BKTR: An efficient spatiotemporally varying coefficient regression package in R and Python

Julien Lanthier
HEC Montréal

Mengying Lei
McGill University

Aurélie Labbe
HEC Montréal

Lijun Sun
McGill University

Abstract

BKTR is a new software library for spatiotemporal regression analysis with varying coefficients that allows for efficient and easy-to-use inference over datasets that vary in time and space. The library is implemented as Python and R packages, providing a flexible and easy to use framework for spatiotemporal regression models. One of the main challenges in spatiotemporal modeling when using local regression is the computational cost. **BKTR** addresses this computational challenge by implementing a tensor regression approach. This approach greatly reduces the computational cost of the model. The calculation speed is further improved using the specialized tensor library **torch** (both in R and Python), which enables optimal matrix and tensor computation on GPUs and TPUs. The framework also utilizes Gaussian process (GP) priors to capture the spatial and temporal dependencies of the data in a Bayesian context. Hence, the full name of the framework, Bayesian Kernelized Tensor Regression, refers to the combined usage of tensor regression and GP models. The Python **pyBKTR** package is available on PyPI and the R **BKTR** package has been submitted to CRAN.

Keywords: Gaussian process, Tensor regression, Local spatiotemporal regression, R, Python.

1. Introduction

With the rise of the Internet of Things (IoT) and a great increase of mobile device and sensor usage, the amount of available data varying through time and space has been growing rapidly. Thus, statistical analysis like spatiotemporal regressions that take into account the spatial and temporal aspects of data have become more and more valuable. Spatiotemporal regressions are especially useful for analyzing and predicting complex phenomena like weather patterns, agriculture output, transportation, disease outbreaks and much more. It is possible to regroup spatiotemporal regressions into two main categories: global and local regressions. The main difference between these two types of regressions are in their approach for modelling relationships between variables over space and time. Global regression assumes that the relationships between variables are constant across space and time. In contrast, local regression allows for the relationship between variables to vary across different locations and time points. Local regression is often viewed as a more flexible and better suited method to capture changes in variables' relationships over time and space.

Even if local regression is usually more flexible and leads to better fit, this method is much more computationally expensive than global regression. This is due to the fact that local regression needs to estimate coefficients at each location and time point studied. In fact, for a response matrix $Y \in \mathbb{R}^{M \times N}$ observed from a set of locations $S = \{s_1, \ldots, s_M\}$ and a set of time points $T = \{t_1, \ldots, t_N\}$, we can define the model over a Cartesian product $S \times T = \{(s_m, t_n) : m = 1, \ldots, M,\ n = 1, \ldots, N\}$ and we can formulate local spatiotemporal regression as:

$$y(s_m, t_n) = \boldsymbol{x}(s_m, t_n)^T \boldsymbol{\beta}(s_m, t_n) + \epsilon(s_m, t_n), \tag{1}$$

where $y(s_m, t_n)$ is the response variable at location s_m and time t_n, $x(x_m, t_n)$ and $\beta(s_m, t_n)$ are the covariates and coefficients at location s_m and time t_n respectively. Local spatiotemporal regression already has been explored and implemented in the literature. For example, Gelfand *et al.* (2003) already suggested using a separable kernel to build a spatiotemporally varying coefficient model (STVC). However, even with the advent of new computing technologies, local regression for spatiotemporal data methodologies like STVC are still unable to run on even medium-sized datasets, due to the sheer number of local regression's parameters. To our knowledge there is, to this day, no readily available software packages allowing to use in an efficient manner a local spatiotemporal regression. The scalable spatiotemporally varying coefficient modelling with bayesian kernelized tensor regression (BKTR) method proposed by Lei *et al.* (2023) overcomes this limitation by using a tensor regression to estimate coefficients. In doing so, the time complexity of each sampling iteration changes from $\mathcal{O}(M^3N^3P^3)$ for the STVC method to $\mathcal{O}(R^3(M^3 + N^3 + P^3))$, where R is usually an arbitrary small value denoting the tensor rank. The BKTR method also uses a Gaussian process (GP) prior with a spatial and a temporal kernel to model the spatiotemporal dependence of the coefficients.

From a software perspective, a wide range of R (R Core Team 2023) packages is currently available on the Comprehensive R Archive Network (CRAN) for exploring the spatial characteristics of datasets. Some general spatial packages including **sp** (Pebesma and Bivand 2005), **spatial** (Venables and Ripley 2002), **spacetime** (Pebesma 2012) and **spatstat** (Baddeley and Turner 2005) enable the analysis and visualization of spatial patterns. Additional packages such as **splm** (Millo and Piras 2012), and **fields** (Douglas Nychka *et al.* 2021) facilitate spatial regressions and kriging. The package **gstat** (Pebesma 2004) initially focused on spatial models, but it is now enabling spatio-temporal modelling using covariance models (Gräler *et al.* 2016).

Significant advancements in spatio-temporal data modeling are linked to the integration of regression models based on the Bayesian paradigm. Implementing Bayesian Markov chain Monte Carlo (MCMC) models can be accomplished through packages like **R2WinBUGS** (Sturtz *et al.* 2005), **rjags** (Plummer 2023) and **rstan** (Stan Development Team 2023) which are R wrappers for the **WinBugs** (Lunn *et al.* 2000), **JAGS** (Plummer 2003) and **Stan** (Carpenter *et al.* 2017) general MCMC frameworks, written in low level languages. An alternative to MCMC for Bayesian inference, which can be more computationally effective, is the integrated nested Laplace approximation (INLA) methodology (Rue *et al.* 2009). This modelling approach has been successfully applied to different spatial dataset (Lindgren and Rue 2015) using the **R-INLA** package. While these packages provide versatile Bayesian frameworks, the complexity of implementing spatio-temporal models, especially with localized spatio-temporal variations, often requires specialized expertise.

Recent years have brought new integrated Bayesian regression software solutions like **spate** (Sigrist *et al.* 2015), simplifying spatio-temporal regression while accounting for temporal aspects of the data. However, **spate** lacks the capability to incorporate local spatial regression, which restrict the inclusion of locally varying temporal patterns. To address this limitation, packages such as **spTimer** (Bakar and Sahu 2015), **spBayes** (Finley *et al.* 2015) and **spTDyn** (Bakar *et al.* 2016) have emerged, making it easier to implement spatio-temporal regression models with spatially varying coefficients. As demonstrated in Table 1, an unmet need for local temporal regression persisted, but this gap is now bridged by the introduction of the **BKTR** package. By incorporating a spatio-temporally varying coefficients in an efficient manner **BKTR** enhance spatio-temporal analyses and broaden the toolkit available to researchers and analysts.

R Package	Regression Types				
	Spatial	Temporal	Bayesian	Local in Space	Local in Time
splm	✓				
fields	✓				
gstat	✓	✓			
spate	✓	✓	✓		
spBayes	✓	✓	✓	✓	
spTimer	✓	✓	✓	✓	
spTDyn	✓	✓	✓	✓	
BKTR	✓	✓	✓	✓	✓

Table 1: Summary of the spatial regression packages available in R

The packages presented in this paper, **BKTR** and **pyBKTR**, implement the BKTR method and provide a user-friendly interface to estimate coefficients for local spatio-temporal regression. The **BKTR** package is implemented in R and is available on CRAN. The **pyBKTR** library is implemented in Python and is available on PyPI (`https://pypi.org/project/pyBKTR`). Both packages provide the same functionalities and are designed to be used in a similar fashion. To mimic the object-oriented patterns of Python, we used the **R6** package (Chang 2021) in **BKTR** for classes and methods. Also, to be able to use a similar approach for tensor operations, we used **Torch** in both R and Python packages which translate to **torch** (Falbel and Luraschi 2023) and **pytorch** (Paszke *et al.* 2019) respectively. The visualization of the results is done using the **ggplot2** package (Wickham 2016) in R and **plotly** (Plotly Technologies Inc. 2015) in Python. Furthermore, to be able to use Wilkinson formulae (Wilkinson and Rogers 1973), like in the R formula object, we use the **Formulaic** (Wardrop 2022) python package. For data frame usage, we use the **pandas** package (The Pandas Development Team 2022) in Python and **data.table** (Dowle and Srinivasan 2023) in R. All the examples shown in this paper are available in a GitHub repository (`https://github.com/julien-hec/bktr-examples`). This paper focuses mainly on the R implementation of **BKTR**, but the syntaxes of the R and Python packages we implemented are very similar. To convert covered examples from R to Python, it should be sufficient to convert all base 1 indexes to base 0 and to change "`$`" to "`.` ", "`<-`" to "`=`" and "`$new()`" to "`()`". Also, the source code and all examples shown in this paper are available on GitHub at `https://github.com/julien-hec/BKTR/` and `https://github.com/julien-hec/pyBKTR/` for **BKTR** and **pyBKTR** respectively. Note that when we refer to the **BKTR** packages in this paper (plural form), we are referring to both the R and Python implementations at the same time.

The rest of this paper is organized as follows. Section 2 presents the BKTR algorithm. Section 3 presents the `BKTRRegressor` class and its attributes. Section 4 presents the different kernels available in the package. Section 5 presents a simulation study to validate our implementation of the BKTR regression. Section 6 presents an experimental study on bike sharing data. Finally, Section 7 concludes the paper.

2. BKTR algorithm

The objective of Bayesian Kernelized Tensor Regression (BKTR) is to model a response variable $\boldsymbol{Y}$ as a function of spatiotemporal covariates $\boldsymbol{\mathcal{X}}$, with the model's coefficients allowed to vary over space and time. The covariates $\boldsymbol{\mathcal{X}}$ represent a tensor of size $M \times N \times P$ where M is the number of locations, N is the number of time points and P is the number of covariates at each location and time point we want to model. The response variable $\boldsymbol{Y}$, for its part, is a matrix of size $M \times N$. An example of application could be to model the housing price of M district through N months, using covariates changing through time and space like temperature, population density and air pollution ($P = 3$).

This section is strongly based on the work of Lei *et al.* (2023) and aims to summarize the BKTR model they described. In Section 2.3, we discuss a previously unexplored aspect of BKTR regarding interpolation.

2.1. Model definition

It is possible to reshape the covariates tensor $\boldsymbol{\mathcal{X}}$ and the response variable $\boldsymbol{Y}$ mentioned above to obtain a vectorized version of Equation 1:

$$\boldsymbol{y} = (\boldsymbol{I}_{MN} \odot \boldsymbol{X}_{(3)})^\top \text{vec}(\boldsymbol{B}_{(3)}) + \boldsymbol{\epsilon}, \tag{2}$$

where $\boldsymbol{y}$ is the vectorized version in $\mathbb{R}^{MN}$ of $\boldsymbol{Y}$, $\boldsymbol{X}_{(3)}$ and $\boldsymbol{B}_{(3)}$ are the mode-3 unfolding of $\boldsymbol{\mathcal{X}}$ and $\boldsymbol{\mathcal{B}}$ respectively. The $\odot$ operator is the Khatri-Rao product (Khatri and Rao 1968) and the product $\boldsymbol{I}_{MN} \odot \boldsymbol{X}_{(3)}$ is a sparse expansion of the covariates. The error term $\boldsymbol{\epsilon}$ is assumed to follow a multivariate normal distribution such that $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \tau^{-1}\boldsymbol{I}_{MN})$, where $\boldsymbol{I}_{MN}$ is an identity matrix of size $MN \times MN$. Assuming that $\boldsymbol{\mathcal{B}}$ admits a CANDECOMP/PARAFAC (CP) (Kolda and Bader 2009) decomposition with rank $R \ll \min\{M, N\}$, i.e., $\boldsymbol{\mathcal{B}} = \sum_{r=1}^{R} \boldsymbol{u}_r \circ \boldsymbol{v}_r \circ \boldsymbol{w}_r$, the model can be rewritten as

$$\boldsymbol{y} = \tilde{\boldsymbol{X}} \text{vec}(\boldsymbol{W}(\boldsymbol{V} \odot \boldsymbol{U})^\top) + \boldsymbol{\epsilon}, \tag{3}$$

where $\tilde{\boldsymbol{X}} = (\boldsymbol{I}_{MN} \odot \boldsymbol{X}_{(3)})^\top$ and $\boldsymbol{U}$, $\boldsymbol{V}$ and $\boldsymbol{W}$ are matrices of size $M \times R$, $N \times R$ and $P \times R$, respectively, containing the concatenated vectors of the CP decomposition of $\boldsymbol{\mathcal{B}}$.

