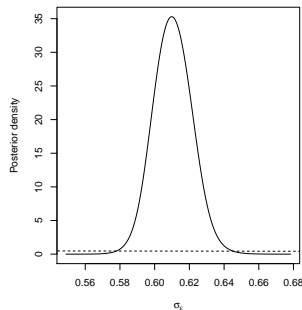
(b) Random effect f_{np}

Figure: Inference obtained for the CO2 dataset using RW2, for observations after year 1990.

Looking at the variance and smoothing parameters:



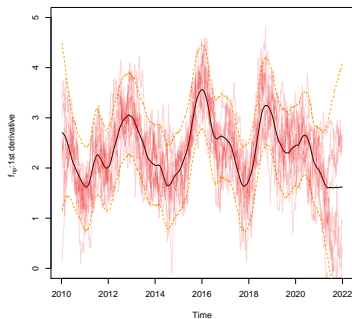
(a) Posterior for the smoothing parameter σ_s



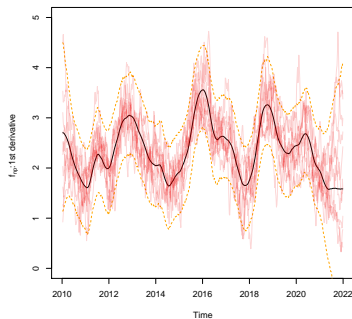
(b) Posterior for the variance parameter σ_ϵ

Figure: Inference for smoothing/variance parameters with PC prior (Simpson et al., 2017) with median 2.

What about the derivatives?

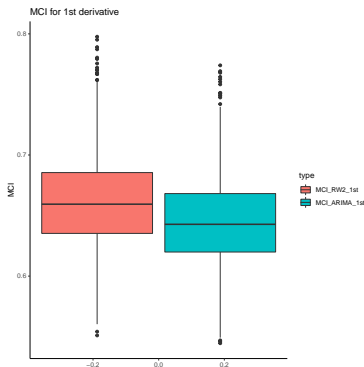


(a) f_{np} using RW2

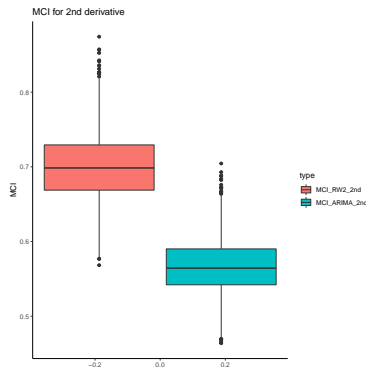


(b) f_{np} using ARIMA

A Simulation Study with 1000 independent replications:



(c) MCI for g'



(d) MCI for g''

Figure: Mean width of 90 percent credible interval (MCI) for g' , g'' using RW2 or ARIMA, replicated for 1000 independent data sets.

- We provide an overview of the extended second order random walk method ([Lindgren and Rue, 2008](#)), as well as its connection with the smoothing spline ([Wahba, 1978](#)) and the ARIMA prior ([Brown and De Jong, 2001](#)).
- The RW2 method gives similar result in terms of inference for g as the ARIMA method, but less smooth inference for higher order derivatives of g compared to ARIMA method.
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