To account for missing values in the response variable $\boldsymbol{Y}$, we can rewrite the model of Equation 3 as:

$$\boldsymbol{y}_\Omega \sim \mathcal{N}\left(\boldsymbol{O}\left(\tilde{\boldsymbol{X}} \text{vec}(\boldsymbol{W}(\boldsymbol{V} \odot \boldsymbol{U})^\top)\right), \tau^{-1}\boldsymbol{I}_{|\Omega|}\right). \tag{4}$$

where $\boldsymbol{y}_\Omega$ is the vectorized version of $\boldsymbol{Y}$ restricted to the observed entries Ω, $\boldsymbol{O}$ is the operator selecting the observed entries of a vector and $|\Omega|$ is the number of observed entries, so that given $\boldsymbol{O}$, $\boldsymbol{y}_\Omega = \boldsymbol{O}\boldsymbol{y}$. To account for the spatial and temporal correlation during CP decomposition, we use GP priors on the spatial and temporal component vectors:

$$\begin{aligned} \boldsymbol{u}_r &\sim \mathcal{GP}(0, \boldsymbol{K}_s),\ r = 1, \dots, R, \\ \boldsymbol{v}_r &\sim \mathcal{GP}(0, \boldsymbol{K}_t),\ r = 1, \dots, R, \end{aligned} \tag{5}$$

where $\boldsymbol{K}_s$ and $\boldsymbol{K}_t$ are covariance matrices of size $M \times M$ and $N \times N$ respectively created from two kernel functions $k_s(s_m, s_{m'}; \Phi)$ and $k_t(t_n, t_{n'}; \Gamma)$, where Φ is a vector of J spatial kernel hyperparameters $\Phi = \{\phi_1, \dots, \phi_J\}$ and Γ is a vector of L temporal kernel hyperparameters $\Gamma = \{\gamma_1, \dots, \gamma_L\}$. The priors of kernel hyperparameters are

$$\begin{aligned} \log(\phi_i) &\sim \mathcal{N}(\mu_{\phi_i}, \tau_{\phi_i}^{-1}),\ i = 1, \dots, J, \\ \log(\gamma_i) &\sim \mathcal{N}(\mu_{\gamma_i}, \tau_{\gamma_i}^{-1}),\ i = 1, \dots, L. \end{aligned} \tag{6}$$

It can be noted that, for BKTR, $\boldsymbol{K_s}$ and $\boldsymbol{K_t}$ are in fact correlation matrices since we set the kernel variance to 1 and capture the variance through $\boldsymbol{W}$.

For the components of the factor matrix $\boldsymbol{W}$, we use the following priors

$$\begin{aligned} \boldsymbol{w}_r &\sim \mathcal{GP}(0, \boldsymbol{\Lambda}_w^{-1}),\ r = 1, \dots, R, \\ \boldsymbol{\Lambda}_w &\sim \mathcal{W}(\boldsymbol{\Psi_0}, \nu_0), \end{aligned} \tag{7}$$

where $\boldsymbol{\Psi_0}$ is a $P \times P$ scale matrix and ν_0 is the number of degrees of freedom.

The prior on the noise precision τ in Equation 4 is $\tau \sim \text{Gamma}(a_0, b_0)$.

An illustration of the BKTR framework taken from (Lei *et al.* 2023) is shown in Figure 1 to help visualize the dependencies between variables and the different steps of the algorithm.

2.2. Sampling

This section only gives a brief overview of the sampling algorithm and its main steps which are described in the algorithm 1. More details about the conditional posterior distributions from which BKTR parameters are sampled can be found in Lei *et al.* (2023).

The BKTR MCMC algorithm uses Gibbs sampling (Geman and Geman 1984) for the parameters $\boldsymbol{U}$, $\boldsymbol{V}$, $\boldsymbol{W}, \tau$ and the precision matrix $\boldsymbol{\Lambda}_w$. For the hyperparameters Φ and Γ, a slice sampling algorithm (Neal 2003) is used since the conditional posterior distribution of these parameters is not easy to sample from.

The sampling process uses K_1 burn-in iterations and K_2 iterations to sample the posterior distribution of the parameters. The number of iterations K_1 and K_2 are arbitrary, chosen by the user and should be large enough to ensure the Markov chains reach a stationary state before sampling begins.

The posterior samples $\{\boldsymbol{\mathcal{B}}^{(k)}\}_{k=1}^{K_2}$ are used to approximate the posterior distribution of the coefficients $\boldsymbol{\mathcal{B}}$. The posterior samples can then be used directly to estimate unobserved response variables and to analyze the spatial and temporal patterns of the coefficients.

2.3. Interpolation

An important addition to the BKTR algorithm is the capacity to do interpolation. By interpolation, we mean the ability to estimate new regression coefficients $\boldsymbol{\mathcal{B}}^{\text{new}}$ and response

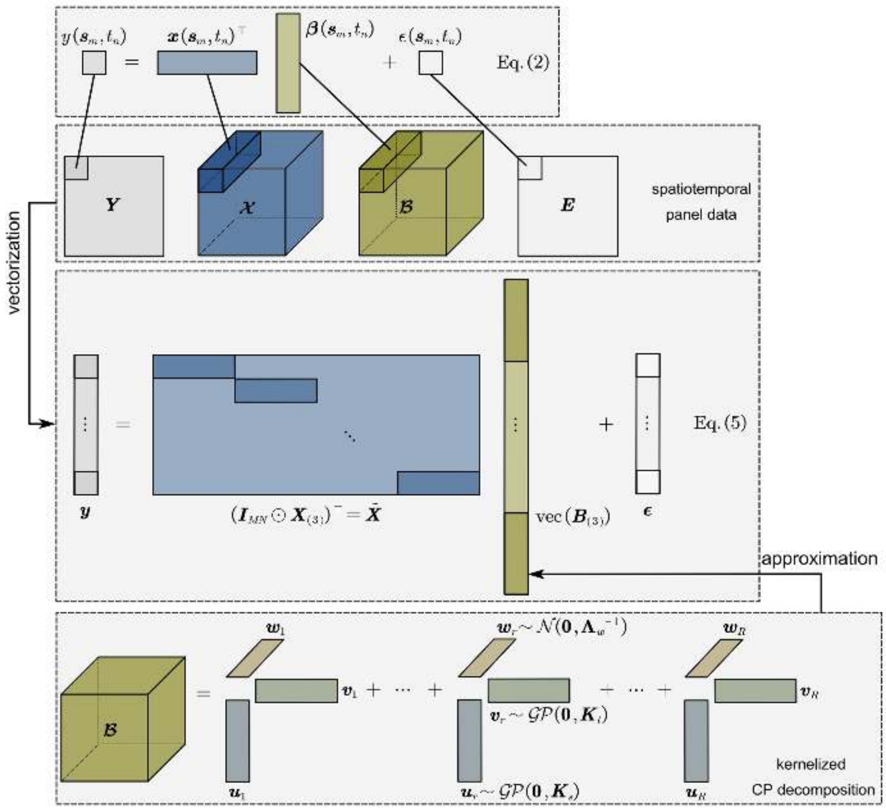

$y(\boldsymbol{s}_m, t_n)$
$=$
$\boldsymbol{x}(\boldsymbol{s}_m, t_n)^\top$
$\boldsymbol{\beta}(\boldsymbol{s}_m, t_n)$
$+$
$\epsilon(\boldsymbol{s}_m, t_n)$
Eq. (2)
$\boldsymbol{Y}$
$\boldsymbol{\mathcal{X}}$
$\boldsymbol{\mathcal{B}}$
$\boldsymbol{E}$
spatiotemporal panel data
vectorization
$\boldsymbol{y}$
$(\boldsymbol{I}_{MN} \odot \boldsymbol{X}_{(3)})^\top = \tilde{\boldsymbol{X}}$
$\mathrm{vec}(\boldsymbol{B}_{(3)})$
$\boldsymbol{\epsilon}$
Eq. (5)
approximation
$\boldsymbol{w}_1$
$\boldsymbol{w}_r \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{\Lambda}_w^{-1})$
$\boldsymbol{w}_R$
$\boldsymbol{\mathcal{B}}$
$\boldsymbol{v}_1 + \cdots +$
$+ \cdots +$
$\boldsymbol{v}_R$
$\boldsymbol{v}_r \sim \mathcal{GP}(\boldsymbol{0}, \boldsymbol{K}_t)$
$\boldsymbol{u}_1$
$\boldsymbol{u}_r \sim \mathcal{GP}(\boldsymbol{0}, \boldsymbol{K}_s)$
$\boldsymbol{u}_R$
kernelized CP decomposition

Figure 1: Illustration of the BKTR framework (Source: Figure 1 from Lei *et al.* (2023))

values $\boldsymbol{Y}^{\mathrm{new}}$ at unobserved time points and locations. In the literature, this process is also often named Bayesian kriging. Interpolation is a different process than imputation, which was already covered in BKTR. Imputation is used when parts of the response variables are missing at some of the M^{obs} locations or N^{obs} time points employed during regression. In contrast, interpolation is accomplished in a completely different step after MCMC sampling, and it is performed at M^{new} new locations and N^{new} time points. To perform interpolation, we need to estimate, for M^{new} unobserved locations and N^{new} unobserved time steps, the posterior distributions of the related coefficients $\boldsymbol{\mathcal{B}}^{\mathrm{new}}$. The formal representation of the $\boldsymbol{\mathcal{B}}^{\mathrm{new}}$ coefficients can be somewhat difficult to visualize, since it cannot be stored in a simple tensor format. Thus, we use a representation similar to the one presented by Takeuchi *et al.* (2017) and we illustrate it in Figure 2. Using this representation, the prediction results of $\boldsymbol{\mathcal{B}}^{\mathrm{new}}$ can be represented by three tensors: $\boldsymbol{\mathcal{B}}^1$ the coefficients for new locations at observed time points, $\boldsymbol{\mathcal{B}}^2$, the coefficients for new time points at observed locations and $\boldsymbol{\mathcal{B}}^3$, the beta coefficients for new locations at new time points. We also include in Figure 2, the equivalent illustration for the newly provided covariates $\boldsymbol{\mathcal{X}}^{\mathrm{new}}$ composed of $\boldsymbol{\mathcal{X}}^1$, $\boldsymbol{\mathcal{X}}^2$, $\boldsymbol{\mathcal{X}}^3$, on top of the related new response variable matrices $\boldsymbol{Y}^{\mathrm{new}}$ composed of $\boldsymbol{Y}^1$, $\boldsymbol{Y}^2$ and $\boldsymbol{Y}^3$.

We estimate the distributions of $\boldsymbol{\mathcal{B}}^{\mathrm{new}}$ via MCMC sampling with an approach similar to the one presented by Gamerman *et al.* (2008). The posterior coefficients $\boldsymbol{\mathcal{B}}^{\mathrm{new}}$ are estimated by doing interpolation on the spatial decomposition $\boldsymbol{U}$ and the temporal decomposition $\boldsymbol{V}$ separately. We can formulate the joint multivariate normal distribution for the r^{th} compo-

Algorithm 1 Simplified BKTR MCMC sampling process

```
    Input: $\boldsymbol{y}_\Omega, \boldsymbol{\mathcal{X}}, R, K_1, K_2, k_s, k_t, \Phi, \Gamma, \tau_\phi, \tau_\gamma, a_0, b_0, \tau$
 1: Intialize $\{\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W}\}$ as normally distributed random values
 2: Set $\mu_{\phi_i} = \log(\phi_i)\ \forall \phi_i \in \Phi,\ \mu_{\gamma_i} = \log(\gamma_i)\ \forall \gamma_i \in \Gamma$
 3: Sample $\Lambda_\omega \sim \mathcal{W}(\boldsymbol{I}_P, P)$
 4: for $k = 1 : K_1 + K_2$ do
 5:     Sample kernel hyperparameters $\Phi, \Gamma$
            ▷ from slice sampling given $\boldsymbol{V}, \boldsymbol{W}, y_\Omega, \boldsymbol{\mathcal{X}}, \Phi, \tau_{\phi_1}, \ldots, \tau_{\phi_J}, \Gamma, \tau_{\gamma_1} \ldots, \tau_{\gamma_L}$
 6:     Sample hyperparameters $\boldsymbol{\Lambda}_w$    ▷ from Wishart distribution given $\boldsymbol{W}$
 7:     Sample factor vec($\boldsymbol{U}$)    ▷ from Normal distribution given $\boldsymbol{W}, \boldsymbol{V}, y_\Omega, \boldsymbol{\mathcal{X}}, \tau, k_s$
 8:     Sample factor vec($\boldsymbol{V}$)    ▷ from Normal distribution given $\boldsymbol{W}, \boldsymbol{U}, y_\Omega, \boldsymbol{\mathcal{X}}, \tau, k_t$
 9:     Sample factor vec($\boldsymbol{W}$)    ▷ from Normal distribution given $\boldsymbol{U}, \boldsymbol{V}, y_\Omega, \boldsymbol{\mathcal{X}}, \tau, \Lambda_\omega$
10:     Sample precision $\tau$    ▷ from Gamma distribution given $\boldsymbol{U}, \boldsymbol{V}, \boldsymbol{W}, y_\Omega, \boldsymbol{\mathcal{X}}, a_0, b_0$
11:     if $k > K_1$ then
12:         Collect the samples $\boldsymbol{U}^{(k-K_1)} = \boldsymbol{U}, \boldsymbol{V}^{(k-K_1)} = \boldsymbol{V}, \boldsymbol{W}^{(k-K_1)} = \boldsymbol{W}$;
13:         Compute and collect $\boldsymbol{\mathcal{B}}^{(k-K_1)}$ given $\boldsymbol{\mathcal{B}} = \sum_{r=1}^{R} \boldsymbol{u}_r \circ \boldsymbol{v}_r \circ \boldsymbol{w}_r$
14:     end if
15: end for
16: return $\{\boldsymbol{\mathcal{B}}^{(k)}\}_{k=1}^{K_2}$ to approximate posterior coefficients and estimate unobserved data.
```

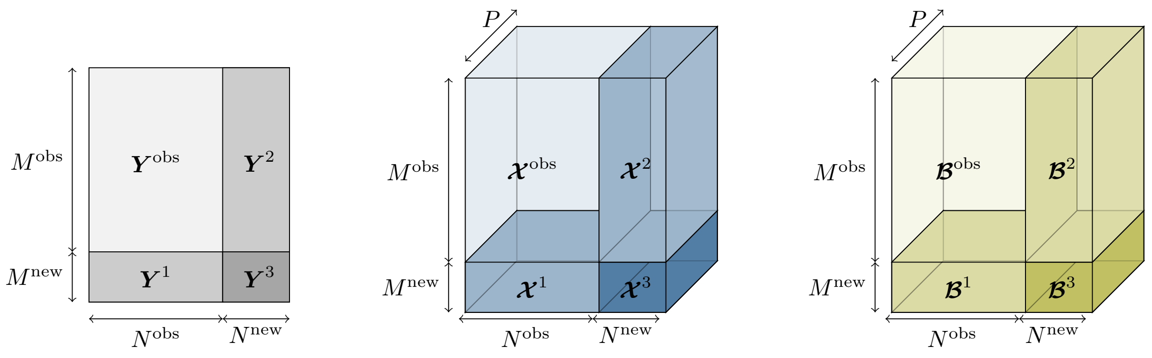

M^{obs}
M^{new}
$\boldsymbol{Y}^{\text{obs}}$
$\boldsymbol{Y}^2$
$\boldsymbol{Y}^1$
$\boldsymbol{Y}^3$
N^{obs}
N^{new}
P
$\boldsymbol{\mathcal{X}}^{\text{obs}}$
$\boldsymbol{\mathcal{X}}^2$
$\boldsymbol{\mathcal{X}}^1$
$\boldsymbol{\mathcal{X}}^3$
$\boldsymbol{\mathcal{B}}^{\text{obs}}$
$\boldsymbol{\mathcal{B}}^2$
$\boldsymbol{\mathcal{B}}^1$
$\boldsymbol{\mathcal{B}}^3$

Figure 2: Illustration of BKTR interpolation data.

nent of the spatial decomposition which includes the observed ($\boldsymbol{u}_r^{\text{obs}}$) and the new ($\boldsymbol{u}_r^{\text{new}}$) decomposition vectors as follows:

$$\begin{pmatrix} \boldsymbol{u}_r^{\text{obs}} \\ \boldsymbol{u}_r^{\text{new}} \end{pmatrix} \mid \Phi \end{pmatrix} \sim \mathcal{N}\left[\begin{pmatrix} \boldsymbol{0}_{M^{\text{obs}}} \\ \boldsymbol{0}_{M^{\text{new}}} \end{pmatrix}, \begin{pmatrix} \boldsymbol{R}_\Phi^{\text{obs}} & \boldsymbol{R}_\Phi^{\text{obs,new}} \\ \boldsymbol{R}_\Phi^{\text{new,obs}} & \boldsymbol{R}_\Phi^{\text{new}} \end{pmatrix}\right], \tag{8}$$

where $\boldsymbol{R}_\Phi^{\text{obs}}$ is the covariance matrix corresponding to the observed locations and $\boldsymbol{R}_\Phi^{\text{new}}$ is the covariance matrix corresponding to the unobserved locations for a known set of spatial kernel hyperparameters Φ. The covariance matrix between the observed and unobserved locations is $\boldsymbol{R}_\Phi^{\text{obs,new}}$ and $\boldsymbol{R}_\Phi^{\text{new,obs}}$ is its transpose. $\boldsymbol{0}_M$ represents a vector of zeros of size M.

The same approach can be used to formulate the joint multivariate normal distribution for the temporal decomposition $\boldsymbol{V}$:

$$\begin{pmatrix} \boldsymbol{v}_r^{\text{obs}} \\ \boldsymbol{v}_r^{\text{new}} \end{pmatrix} \mid \Gamma \sim \mathcal{N}\left[\begin{pmatrix} \mathbf{0}_{N^{\text{obs}}} \\ \mathbf{0}_{N^{\text{new}}} \end{pmatrix}, \begin{pmatrix} \boldsymbol{R}_\Gamma^{\text{obs}} & \boldsymbol{R}_\Gamma^{\text{obs,new}} \\ \boldsymbol{R}_\Gamma^{\text{new,obs}} & \boldsymbol{R}_\Gamma^{\text{new}} \end{pmatrix}\right]. \tag{9}$$

From Equation 8 and Equation 9, the conditional distribution of the decompositions at new locations and time steps are

$$\begin{aligned} \boldsymbol{u}_r^{\text{new}} | \boldsymbol{u}_r^{\text{obs}} &\sim \mathcal{N}(\boldsymbol{R}_\Phi^{\text{new,obs}} \boldsymbol{R}_\Phi^{\text{obs}^{-1}} \boldsymbol{u}_r^{\text{obs}},\ \boldsymbol{R}_\Phi^{\text{new}} - \boldsymbol{R}_\Phi^{\text{new,obs}} \boldsymbol{R}_\Phi^{\text{obs}^{-1}} \boldsymbol{R}_\Phi^{\text{obs,new}}),\ r = 1, \ldots, R, \\ \boldsymbol{v}_r^{\text{new}} | \boldsymbol{v}_r^{\text{obs}} &\sim \mathcal{N}(\boldsymbol{R}_\Gamma^{\text{new,obs}} \boldsymbol{R}_\Gamma^{\text{obs}^{-1}} \boldsymbol{v}_r^{\text{obs}},\ \boldsymbol{R}_\Gamma^{\text{new}} - \boldsymbol{R}_\Gamma^{\text{new,obs}} \boldsymbol{R}_\Gamma^{\text{obs}^{-1}} \boldsymbol{R}_\Gamma^{\text{obs,new}}),\ r = 1, \ldots, R. \end{aligned} \tag{10}$$

From this point, we can obtain the parameters in Equation 10 using posterior samples that were captured during the K_2 sampling iterations of the MCMC sampling described in the Algorithm 1. To estimate the distribution parameters of $\boldsymbol{u}_r^{\text{new}}$ and $\boldsymbol{v}_r^{\text{new}}$, we can use the accumulated estimated values of all spatial and temporal kernel hyperparameters Φ and Γ to evaluate, at each sampling iteration, the covariance matrices $\boldsymbol{R}_\Phi^{\text{obs}}$, $\boldsymbol{R}_\Phi^{\text{new}}$, $\boldsymbol{R}_\Phi^{\text{obs,new}}$, $\boldsymbol{R}_\Gamma^{\text{obs}}$, $\boldsymbol{R}_\Gamma^{\text{new}}$ and $\boldsymbol{R}_\Gamma^{\text{obs,new}}$. From the sampled distributions, we are able to obtain a spatial decomposition values at new locations $\boldsymbol{u}_r^{\text{new}^*}$ and temporal decomposition values at new time points $\boldsymbol{v}_r^{\text{new}^*}$ for each of the K_2 sampling iterations. From $\boldsymbol{u}_r^{\text{new}^*}$, $\boldsymbol{v}_r^{\text{new}^*}$ and the corresponding $\boldsymbol{w}_r$ of each sampling iteration, we are then able to approximate the values of $\boldsymbol{\mathcal{B}}^{\text{new}^*}$. Finally, by combining the K_2 sampled $\boldsymbol{\mathcal{B}}^{\text{new}^*}$ values, we can obtain a sample of the distribution of $\boldsymbol{\mathcal{B}}^{\text{new}}$.

After this sampling process, it is fairly simple, following Equation 2, to get the expectation of the response variable $E(\boldsymbol{Y}^{\text{new}}|\boldsymbol{Y}^{\text{obs}})$ utilizing $\boldsymbol{\mathcal{B}}^{\text{new}}$ and the corresponding covariates $\boldsymbol{\mathcal{X}}^{\text{new}}$.

An important aspect of using kriging for predictions is that it is mainly effective when new locations and time points are close to observed records. Thus, BKTR predictions made in a relatively close spatial and temporal neighborhoods should be very effective. However, in tasks like predicting temporal values located very far in the future, the current prediction methodology might yield poor results due to the fact that kriging relies on nearby results to make predictions.

This interpolation sampling process is implemented in both **BKTR** packages. The performance and results of this implementation are reviewed extensively on simulated data in Section 5.5 and on real world data in Section 6.3.

3. BKTR regressor class

The **BKTR** packages provide a `BKTRRegressor` class that encapsulates the core concepts and functionalities of the BKTR algorithm. This class provides a simple interface to fit the BKTR model for a given data set and allows to visualize fitted coefficients as well as to predict values for new or missing observations. Even though the `BKTRRegressor` class has been designed in a user friendly manner, its flexibility and number of parameters need to be carefully considered. Thus, this section is dedicated to explaining the different data inputs, parameter inputs and all the attributes and methods of the `BKTRRegressor` class.

3.1. Input data

For the BKTR algorithm, three data frame inputs need to be provided during the initialization of a `BKTRRegressor` object.

- A data frame `spatial_positions_df` with M rows and $1 + d_s$ columns containing information about the spatial locations. The first column is used to label each spatial location and the other d_s columns encapsulate the spatial position of each location in d_s dimensions. When we consider for example a location to be represented by longitude and latitude, we would have $d_s = 2$ and a three column data frame. For consistency, the first column containing location labels should contain only unique values and needs to be named `location`.

- A data frame `temporal_positions_df` with N rows and $1 + d_t$ columns containing information about each discrete timestamp. The first column labels each time point and the subsequent d_t columns are used to capture the timestamps temporal position. Typically, like when using dates as time points, $d_t = 1$ can be used, resulting in a two columns data frame. For consistency, the first column containing time point labels should contain only unique values and needs to be named `time`.

- A principal data frame `data_df` with MN rows and $3 + P$ columns, containing a location label column, a time point label column, a column containing the response variable and P columns for the covariates. The first column of the data frame needs to be named `location`, it must contain the same values as the `spatial_positions_df`'s `location` column and each value must appear a N times. Similarly, the second column of the data frame needs to be named `time`, it must contain the same values as the `temporal_positions_df`'s `time` column and each value must appear M times. In other words, the `data_df` data frame must contain in the `location` and `time` columns all the possible combinations of `spatial_positions_df` locations and `temporal_positions_df` time points. In general, it is preferred but not mandatory that the third column of the data frame contains the response variable data.

It is important to note that `data_df` can also contain missing values in the response variable y column. Those missing values must be properly encoded as `NaN` and represent, in fact, a flattened version of the matrix Ω in Equation 4.

To give us a better idea of what would be a valid shape for `BKTRRegressor` input data, let's take a look at the BIXI data presented in Section 6. To keep the visualization succinct, we will take a subset of two locations ($M = 2$), three time points ($N = 3$) and two covariates ($P = 2$). We can start by looking at a valid `spatial_positions_df`:

```
R> bixi_data <- BixiData$new()
R> ex_locs <- c('7114 - Smith / Peel', '6435 - Victoria Hall')
R> ex_times <- c('2019-04-17', '2019-04-18', '2019-04-19')
R> print(bixi_data\$spatial_positions_df[location %in% ex_locs])
```

```
               location latitude longitude
1: 6435 - Victoria Hall 45.48129 -73.60033
2:  7114 - Smith / Peel 45.49284 -73.55642
```

Then look at a valid `temporal_positions_df`:

```
R> print(bixi_data$temporal_positions_df[time %in% ex_times])
```

```
         time time_index
1: 2019-04-17          2
2: 2019-04-18          3
```

And finally look at the corresponding valid `data_df`:

```
R> print(bixi_data$data_df[
R>   location %in% ex_locs & time %in% ex_times,
R>   c(1:4, 17)
R> ])
```

```
              location       time nb_departure area_park  humidity
1: 6435 - Victoria Hall 2019-04-17    0.2178218 0.2254071 0.1919343
2: 6435 - Victoria Hall 2019-04-18    0.3366337 0.2254071 0.4697535
3: 6435 - Victoria Hall 2019-04-19    0.2178218 0.2254071 0.9350261
4:  7114 - Smith / Peel 2019-04-17    0.7821782 0.0652808 0.1919343
5:  7114 - Smith / Peel 2019-04-18    0.3861386 0.0652808 0.4697535
6:  7114 - Smith / Peel 2019-04-19    0.6534653 0.0652808 0.9350261
```

Another important data related input for the `BKTRRegressor` is the `formula`. By default, if no `formula` is provided, the third column of `data_df` will be used as the response variable $\boldsymbol{y}$ and the remaining columns will be used as covariates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_P$. If a `formula` is provided, the model matrices $\boldsymbol{y}$ and $\boldsymbol{X}$ will be extracted from the `data_df` and the `formula`. The `formula` must be in form of `y ~ x1 + x2 + . .. + xP` and correspond to a valid R formula (Wilkinson and Rogers 1973). All the terms in the `formula` must correspond to valid column names of the `data_df` data frame. For R users, the `formula` must be a `formula` object. For Python users, the `formula` must be a string that can be parsed by the **Formulaic** library. In both cases, it is important to note that by default, an intercept term is automatically added to the model matrix $\boldsymbol{X}$ and can be removed by adding a `-1` term to the `formula`.

The covariates $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_P$ can describe the spatial and temporal attributes of the observations. By nature, the **BKTR** packages are designed to be able to take into accounts spatial attributes that vary through time (e.g., population density that varies through time) or temporal attributes that vary through space (e.g., temperature that varies through different countries). However, it is not uncommon to have spatial attributes that are constant through time and temporal attributes that are constant through space like in the BIXI example of Section 6. When this is the case and the data is provided in a compressed manner, we provide a `reshape_covariate_dfs` utility function (see Appendix B) that can help users to obtain a valid `data_df`.

3.2. Input parameters

On top of data frames, the user must provide sampling parameters to be able to initialize a regressor. Those parameters include `burn_in_iter` and `sampling_iter` which are integer inputs representing the number of iterations for the burn-in phase (K_1) and the sampling phase (K_2) respectively. There is also `rank_decomp` which is an integer input representing the rank of the CP decomposition (R). The default values for iterations are 500 iterations for each of K_1 and K_2 whereas the default value for the rank decomposition is 10. Two different `Kernel` objects can also be provided (which are further described in Section 4.2), one for the spatial kernel `spatial_kernel` and one for the temporal kernel `temporal_kernel`. The user can also provide some distribution parameters like `sigma_r` which is a float representing the variance of the white noise process (τ^{-1}). We can supply `a_0` and `b_0` representing the initial values for the shape (α) and rate (β) of the gamma function generating τ. To ensure weak priors for `a_0` and `b_0` and since their selection is non-trivial along with `sigma_r`, we provide default values for those parameters of `a_0=1E-6`, `b_0=1E-6`, `sigma_r=1E-2` respectively. The kernels `spatial_kernel` and `temporal_kernel` are provided default `Kernel` objects as well. The default used spatial kernel is a Matérn kernel 5/2 having a smoothness factor $\nu = 5$ (see Table 4) while the default temporal kernel is a Squared Exponential (SE) kernel. The `BKTRRegressor` class can also take a boolean value input for the `has_geo_coords` parameter. This parameter, that has a default truthful value, indicates if we need to apply or not a Mercator projection (Snyder 1987) to the spatial locations. We usually need to apply a projection when the spatial positions are encoded in longitude and latitude so that we keep the kernel valid. The `geo_coords_scale` parameter is directly associated to the Mercator projection and dictates the scale in which it should be projected. More information about the projection are available in the Appendix C.

When using all the defaults parameters mentioned above, it is very simple to run a BKTR regression on a given dataset. Here is a very simple example of the usage of the `BKTRRegressor` on the full version of the BIXI data mentioned in Section 3.1:

```
R> bktr_regressor <- BKTRRegressor$new(
+    data_df=bixi_data$data_df,
+    spatial_positions_df=bixi_data$spatial_positions_df,
+    temporal_positions_df=bixi_data$temporal_positions_df)
```

Once the regressor is initialized, the user can launch the MCMC sampling process by calling the `mcmc_sampling` method which stores its results inside the `BKTRRegressor` object. Depending on the number of iterations and the size of the data, this process can take a long time to complete. Thus, we added a progress log showing the current MCMC iteration number, the elapsed time and the current error values. The displayed in-sample errors are the mean absolute error (MAE) and the root mean square error (RMSE) of the response variable. The following code chunk shows the usage of the `mcmc_sampling` method, but with a truncated output for the sake of brevity.

```
R>  bktr_regressor$mcmc_sampling()

* Iter 1     | Elapsed    0.48s | MAE  0.1036 | RMSE  0.1465 *
...
* Iter 1500  | Elapsed    2.83s | MAE  0.0543 | RMSE  0.0734 *
* Iter TOTAL | Elapsed 4528.07s | MAE  0.0525 | RMSE  0.0714 *
```

3.3. Attributes and visualizations

Once a `BKTRRegressor` object has been initialized, the user can access its attributes and methods shown in Table 2. Note that except for the `mcmc_sampling` method, all the other

BKTRRegressor Methods	
`mcmc_sampling`	Launch the MCMC sampling process for a predefined number of iterations and a given set of parameters
`predict`	Allows to estimate the response variable $\boldsymbol{y}$ and the $\boldsymbol{\mathcal{B}}$ coefficients for new locations or time points
`get_beta_summary_df`	Get a summary of estimated beta values (mean, stdev, quantiles). Labels can be provided for spatial locations, time points and features. When no labels are given for a dimension, all its betas are shown.
BKTRRegressor Attributes	
`summary`	Summary of the MCMC regressor object
`beta_covariates_summary_df`	Data frame summarizing beta covariates per feature (mean, stdev, quantiles)
`y_estimates`	Data frame for the estimated target variable
`imputed_y_estimates`	Data frame of the estimated and imputed target variable including missing data (Ω)
`beta_estimates`	Data frame estimated values for betas
`hyperparameters_per_iter_df`	Data frame of estimated MCMC hyperparameters (kernels' and τ) values per iteration

Table 2: `BKTRRegressor` attributes and methods

methods and attributes are available only after the MCMC sampling process is completed. When called on a `BKTRRegressor` object, the built-in `summary` and `print` R functions will simply display the `summary` attribute.

The `predict` method allows to estimate the response variable $\boldsymbol{Y}$ and the $\boldsymbol{\mathcal{B}}$ coefficients for new locations and/or time points which we referred as interpolation in Section 2.3. The method takes as input a data frame containing the covariates for the new locations and/or time points `new_data_df`, a data frame containing the spatial positions of the new locations `new_spatial_positions_df` and finally a data frame containing the temporal positions of the new time points `new_temporal_positions_df`. It is possible to provide either a `new_spatial_positions_df` or a `new_temporal_positions_df` or both. In R, it can also be called via the `predict` built-in function using the `BKTRRegressor` object as first argument followed by all the other arguments in the same order as described above. Extensive usage examples of the `predict` method are provided in Section 5.5 and Section 6.3.

The `get_beta_summary_df` method allows to get a summary of the estimated $\boldsymbol{\mathcal{B}}$ coefficients. It can take as inputs a list of labels for the spatial locations, a list of time point labels and a list of feature labels. When no labels are given for one of the input, all the $\boldsymbol{\mathcal{B}}$ coefficients for the corresponding dimension are shown. The method returns a data frame containing the mean, standard deviation, quantiles for each of the queried $\boldsymbol{\mathcal{B}}$ coefficient for the sampled posterior distribution. A usage example of the `get_beta_summary_df` method is provided in Section 6.1.

Multiple visualization functions are also available in the **BKTR** packages. Those visualization functions are shown in Table 3. All functions take a `BKTRRegressor` object as a first input for which the sampling process must be completed. We can also specify, via the `show_figure` boolean parameter, to either return a plot object (ggplot2 in R and plotly in Python) or to

`BKTRRegressor` Plot Functions	
`plot_temporal_betas`	Plot beta values through time for a given spatial point and a set of feature labels.
`plot_spatial_betas`	Plot beta values through space for a given time point and a set of feature labels.
`plot_covariates_beta_dists`	Plot the distribution of beta estimates grouped by features. A subset of features can be provided to plot only a subset of them.
`plot_hyperparams_dists`	Plot the distribution of τ and kernels' hyperparameters for all sampling iterations. `hyperparameters` allows to plot only a subset of parameters.
`plot_hyperparams_per_iter`	Plot the values of τ and kernels' hyperparameters through sampling iterations (trace plot). The argument `hyperparameters` allows to plot only a subset of parameters.
`plot_y_estimates`	Plot the estimated values for the response variable $\hat{\boldsymbol{y}}_\Omega$ alongside their corresponding observed values $\boldsymbol{y}_\Omega$.

Table 3: Plot functions that can be used on a `BKTRRegressor` object after MCMC sampling

just display the plot. The plot object can then be used to customize the plot further if needed or to save it as an image. Also, all visualization functions can use the `width` or the `height` parameters to customize the size of the plotting area.

Most of the attributes, methods and visualization functions described in this section are further explored and tested in the Section 5 and Section 6.

4. BKTR Kernels

Kernels play a crucial role in Gaussian processes. They are used to model the similarity or dissimilarity between observations. This similarity can then serve to generate a covariance matrix that can be used as a prior distribution for given parameters. The choice of a kernel is very important as it influences properties of the gaussian process and makes hypotheses about the underlying structure of the function being modeled. For example, a squared exponential kernel (SE) is highly smooth, often referred to as the Gaussian Kernel. Consequently, it assigns a high covariance to input points that are defined as close and low covariance to points that are distant. In contrast, a periodic kernel assigns high covariance to points that are separated by a multiple of a given period, resulting in a GP that can capture periodic patterns in the data (Duvenaud 2014). Thus, the pattern difference between the SE and periodic kernel highlights the importance of choosing a sensible kernel when modeling a function with a GP.

In BKTR, we use kernels to model relationships between spatial locations and between time points. A `BKTRRegressor` object uses two distinct kernels which are the `spatial_kernel` and the `temporal_kernel`. The `spatial_kernel` is used to generate the spatial covariance matrix $\boldsymbol{K}_s$ and the `temporal_kernel` is used to generate the temporal covariance matrix $\boldsymbol{K}_t$ that are defined in Equation 5. The `spatial_kernel` and `temporal_kernel` objects can come from any kernel class implemented in the `kernels` module of **BKTR** (see Section 4.2). We can say that **BKTR** kernel classes themselves need two main components to be defined: the kernel parameters (see Section 4.1), and the kernel function (explained in Section 4.2). The kernels implemented in **BKTR** take inspiration from the kernels existing in the **GPyTorch** package (Gardner *et al.* 2018) and the **Scikit-learn** package (Pedregosa *et al.* 2011).

4.1. Kernel Parameters

All kernels implemented in **BKTR** have a set of parameters `KernelParameter` that can be optimized during the training process of the MCMC sampling. This set of parameters can be accessed via the `parameters` attribute of a kernel after its initialization. Kernels in general contain sensible default parameters. However, the user can change the behavior of a given `Kernel`'s parameter by providing a `KernelParameter` object to the related parameter argument.

The `KernelParameter` class can take multiple arguments at initialization:

- `value`: an initial value used for the parameter during slice sampling or the constant value used for the parameter when it is not optimized
- `is_fixed`: a boolean argument indicating if the hyperparameter value is fixed or optimized during sampling
- `lower_bound`: a value that indicates what is the minimum value that can be taken by the parameter during sampling
- `upper_bound`: a value that indicates what is the maximum value that can be taken by the parameter during sampling
- `slice_sampling_scale`: a value indicating the scale parameter for the slice sampling algorithm
- `hparam_precision`: a value indicating the precision of the hyperparameter

The `value` argument is the only required argument to initialize `KernelParameter`. The other arguments have default values if not provided. The `is_fixed` argument is set to false by default, which means that the parameter will necessarily be optimized during the training process. The `lower_bound` and `upper_bound` arguments are set to `1E-3` and `1E3` respectively by default, which means that the parameter will be sampled in a range of $[10^{-3}, 10^{3}]$ during the training process. The `slice_sampling_scale` argument is set to `2` by default, which represent the slice sampling step size during the MCMC sampling process. Finally, the `hparam_precision` argument is set to `1E-3` by default.

4.2. Kernel Classes

BKTR `Kernel` classes are core components encapsulating behavior and attributes used to compute the covariance matrix during Gaussian processes. They contain information about observations' positions, all the kernel's hyperparameters and a kernel function.

For a kernel to induce a covariance matrix, it needs an initial input encoding the positions of the observations. This position vector is set for a `Kernel` object using the `set_positions_df` method. This method accepts a data frame having a number of rows equal to the number of

Kernel Class	Optimizable Parameters	Kernel Function
`KernelWhiteNoise` White noise		$k(x,x') = I_{\lvert x\rvert}$, where $\lvert x\rvert$ is the the number of elements in the position vector x.
`KernelSE` Squared exponential	`lengthscale` (ℓ)	$k(x,x';\ell) = \exp\Big(-\frac{d(x,x')^2}{2\ell^2}\Big)$
`KernelRQ` Rational quadratic	`alpha` (α) `lengthscale` (ℓ)	$k(x,x';\alpha,\ell) = \Big(1+\frac{d(x,x')^2}{2\alpha\ell^2}\Big)^{-\alpha}$
`KernelPeriodic` Periodic	`lengthscale` (ℓ) `period_length` (t)	$k(x,x';\ell,t) = \exp\Big(-\frac{2\sin^2(\frac{\pi d(x,x')}{t})}{\ell^2}\Big)$
`KernelMatern` Matérn	`lengthscale` (ℓ)	$k(x,x';\ell,\nu) = \begin{cases}\exp(-\frac{D}{\ell}), & \text{if } \nu=1\\ (1+\frac{\sqrt{3}D}{\ell})\exp(-\frac{D}{\ell}), & \text{if } \nu=3,\\ (1+\frac{\sqrt{5}D}{\ell}+\frac{5D^2}{3\ell^2})\exp(-\frac{D}{\ell}), & \text{if } \nu=5\end{cases}$ where $D=d(x,x')$ and ν is a Matérn kernel input called the `smoothness_factor`. The `smoothness_factor` input can be either `1`, `3` or `5`, which correspond to so called Matérn $\frac{1}{2}$, $\frac{3}{2}$ and $\frac{5}{2}$ kernels respectively.
`KernelAddComposed` Composed via addition		$k(x,x';\Lambda_a,\Lambda_b) = k_a(x,x';\Lambda_a) + k_b(x,x';\Lambda_b)$, where k_a and k_b are two kernel functions and Λ_a and Λ_b their sets of parameters.
`KernelMulComposed` Composed via multiplication		$k(x,x';\Lambda_a,\Lambda_b) = k_a(x,x';\Lambda_a) * k_b(x,x';\Lambda_b)$, where k_a and k_b are two kernel functions and Λ_a and Λ_b their sets of parameters.

Table 4: List of kernel classes implemented in the **BKTR** packages and their respective parameters and equations. The $d(x,x')$ function is the Euclidean distance function applied on the observations' positions. Note that only the parameters that are objects coming from the `KernelParameter` class (parameters that can be sampled) are listed in the Optimizable Parameters column.

observations and number of column equal to $1+K$, where the first column is for labeling each observation and the other columns contains the location information for the K dimensions of each observation.

When using stationary kernels, we can initially calculate a distance between observations

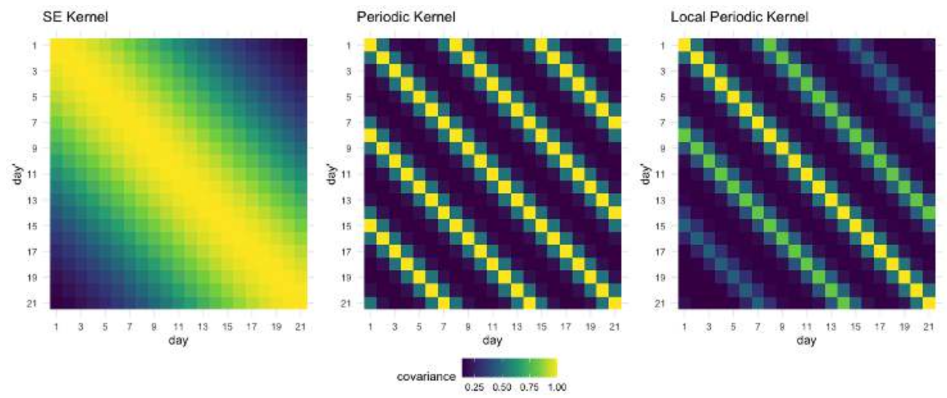


Figure 3: Heatmap plots of the covariance matrix for three different kernels implemented in the **BKTR** package calculated on 21 consecutive days. Presented kernels are, in order, a `KernelSE` with a `lengthscale` of 10, a `KernelPeriodic` with a `period_length` of 7 and a local periodic kernel (`KernelMulComposed`) resulting from the multiplication of two other kernels. The local periodic kernel plot shows that it contains the periodicity of the `KernelPeriodic` kernel and the decay of the `KernelSE` kernel.

$d(x, x')$ and use it for the generation of the covariance matrix. To ensure the validity of covariance matrices, in **BKTR**, we use the Euclidean distance function:

$$d(x_i, x_j) = \sqrt{\sum_{k=1}^{K} (x_{ik} - x_{jk})^2}, \tag{11}$$

where x_i and x_j are two given observations' positions from the position vector $\boldsymbol{x}$ and K is the number of dimensions of a given position.

With this position information, we can use all the different kernel classes available in the **BKTR** package, which are enumerated in Table 4. Different kernels yield completely different covariance matrices according to their function and parameters. For instance, the `KernelSE` kernel yields a covariance matrix with a smooth decreasing function from the diagonal, whereas the `KernelPeriodic` kernel yields a covariance matrix with a periodic pattern from the diagonal. Those different covariance matrices can be visualized using the `plot` method of any implemented `Kernel` class and the two aforementioned kernel examples are shown in Figure 3 (first two subfigures).

Like in the case of the local periodic kernel, it is sometimes useful to combine different kernels to obtain a composition of different covariance matrices. This feature is implemented in the **BKTR** package with the `KernelAddComposed` class when adding two kernels and `KernelMulComposed` class when multiplying two kernels. We can look at an example of a composed kernel in **BKTR** by creating a local periodic kernel when multiplying a `KernelSE` kernel with a `KernelPeriodic` kernel. The `KernelSE` kernel is used to model the smooth decreasing function from the diagonal and the `KernelPeriodic` kernel is used to model the periodic function from the diagonal. In the BIXI example used by Lei *et al.* (2023), a local periodic kernel was used to model the BIXI stations' demand with a constant period of seven days. We can easily create and visualize this local periodic kernel using the `KernelComposed` class as shown in the following code snippet:

```
R> library(data.table)
R> days_df <- data.table(day=1:21, position=1:21)
R> se_lengthscale <- KernelParameter$new(value=10)
R> per_length <- KernelParameter$new(value=7, is_fixed=TRUE)
R> kernel_periodic <- KernelPeriodic$new(period_length=per_length)
R> kernel_se <- KernelSE$new(lengthscale=se_lengthscale)
R> kernel_local_periodic <- kernel_periodic * kernel_se
R> kernel_local_periodic$set_positions(days_df)
R> kernel_local_periodic$kernel_gen()
R> kernel_local_periodic$plot()
```

The resulting kernel plot is illustrated as the rightmost plot of the Figure 3. The `lengthscale` parameter of the SE kernel was set to a value of 10 in this example, and the `period_length` of the periodic kernel was set to 7 to enhance kernel properties visualization.

5. Simulation-based study

To showcase the capabilities of the **BKTR** package, we will first generate simulated datasets with known ground truths and then use our software library to estimate the underlying parameters. This aims to demonstrate the package's capabilities and to illustrate the different insights that can be obtained from the results of **BKTR**. Subsequently, we will show the imputation and interpolation abilities of the **BKTR** packages on the aforementioned simulated dataset. The imputation and interpolation results will also be compared with the results of the Python library implementation.

5.1. Simulation data

For the simulation, we will use the `simulate_spatiotemporal_data` utility function implemented in the **BKTR** packages to simulate a spatiotemporal dataset with four different data frames: spatiotemporal locations, time points, covariates (including the response variable and an intercept term) and beta coefficients.

The function generates M spatial locations in a d_s dimension Euclidean space with each dimension being in a range of $[0, S_s]$, where S_s is the scale parameter of the spatial dimensions. It also generates N sequential time points that are in a range of $[0, S_t]$, where S_t is the time scale parameter. Resulting time points therefore have a time resolution of $S_t/(N-1)$.

The covariates are simulated using an intercept term, p_s spatial covariates and p_t temporal covariates.

$$\begin{aligned}
\boldsymbol{\mathcal{X}}(:,:,p=1) &= 1 && \text{(intercept)},\\
\boldsymbol{\mathcal{X}}(:,:,p=2,\ldots,1+p_s) &= 1_N^\top \otimes \boldsymbol{x}_s^p,\ \text{with } \boldsymbol{x_s^p} \sim \mathcal{N}(\boldsymbol{\mu}_s^p, \boldsymbol{I}_M) && \text{(spatial covariates)}, \quad (12)\\
\boldsymbol{\mathcal{X}}(:,:,p=2+p_s,\ldots,P) &= \boldsymbol{x}_t^p \otimes 1_M^\top,\ \text{with } \boldsymbol{x_t^p} \sim \mathcal{N}(\boldsymbol{\mu}_t^p, \boldsymbol{I}_N) && \text{(temporal covariates)},
\end{aligned}$$

where P is the total number of covariates and is $1 + p_s + p_t$, and $\boldsymbol{\mu}_s^p$ and $\boldsymbol{\mu}_t^p$ are vectors of length M and N, respectively.

The $\boldsymbol{\beta}$ values are generated from a multivariate normal distribution:

$$\text{vec}(\boldsymbol{\beta}_{(3)}) \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{K}_t^{\text{sim}} \otimes \boldsymbol{K}_s^{\text{sim}} \otimes \boldsymbol{\Lambda}_w^{-1}), \quad (13)$$

with $\boldsymbol{K}_s^{\text{sim}}$ and $\boldsymbol{K}_t^{\text{sim}}$ being covariance matrices generated by the spatial and temporal kernels, respectively. Both kernels are input parameters for the `simulate_spatiotemporal_data` function.

The response variable $\boldsymbol{Y}$, for its part, is created from the product of the covariates and the $\boldsymbol{\mathcal{B}}$ values to which we add an error term $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}_{MN}, S_\epsilon \boldsymbol{I}_{MN})$, where S_ϵ is the scale parameter of the error term and $\boldsymbol{I}_{MN}$ is an identity matrix of size $MN \times MN$.

In summary, the `simulate_spatiotemporal_data` function input parameters are

- M: `nb_spatial_locations` (number of spatial locations)
- N: `nb_time_points` (number of time points)
- d_s: `nb_spatial_dimensions` (number of spatial dimensions in the Euclidean space)
- S_s: `spatial_scale` (scale of the spatial dimensions)
- S_t: `time_scale` (scale of the time dimension)
- $\boldsymbol{\mu}_s$: `spatial_covariates_means` (mean vector of the spatial covariates)
- $\boldsymbol{\mu}_t$: `temporal_covariates_means` (mean vector of the temporal covariates)
- $k_s^{\text{sim}}(s_m, s_{m'}; \Phi^{\text{sim}})$: `spatial_kernel` (spatial kernel generating $\boldsymbol{K}_s^{\text{sim}}$)
- $k_t^{\text{sim}}(t_n, t_{n'}; \Gamma^{\text{sim}})$: `temporal_kernel` (temporal kernel generating $\boldsymbol{K}_t^{\text{sim}}$)
- S_ϵ: `noise_scale` (scale parameter for the added noise)

The `simulate_spatiotemporal_data` function returns a list (dictionary in Python) containing four data frames: `data_df`, `spatial_locations_df`, `time_points_df` and `beta_df`. The first three data frames can directly be passed to the initialization of a `BKTRRegressor`. The `beta_df` data frame represents the true $\boldsymbol{\mathcal{B}}$ values and has a shape of $MN \times (2 + P)$ (including two columns for the labels). The dataset generated has spatial covariates that are independent of the spatial locations and temporal covariates that are independent of the time points. Therefore, we used a process similar to the `reshape_covariate_dfs` utility function (see Appendix B) to create a valid `data_df` data frame.

It is important to note that because of the double Kronecker product used in the Equation 13, the covariance matrix that will be generated will use a sizeable amount of memory since its shape will be $MNP \times MNP$. For this reason, we decided to sample from a matrix normal distribution instead of generating the whole covariance matrix. The used matrix normal distribution is defined as follows:

$$\text{vec}(\boldsymbol{\beta}_{(3)}) \sim \mathcal{MN}(\mathbf{0}_{N\times MP}, \boldsymbol{K}_t^{\text{sim}}, \boldsymbol{K}_s^{\text{sim}} \otimes \boldsymbol{\Lambda}_w^{-1}), \tag{14}$$

From this distribution we can significantly reduce memory usage by sampling a tensor of size $N \times MP$ from MNP independent $\mathcal{N}(0, 1)$ distributions. The generated tensor can then be multiplied by the Cholesky decomposition of $\boldsymbol{K}_t^{\text{sim}}$ and be followed by a matrix multiplication with the Cholesky decomposition of $\boldsymbol{K}_s^{\text{sim}} \otimes \boldsymbol{\Lambda}_w^{-1}$.

In the sequel, we use two different shapes of simulated datasets coming from the function `simulate_spatiotemporal_data`. The former, that we will call the *Smaller* dataset, will hold a $\boldsymbol{\mathcal{B}}$ tensor with 2,400 values having $M = 20$ spatial locations, $N = 30$ time points, two spatial covariate with $\boldsymbol{\mu}_s = [0, 2]$ and one temporal covariate $\boldsymbol{\mu}_t = [1]$. The other type of simulated dataset, that we will call the *Larger* one, will use a $\boldsymbol{\mathcal{B}}$ with 90,000 values having $M = 100$ spatial locations, $N = 150$ time points, three spatial covariates with $\boldsymbol{\mu}_s = [0, 2, 4]$ and two temporal covariates $\boldsymbol{\mu}_t = [1, 3]$. Both datasets have a noise scale of $S_\epsilon = 1$, a spatial scale of $S_s = 10$, a temporal scale of $S_t = 10$ and spatial data in $d = 2$ dimensions. Spatial and temporal kernel functions used to obtain covariance matrices will vary on a case by case basis, depending on subsections.

5.2. Simulation analysis

We start by simulating a completely new dataset using the function presented in the last section `simulate_spatiotemporal_data`. We simulate a dataset of the *Larger* shape using a spatial Matérn 5/2 Kernel with a lengthscale parameter value $\phi_1^{\text{sim}} = 14$ and a temporal squared exponenential kernel with a lengthscale parameter $\gamma_1^{\text{sim}} = 5$.

```
R> TSR$set_params(seed = 1)
R> matern_lengthscale <- KernelParameter$new(value = 14)
R> se_lengthscale <- KernelParameter$new(value = 5)
R> spatial_kernel <- KernelMatern$new(
+    lengthscale = matern_lengthscale,
+    smoothness_factor = 5)
R> temporal_kernel <- KernelSE$new(lengthscale = se_lengthscale)
R>
R> # Simulate data
R> simu_data <- simulate_spatiotemporal_data(
+    nb_locations=100,
+    nb_time_points=150,
+    nb_spatial_dimensions=2,
+    spatial_scale=10,
+    time_scale=10,
+    spatial_covariates_means=c(0, 2, 4),
+    temporal_covariates_means=c(1, 3),
+    spatial_kernel=spatial_kernel,
+    temporal_kernel=temporal_kernel,
+    noise_variance_scale=1)
```

Once the data are simulated, we can fit a BKTR model to it. We will use new kernels for the spatial and temporal dimensions to make sure that the model is able to recover parameters used to simulate the data.

```
R> bktr_regressor <- BKTRRegressor$new(
+    data_df = simu_data$data_df,
+    spatial_kernel = KernelMatern$new(smoothness_factor = 5),
+    spatial_positions_df = simu_data$spatial_positions_df,
+    temporal_kernel = KernelSE$new(),
+    temporal_positions_df = simu_data$temporal_positions_df,
+    has_geo_coords=FALSE)
R> bktr_regressor$mcmc_sampling()

[1] "Iter 1     | Elapsed Time:     1.60s | MAE:  2.9356 | RMSE:  3.7555"
...
[1] "Iter 1000  | Elapsed Time:     1.84s | MAE:  0.8026 | RMSE:  1.0075"
[1] "Iter TOTAL | Elapsed Time:  1684.75s | MAE:  0.7976 | RMSE:  1.0008"
```

The `mcmc_sampling` method prints the results for each iteration and we truncated the output for brevity. We can print the summary of the BKTR model to get a quick overview of its parameters and to assess quality of the fit.

```
>  summary(bktr_regressor)

======================================================================
                        BKTR Regressor Summary
======================================================================
Formula: y ~ .

Burn-in iterations: 500
Sampling iterations: 500
Rank decomposition: 10
Nb Spatial Locations: 100
Nb Temporal Points: 150
Nb Covariates: 6
======================================================================
In Sample Errors:
  RMSE: 1.001
  MAE: 0.798
Computation time: 1684.75s.
======================================================================
-- Spatial Kernel --
Matern 5/2 Kernel
Parameter(s):
                       Mean   Median       SD  Low2.5p  Up97.5p
lengthscale          13.608   13.602    0.576   12.515   14.799

-- Temporal Kernel --
SE Kernel
Parameter(s):
                       Mean   Median       SD  Low2.5p  Up97.5p
lengthscale           4.534    4.545    0.237    4.007    4.974
======================================================================
Beta Estimates Summary (Aggregated Per Covariates)

                       Mean   Median       SD
Intercept             2.405    2.622    1.688
```

```
s_cov_0              2.450    2.634    1.410
s_cov_1             -4.224   -4.166    2.775
s_cov_2             -1.935   -1.954    0.470
t_cov_0             -2.373   -2.612    1.493
t_cov_1              0.071    0.160    0.799
==================================================================
```

The model was able to recover the kernel parameters used to simulate the data. The estimated lengthscale ϕ_1 for the spatial kernel is 13.608 while the underlying value was $\phi_1^{\text{sim}} = 14$. The estimated lengthscale γ_1 for the temporal kernel is 4.534 while the true value was $\gamma_1^{\text{sim}} = 5$. The estimated noise variance is $1.001^2 = 1.002$ while the true value was 1. We can also compare the estimated $\boldsymbol{\mathcal{B}}$ coefficients with their simulated values.

```
R> beta_err <- unlist(abs(
+    bktr_regressor$beta_estimates[, -c(1, 2)]
+    - simu_data$beta_df[, -c(1, 2)]))
R> print(sprintf('Beta RMSE: %.4f', sqrt(mean(beta_err^2))))
R> print(sprintf('Beta MAE: %.4f', mean(abs(beta_err))))

[1] "Beta RMSE: 0.1449"
[1] "Beta MAE: 0.0855"
```

It is possible to observe that the model was able to find $\boldsymbol{\mathcal{B}}$ coefficients close to the ones used to simulate the data, with a $\text{MAE}_{\boldsymbol{\mathcal{B}}}$ of 0.0855 and a $\text{RMSE}_{\boldsymbol{\mathcal{B}}}$ of 0.1449.

We can plot, using the `plot_hyperparams_traceplot` function, the estimated hyperparameters values (kernels' and τ) through iterations to see how they evolved during the MCMC sampling. This function will plot a subset of the aforementioned hyperparameters if a vector of hyperparameter names is provided as the `hyperparameters` argument. In our case, we find interesting to plot the evolution of all kernel hyperparameters, which we can do using the following code:

```
R> plot_hyperparams_traceplot(bktr_regressor, c(
+    'Spatial - Matern 5/2 Kernel - lengthscale',
+    'Temporal - SE Kernel - lengthscale'))
```

The plot resulting from the `plot_hyperparams_traceplot` function is shown in Figure 4. In the figure, we can observe that during the sampling iterations, the posterior distribution of the hyperparameters was truly hovering around the true values used to simulate the data, which were $\phi_1^{\text{sim}} = 14$ for the spatial kernel's lengthscale and $\gamma_1^{\text{sim}} = 5$ for the temporal kernel's lengthscale. This is a good indication of the strength of the BKTR model, which is able to recover the underlying hyperparameters used to simulate the data. It is also interesting to note that it would have been possible to plot the posterior distribution of the hyperparameters using the `plot_hyperparams_dists` function with the same parameters.

To visualize the proximity of the fitted model's response variable values $\hat{\boldsymbol{y}}_\Omega$ to the observed reponse variable $\boldsymbol{y}_\Omega$, we can use the `plot_y_estimates` function of BKTR.

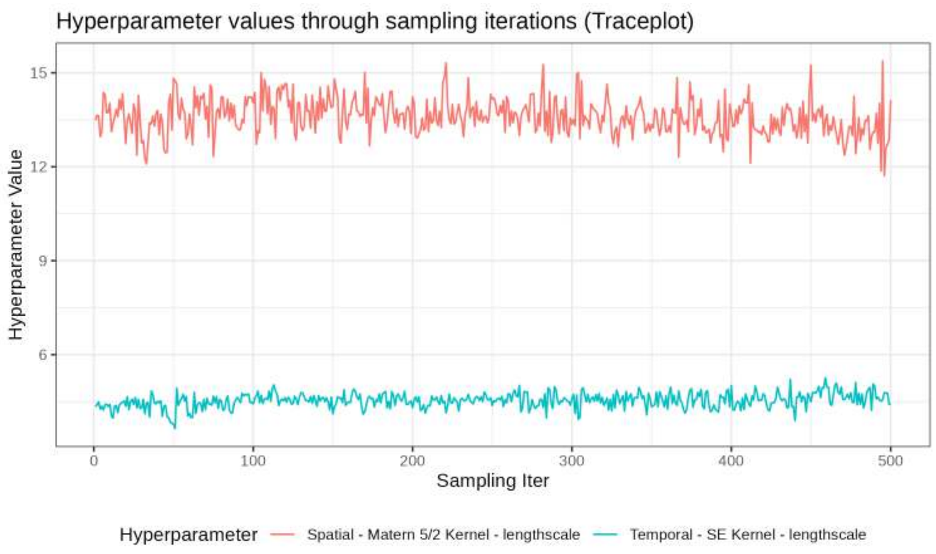


Figure 4: Traceplot of the hyperparameters through sampling iterations for a simulated dataset with 100 spatial locations, 150 temporal points, 6 covariates using a rank decomposition of 10, 500 burn-in iterations and 500 sampling iterations.

```
R> plot_y_estimates(bktr_regressor, fig_title = NULL)
```

When modeling the response variable effectively, the `plot_y_estimates` function should show points that closely align with a diagonal reference line, representing an ideal prediction. In Figure 5, the output of the function applied to the simulated data reveals estimated values that closely match the true $\boldsymbol{y}_\Omega$ values.

5.3. Influence of device and floating point format

In this section, we look into the influence of the device and floating point format used during tensor operations. The goal of this exercise is to be able to select a default type of floating point format and calculation device when using **BKTR**.

As some reader might have caught, there is a `TSR` component that we used during all our operations so far. `TSR` is a wrapper containing all used tensor operations functions, and is further detailed in Appendix A. This object allows us to set the seed for our operations via the `seed` argument of the `set_params` method. On top of the `seed` argument, the `set_params` method can also receive information about where the calculation should be done (on which device) and using which type of floating point format. This information can be passed via the `fp_device` and `fp_type` parameters of the `set_params` method. The available values for `fp_device` at the moment are `'cpu'` and `'cuda'`, where `'cpu'` use the central processing unit of the computer (CPU) and `'cuda'` use the graphic processing unit (GPU) if there is one on the system being used. For the floating point format, there are also two different values that can be passed to the `fp_type` parameter, which are `'float32'` for using single precision number format and `'float64'` to use double precision.

In some software packages or applications, using single precision instead of double precision can degrade the precision of the obtained results, while providing major computational speed

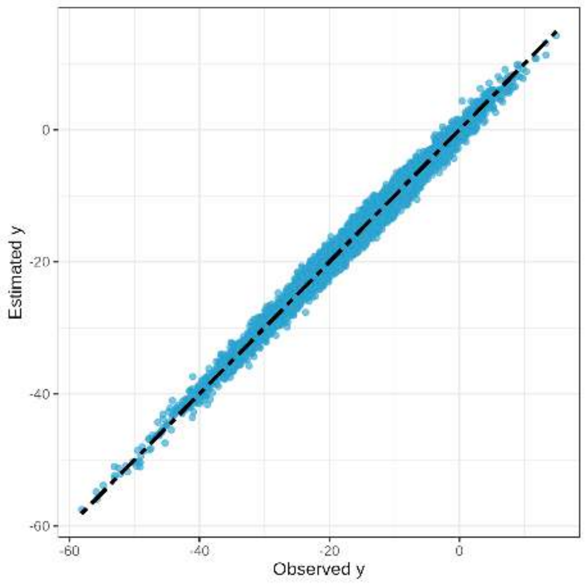


Figure 5: Scatter plot of estimated response variable vs. observed values in a simulated dataset with 100 spatial locations, 150 temporal points, 6 covariates using a rank decomposition of 10, 500 burn-in iterations and 500 sampling iterations.

`fp_device`	`fp_type`	Performance Metrics		
		$\text{MAE}_{\mathcal{B}}/\text{RMSE}_{\mathcal{B}}$	$\text{MAE}_{\boldsymbol{Y}}/\text{RMSE}_{\boldsymbol{Y}}$	Time (s)
`'cpu'`	`'float64'`	0.078±0.01/0.125±0.02	0.792±0.00/0.992±0.00	713±9
	`'float32'`	0.080±0.01/0.126±0.02	0.787±0.01/0.987±0.01	525±11
`'cuda'`	`'float64'`	0.075±0.01/0.125±0.03	0.793±0.00/0.994±0.01	221±10
	`'float32'`	0.080±0.02/0.123±0.03	0.787±0.01/0.986±0.01	210±9

Table 5: **BKTR** regression fitting performance comparison on simulated data using different processing device (`fp_device`) and floating point format (`fp_type`).

upticks. When using a sizeable amount of data, running matrix and tensor operations on GPU instead of CPU can usually provide great computational speed gains. Therefore, we test the four possible combinations of device and floating point format on simulated data to assess their performance. We use, for each combination, 10 new different simulation datasets of the *Larger* size (mentioned in 5.1, on which we fit the **BKTR** package using 500 burn-in iterations, 500 sampling iterations and a rank decomposition of 10. The obtained results are shown in Table 5.

The results show that there is no significant difference in the parameter estimation precision when using different floating point format or device. However, it is interesting to see that the usage of `'float32'` over `'float64'` leads to important computational speed improvement when we compare the mean of sampling runtime, with an improvement of 36% on CPU and a lesser uptick of 5% on GPU. Looking at the influence of the device, it is also possible to perceive that using GPU improves the execution speed for both floating point format (223% using `'float64'`and 138% using `'float32'`). Thus, for every example moving forward, we will use an `fp_type` of `'float32'` and `'cuda'` as a `fp_device`.

5.4. Imputation Results

In this section, we will take a look at the effectiveness of the **BKTR** packages at imputation. By imputation, we mean being able to find the best estimate for response values that were missing in the dataset. For our testing purposes, we simulate again datasets of the *Larger* shape. Then, from those datasets, we remove at random a certain percentage of response variable values and replace them by `NaN`. We use three scenarios of missing values rate which are 10%, 50% and 90%.

In Section 5.2 and Section 5.3 we obtained results that were extremely close to the ground truth. This can be seen through the fact that the $\text{RMSE}_{\boldsymbol{Y}}$ always stayed around 1 which was the value of the noise scale S_ϵ and that for all floating point format and device used in Section 5.3, we obtained $\text{MAE}_{\boldsymbol{\mathcal{B}}}$ that were below 0.1. One of the factors that could have helped **BKTR** to capture the underlying structure of the data so well might have been that the kernels used during simulation were very smooth. These kernels resulted in spatial and temporal covariance matrices with high values, making the synthetic data highly correlated within space and time. Thus, to verify the effect of the kernel parameters on the beta convergence and the imputation method, we will test the imputation implementation on two different lengthscale values scenarios. The first scenario will use lengthscale values of 3 for both kernel, $\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 3$ and the second scenario will use a value of $\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 6$. Both of those scenarios are coupled with each missing percentage scenario, analyzing a total of 6 different settings. For all different settings, we simulate 10 new datasets, on which we fit $K_1 = 500$ burn-in iterations, $K_2 = 500$ sampling iterations and a rank decomposition $R = 10$.

After the completion of the MCMC sampling, we use the `imputed_y_estimates` attribute to get the imputed values and compare them with equivalent initial values that were removed to get the $\text{MAE}_{\boldsymbol{Y}}$ and $\text{RMSE}_{\boldsymbol{Y}}$. We also look at the impact of missing values on the evaluation of underlying beta values in each scenario by calculating $\text{MAE}_{\boldsymbol{\mathcal{B}}}$ and $\text{RMSE}_{\boldsymbol{\mathcal{B}}}$. We compare the results obtain with the **BKTR** package implemented in R with the results of the **pyBKTR** package implemented in Python. The results of this experiment are shown in Table 6.

We observe that estimation of missing $\boldsymbol{Y}$ values seems much more accurate when using kernel parameters creating matrices with higher correlations. Moreover, it is possible to notice that reaching 90% of missing values, in all scenarios, is related to an important increase in $\text{MAE}_{\boldsymbol{Y}}$ and $\text{RMSE}_{\boldsymbol{Y}}$. Nonetheless, it is quite impressive to see that the $\text{RMSE}_{\boldsymbol{Y}}$ still has an average value of 1.05 even when there is 50% of $\boldsymbol{Y}$ values missing for lengthscale values of 6. The results in R and Python are very similar, showing us that the calculation implementations correspond well in both languages.

5.5. Interpolation Results

For interpolation, we start by exploring how to use the `predict` method of the `BKTRRegressor` class to complete interpolation. As mention in section 3.3, the shape of the provided data is crucial and can be non-trivial to visualize. Thus, we take the time to show how to use the `predict` method using a dataset of a *Larger* shape with simulation's kernels values of $\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 6$.

Since interpolation has not been explored previously for BKTR, we test the `predict` method results on the two types of datasets *Smaller* and *Larger*. We also look at the results for both the R and the Python packages. For each dataset, we also use two different values (3 and 6) for both the spatial kernel lengthscale ϕ_1^{sim} and the temporal kernel lengthscale γ_1^{sim}.

Simulation Settings	Missing	Lang.	Performance Metrics	
			$\text{MAE}_{\boldsymbol{\mathcal{B}}}/\text{RMSE}_{\boldsymbol{\mathcal{B}}}$	$\text{MAE}_{\boldsymbol{Y}}/\text{RMSE}_{\boldsymbol{Y}}$
$\phi_1^{\text{sim}} = 3$ $\gamma_1^{\text{sim}} = 3$	10%	R	0.76±0.21/1.21±0.31	0.87±0.02/1.10±0.03
		Python	0.83±0.33/1.38±0.66	0.87±0.02/1.10±0.03
	50%	R	0.67±0.14/1.04±0.22	0.93±0.03/1.17±0.0
		Python	0.72±0.11/1.17±0.17	0.91±0.02/1.16±0.04
	90%	R	1.02±0.20/1.50±0.33	2.47±0.39/3.54±0.61
		Python	0.95±0.08/1.43±0.14	2.27±0.26/3.31±0.52
$\phi_1^{\text{sim}} = 6$ $\gamma_1^{\text{sim}} = 6$	10%	R	0.23±0.05/0.38±0.09	0.81±0.02/1.02±0.02
		Python	0.18±0.04/0.28±0.07	0.81±0.01/1.02±0.02
	50%	R	0.20±0.06/0.31±0.11	0.83±0.01/1.05±0.01
		Python	0.18±0.03/0.28±0.07	0.83±0.01/1.04±0.01
	90%	R	0.40±0.07/0.60±0.13	1.24±0.10/1.68±0.19
		Python	0.39±0.06/0.60±0.10	1.23±0.10/1.65±0.17

Table 6: **BKTR** imputation performance comparison on simulated data. Mean ± standard deviation of the MAE and RMSE for $\boldsymbol{Y}$ and $\boldsymbol{\mathcal{B}}$ computed across 10 distinct simulated datasets for different simulation scenarios.

Dataset	Simulation Settings	Lang.	Performance Metrics	
			$\text{MAE}_{\boldsymbol{\mathcal{B}}}/\text{RMSE}_{\boldsymbol{\mathcal{B}}}$	$\text{MAE}_{\boldsymbol{Y}}/\text{RMSE}_{\boldsymbol{Y}}$
Smaller $M = 20$ $N = 30$ $P = 4$	$\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 3$	R	0.81±0.19/1.08±0.27	1.79±0.69/2.48±1.03
		Python	0.76±0.19/1.03±0.27	1.68±0.50/2.35±0.97
	$\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 6$	R	0.51±0.11/0.71±0.19	1.16±0.12/1.49±0.16
		Python	0.52±0.10/0.71±0.19	1.11±0.13/1.42±0.21
Larger $M = 100$ $N = 150$ $P = 6$	$\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 3$	R	1.23±0.73/2.26±1.96	2.18±0.58/3.20±0.93
		Python	1.26±0.64/2.13±1.24	2.60±1.23/3.93±2.17
	$\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 6$	R	0.27±0.08/0.44±0.14	1.00±0.13/1.27±0.17
		Python	0.25±0.08/0.40±0.15	0.96±0.18/1.23±0.29

Table 7: BKTR interpolation performance comparison on simulated data. Mean ± standard deviation of the MAE and RMSE for $\boldsymbol{Y}$ and $\boldsymbol{\mathcal{B}}$ computed across 10 distinct simulated datasets for different simulation scenarios.

For each of the four aforementioned scenarios, we simulate 10 different datasets, from which we randomly keep aside four spatial locations and six time points during the training phase of **BKTR**. We fit the regression on $K_1 = 500$ burn-in iterations and $K_2 = 500$ sampling iterations with a rank decomposition of 10. Then, we use the predict method to try to find the $\boldsymbol{Y}$ and $\boldsymbol{\mathcal{B}}$ values of the kept aside locations. Subsequently, we calculate the error between the initial data and the kept aside data via the $\text{MAE}_{\boldsymbol{\mathcal{B}}}$, $\text{RMSE}_{\boldsymbol{\mathcal{B}}}$, $\text{MAE}_{\boldsymbol{Y}}$, $\text{RMSE}_{\boldsymbol{Y}}$ that we show in Table 7. From this table, we can observe again that using kernels that have higher correlation $\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 6$ give results with a lower error in all scenario. The best results were obtained from the *Larger* dataset and the highest lengthscale values, giving a $\text{RMSE}_{\boldsymbol{Y}}$ of 1.27 and 1.23 for R and Python respectively.

Another task we want to perform with simulated data is to examine the interpolation errors through the different segments of predictions that were presented in Section 2.3. Therefore,

Interpolated Portion	Performance Metrics	
	$\text{MAE}_{\boldsymbol{\mathcal{B}}}/\text{RMSE}_{\boldsymbol{\mathcal{B}}}$	$\text{MAE}_{\boldsymbol{Y}}/\text{RMSE}_{\boldsymbol{Y}}$
$\boldsymbol{Y}^1$ and $\boldsymbol{\mathcal{B}}^1$; $M_{\text{new}} = 10 \times N_{\text{obs}} = 130$	0.24±0.06/0.38±0.10	1.05±0.14/1.34±0.22
$\boldsymbol{Y}^2$ and $\boldsymbol{\mathcal{B}}^2$; $M_{\text{obs}} = 90 \times N_{\text{new}} = 20$	0.22±0.03/0.35±0.06	0.81±0.01/1.01±0.01
$\boldsymbol{Y}^3$ and $\boldsymbol{\mathcal{B}}^3$; $M_{\text{new}} = 10 \times N_{\text{new}} = 20$	0.24±0.06/0.37±0.10	1.02±0.14/1.31±0.20
Total $\boldsymbol{Y}^{\text{new}}$ and $\boldsymbol{\mathcal{B}}^{\text{new}}$	0.23±0.04/0.37±0.07	0.92±0.07/1.18±0.11

Table 8: **BKTR** interpolation performance breakdown on the different portions of the predicted data. Mean ± standard deviation of the MAE and RMSE for $\boldsymbol{Y}$ and $\boldsymbol{\mathcal{B}}$ computed across 10 distinct simulated datasets for different interpolation portions.

we estimate the $\text{RMSE}_{\boldsymbol{Y}}$ and $\text{MAE}_{\boldsymbol{Y}}$ errors on $\boldsymbol{Y}^{\text{new}}$ distributed across $\boldsymbol{Y}^1, \boldsymbol{Y}^2, \boldsymbol{Y}^3$, as well as the $\text{RMSE}_{\boldsymbol{\mathcal{B}}}$ $\text{MAE}_{\boldsymbol{\mathcal{B}}}$ errors on $\boldsymbol{\mathcal{B}}^{\text{new}}$ across $\boldsymbol{\mathcal{B}}^1, \boldsymbol{\mathcal{B}}^2, \boldsymbol{\mathcal{B}}^3$. We do so with a scenario that use a simulation dataset of the *Larger* shape and simulation kernel lengthscale values of $\phi_1^{\text{sim}} = \gamma_1^{\text{sim}} = 6$. We keep aside 10 locations and 20 time points during regression and use interpolation on them afterward. This translates to having $M^{\text{obs}} = 90$ observed locations and $M^{\text{new}} = 10$ new locations. For the time points, the equivalent sizes are $N^{\text{obs}} = 130$ and $N^{\text{new}} = 20$. We fit the BKTR regression on the synthetic data using $K_1 = 1000$, $K_2 = 500$ and $R = 10$. We repeat the simulation, regression and interpolation exercise 10 times and the results are shown in Table 8.

From this table, we can observe, via all error metrics, that the interpolation struggles more doing interpolation for new locations ($\boldsymbol{Y}^1$ and $\boldsymbol{\mathcal{B}}^1$) than for new time points ($\boldsymbol{Y}^2$ and $\boldsymbol{\mathcal{B}}^2$). Since, time points span only one dimension, compared to the two dimensions of spatial points, we could think that the covariance pattern between observations his easier to estimate for new time points than new locations. It also seems like the new points situated at new location and new timestamps, $\boldsymbol{Y}^3$ and $\boldsymbol{\mathcal{B}}^3$, have error values very similar to the one of new locations, suggesting that the majority of the errors in this example comes from predicting values for unseen locations.

6. Experimental study

This section aims to test the capacity of the **BKTR** package on real world data. We achieve this task using the same bike sharing demand dataset that was used by Lei *et al.* (2023). A great portion of this dataset was initially gathered by Wang *et al.* (2021) who used information from multiple sources to create a feature rich set of data points.

This dataset contains five distinct data frames

- `bixi_station_departures` (the response variable)
- `bixi_temporal_features` (the temporal covariates)
- `bixi_spatial_features` (the spatial covariates)
- `bixi_spatial_locations` (the location of each spatial point)
- `bixi_temporal_locations` (the location of each temporal point)

The `station_departures` data frame comes from BIXI Montréal (2023), which is a Montreal, Canada based bike sharing company. The response variable is the total daily bike departure for each station held by BIXI during its 2019 season. The database contains $M = 587$ rows each representing one station and $N = 196$ columns representing different days from April 15 to October 27, 2019. The value of each data point in this data frame is equivalent to the total number of bike departures for a station on a given day. The `bixi_temporal_features` data includes daily meteorological covariates that vary through time like temperature, precipitation, humidity, etc. This information was collected from the Environment and Climate Change Canada Historical Climate Data website. Temporal features also include data regarding if each date was a holiday or not, according to the Quebec government. The `station_features` data frame includes data related to the location of each bike sharing stations like surrounding population (taken from the 2016 Canada census data at a dissemination block level), walk score (Walk Score 2023) and a number of other information collected with DMTI Spatial Inc. (2019) concerning point of interests in a surrounding radius of each station like the number of university, the number of metro stations, etc. The data frame `temporal_locations` is simply representing the position (`time_index`) of each of the $N = 196$ day relative to each other. Since there is no day missing, it simply translates to a range from 0 to 195 associated to the order of each date. The last data frame, `spatial_locations`, encodes the position for each of the $M = 587$ bike station with geographic coordinates (e.g., latitude and longitude).

All data frames are available, as is, in the **BKTR** library. A normalize version of all datasets can also be accessed through the `BixiData` class of the `examples` module in both the **BKTR** packages. As mentioned previously, when the spatial covariates do not vary through time, the temporal covariates do not vary through space, and they are provided in the form of two different data frames, the **BKTR** packages offer a convenience function allowing to merge those data frames called `reshape_covariate_dfs`. It was already used to merge `bixi_station_departures`, `bixi_temporal_features` and `bixi_spatial_features` into the `data_df` data frame which can be found in the `BixiData` class as well. Note that the data frames used in this section are the same as the ones used by Lei *et al.* (2023), except for having their column header renamed to achieve a consistent naming convention.

As a result, in this section, we will directly work with `data_df`, `spatial_positions_df` and `temporal_positions_df` from the `BixiData` class. With this dataset, we will try to explore and compare the full capacity of the **BKTR** package on real world data.

6.1. Analysis

In this section we fit a `BKTRRegressor` to the data present in the `BixiData` class, and then interpret the results using different properties and visualizations that the **BKTR** package offers.

We will begin by fitting the number of bike departures using three covariates: the mean temperature, the total precipitation in mm and the total park area. To accomplish this task, we will pass the formula `nb_departure ~ 1 + mean_temp_c + area_park + walkscore` to the initialization of the `BKTRRegressor` object. We will then run a MCMC sampling for 1500 iterations, including $K_1 = 1000$ burn-in iterations and $K_2 = 500$ sampling iterations. Additionally, we will utilize a rank decomposition of 8, a spatial Matérn 5/2 kernel and a local periodic temporal kernel like the one presented in Section 4.2. To initialize a `BKTRRegressor` object with the aforementioned parameters, we can simply run the following code chunk (output omitted for brevity).

```
R> TSR$set_params(seed = 1, fp_type = 'float32', fp_device = 'cuda')
R> bixi_data <- BixiData$new()
R> <- KernelParameter$new(value = 7, is_fixed = TRUE)
R> k_local_periodic <- KernelSE$new() * KernelPeriodic$new(
+    period_length = KernelParameter$new(value = 7, is_fixed = TRUE))
R> bktr_regressor <- BKTRRegressor$new(
+    formula = nb_departure ~ 1 + mean_temp_c + area_park + total_precip_mm,
+    data_df = bixi_data$data_df,
+    spatial_positions_df = bixi_data$spatial_positions_df,
+    temporal_positions_df = bixi_data$temporal_positions_df,
+    rank = 8,
+    spatial_kernel = KernelMatern$new(smoothness_factor = 5),
+    temporal_kernel = kernel_local_periodic,
+    burn_in_iter = 1000,
+    sampling_iter = 500)
R> bktr_regressor$mcmc_sampling()
```

After sampling completion, we can obtain the summary of the `BKTRRegressor` object.

```
> summary(bktr_regressor)
```

```
======================================================================
                        BKTR Regressor Summary
======================================================================
Formula: nb_departure ~ 1 + mean_temp_c + area_park + total_precip_mm

Burn-in iterations: 1000
Sampling iterations: 500
Rank decomposition: 8
Nb Spatial Locations: 587
Nb Temporal Points: 196
Nb Covariates: 4
======================================================================
In Sample Errors:
  RMSE: 0.072
  MAE: 0.053
Computation time: 1235.50s.
======================================================================
-- Spatial Kernel --
Matern 5/2 Kernel
Parameter(s):
                       Mean   Median       SD  Low2.5p  Up97.5p
lengthscale          21.128   20.877    1.401   18.658   23.738

-- Temporal Kernel --
```

```
Composed Kernel (Mul)
  SE Kernel
  Parameter(s):
                         Mean   Median       SD  Low2.5p  Up97.5p
  lengthscale           6.448    6.437    0.114    6.252    6.685
  *
  Periodic Kernel
  Parameter(s):
                         Mean   Median       SD  Low2.5p  Up97.5p
  lengthscale           0.941    0.942    0.020    0.899    0.979
  period length          Fixed Value: 7.000
======================================================================
Beta Estimates Summary (Aggregated Per Covariates)

                       Mean   Median       SD
Intercept             0.447    0.376    0.306
mean_temp_c          -0.011   -0.008    0.042
area_park            -0.005   -0.011    0.185
total_precip_mm      -0.260   -0.214    0.189
======================================================================
```

The displayed model summary is again divided in four different sections. In the kernel section, we see that even the kernel composed via the multiplication of two kernels shows a parameter summary in a very comprehensive fashion. In the beta coefficients estimates section, we observe that the `total_precip_mm` has the lowest coefficient estimate, which means that it has, in average, the most negative effect on the number of bike departures. The summary reveals that it took 1235.5 seconds to complete MCMC sampling and fit over 460k coefficients. It is interesting to note that GPU acceleration played a significant role in handling this extensive dataset scenario, as running the same code once on our system with `fp_type='cpu'` took approximately 9.5h hours to complete (34,224s).

Another way to visualize some aspects of the fitted model is to plot the coefficient estimates of covariates through time for a given spatial point. This can be done by calling the `plot_temporal_betas` function on a `BKTRRegressor` object.

```
R> plot_temporal_betas(
+    bktr_regressor,
+    plot_feature_labels = c('mean_temp_c', 'area_park', 'total_precip_mm'),
+    spatial_point_label = '7114 - Smith / Peel')
```

The result of this call is shown in Figure 6. This plot helps us visualize the non stationarity of the coefficients via the evolution of the influence of the covariates through time. For instance, we can see that the influence of the mean temperature on the number of bike departures is lower during the beginning and the ending months of the season compared to the mid summer months. For this station, precipitations negatively impacts departures during summer.

In the same way, we can plot the coefficient estimates of the covariates through space for a given time point. This can be done similarly by calling the `plot_spatial_betas` function.

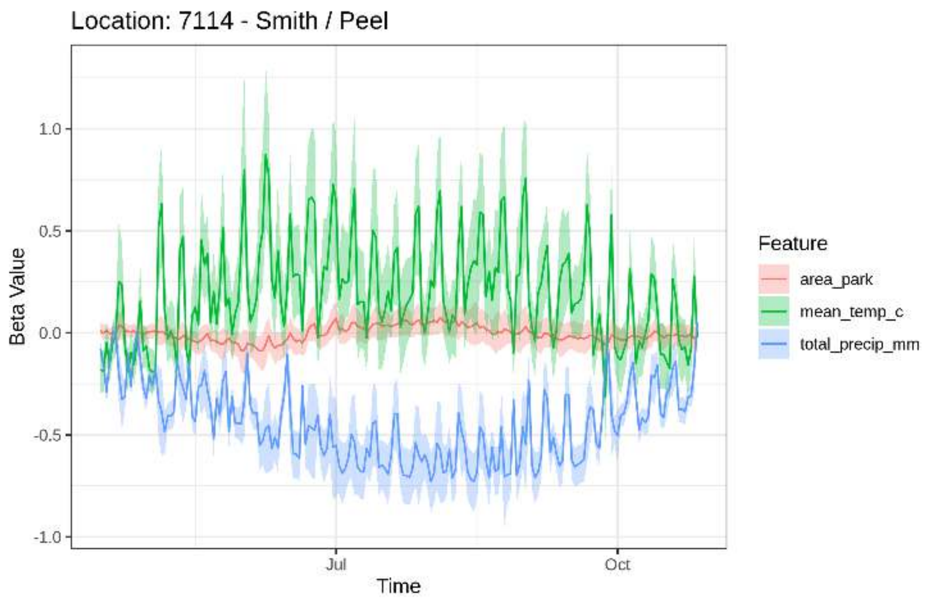


Figure 6: Result of the `plot_temporal_betas` function to plot the coefficient estimates of the covariates through time for a given spatial location.

```
R> plot_spatial_betas(
+    bktr_regressor,
+    plot_feature_labels = c('mean_temp_c', 'area_park', 'total_precip_mm'),
+    temporal_point_label = '2019-07-19',
+    nb_cols = 3)
```

The result of this function call is shown in Figure 7. Again, this plot helps us to better visualize non stationarity with the evolution of the influence of the covariates through space. We can observe that the precipitation has more negative influence on the number of bike departures in the center of the city when compared to the periphery of the city.

We can demonstrate the proximity of **BKTR**'s estimated response variables to the actual values by utilizing the `plot_y_estimates` function, employing the same code as presented in Section 5.2. The outcomes of this function are visualized in Figure 8. These plots show estimated values that, while slightly further from the diagonal compared to those in Figure 5, still display a relevant correlation between estimated and observed response variables.

We can see that the **BKTR** package provides a very easy way to fit local regression models on a given dataset. And that it also provides useful and user-friendly integrated functions to help visualize and understand the fitted model.

6.2. Imputation Example

In this section, we will explore how to use **BKTR** to estimate the values for missing data points in the response variable $\boldsymbol{Y}$ of the BIXI dataset. Imputation for **BKTR** can only be done at the response variable level, which means that it is not possible at the moment to estimate missing covariate values. It is possible to observe that there is already some missing values in the `data_df` data frame of the BIXI dataset for the response variable column `nb_departure`,

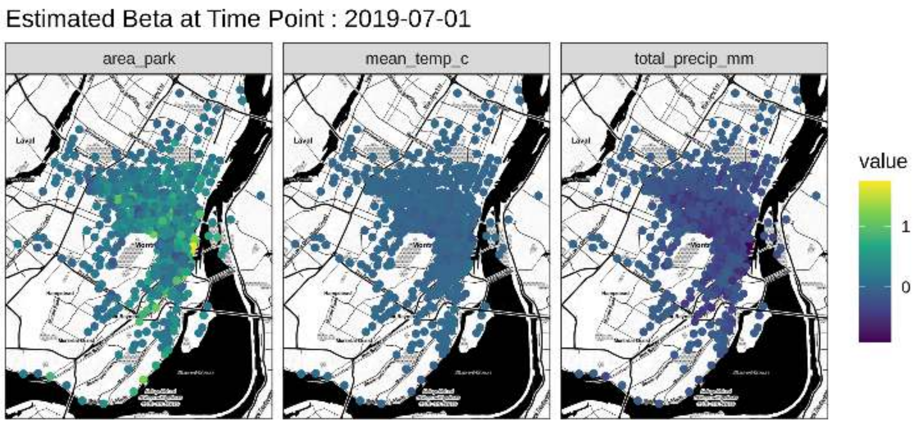


Figure 7: Result of the `plot_spatial_betas` function to plot the coefficient estimates of the covariates through space for a given time point.

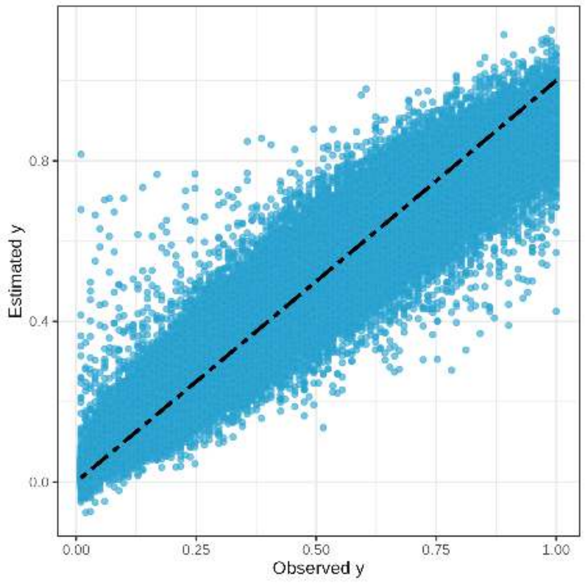


Figure 8: Scatter plot of **BKTR** estimated response variable vs. observed values in the BIXI dataset.

as the next code snippet can illustrate.

```
R> y_is_na <- is.na(bixi_data$data_df$nb_departure)
R> nb_y_na <- sum(y_is_na)
R> sprintf(
+   'There is %.d missing `nb_departure` values representing ~%.2f%%',
+   nb_y_na,
+   nb_y_na / length(y_is_na) * 100))
```

```
"There is 14940 missing `nb_departure` values representing ~12.99%"
```

This shows us that there is already around 13% of the response variable values missing in our dataset. Let's take a look at the first three missing values of the data frame to be able to find at which location and which moment those values were situated.

```
R> bixi_data$data_df[which(y_is_na)[1:3], 1:3]
```

```
                                           location       time nb_departure
1: 10002 - Métro Charlevoix (Centre / Charlevoix) 2019-04-22           NA
2: 10002 - Métro Charlevoix (Centre / Charlevoix) 2019-05-08           NA
3: 10002 - Métro Charlevoix (Centre / Charlevoix) 2019-05-16           NA
```

Knowing that the location *10002 - Métro Charlevoix (Centre / Charlevoix)* is missing multiple values, we can effortlessly use the `imputed_y_estimates` attribute from the fitted regressor instance of Section 6.1 to estimate those data points.

```
R> bktr_regressor$imputed_y_estimates[which(y_is_na)[1:3]]
```

```
                                           location       time     y_est
1: 10002 - Métro Charlevoix (Centre / Charlevoix) 2019-04-22 0.8021128
2: 10002 - Métro Charlevoix (Centre / Charlevoix) 2019-05-08 1.0260799
3: 10002 - Métro Charlevoix (Centre / Charlevoix) 2019-05-16 1.0563858
```

After observing the ease of imputing missing response variables in BIXI, we can further validate its efficiency by arbitrarily masking 20% of the non-missing `nb_departures` values. We then fit a `BKTRRegressor` object using the exact same code as in Section 6.1 for the dataset for which we added missing data. Afterwards, we can compare the imputed results `bktr_regressor$imputed_y_estimates` with the original dataset response variable values to validate imputation performance.

```
R> y_is_not_na <- which(!y_is_na)
R> nb_masked_vals <- round(length(y_is_not_na) * 0.2)
R> masked_indices <- sample(y_is_not_na, nb_masked_vals)
R> new_data_df <- bixi_data$data_df
R> new_data_df[masked_indices, 'nb_departure'] <- NA
R> bktr_regressor <- BKTRRegressor$new(new_data_df,
+    ...) # Same parameters as previous section
R> bktr_regressor$mcmc_sampling()
R> y_err <- (bixi_data$data_df$nb_departure[masked_indices]
+    - bktr_regressor$imputed_y_estimates$y_est[masked_indices])
R> sprintf('MAE: %.2f  ||  RMSE: %.2f', mean(abs(y_err)),
+  sqrt(mean(y_err ^ 2)))
```

```
MAE: 0.0566  ||  RMSE: 0.0774
```

The imputed data error calculated $\text{RMSE}_{\boldsymbol{Y}} = 0.077$ and $\text{MAE}_{\boldsymbol{Y}} = 0.057$ gives results that are very close to the ones observed in-sample via Section 6.1 summary which was $\text{RMSE}_{\boldsymbol{Y}} = 0.072$ and $\text{MAE}_{\boldsymbol{Y}} = 0.053$. Therefore, we find **BKTR** being a powerful tool for spatiotemporal data imputation.

6.3. Interpolation Example

In the BIXI case, interpolation can prove to be highly valuable in estimating the number of departures at newly planned locations. This estimation could help significantly the allocation planning of number of docks needed at a given new location. Furthermore, when there is complete absence of data for a given time period (e. g., due to a reporting datacenter shortage with a duration of two days), we could simply use interpolation to gather an estimate of the number of departure per station during that time period. To test the interpolation capabilities of **BKTR**, we select arbitrarily three bike stations and two contiguous days in the dataset. We then temporarily remove those days and stations from the initial dataset and put them aside. Next, we fit the regressor on the remaining data, and finally we use the `predict` method on the set-aside data with the goal of estimating the number of departures at those days and locations.

We start by setting aside the following three locations *4002 - Graham / Wicksteed*, *7079 - Notre-Dame / Gauvin* and *6236 - Laurier / de Bordeaux*. We also set aside two time points equivalent to the dates *2019-05-01* and *2019-05-02*. We then separate the three main BIXI data frames in two portions which are the observed data and the new data.

```
R> library(data.table)
R> TSR$set_params(seed=0, fp_type='float32')
R> bixi_data <- BixiData$new()
R> data_df <- bixi_data$data_df
R> spa_df <- bixi_data$spatial_positions_df
R> tem_df <- bixi_data$temporal_positions_df
R> # New locations and times
R> new_s <- c('4002 - Graham / Wicksteed',
+    '7079 - Notre-Dame / Gauvin',
+    '6236 - Laurier / de Bordeaux')
R> new_t <- c('2019-05-01', '2019-05-02')
R> # Cast to IDate to match implicit cast of data.table
R> new_t <- as.IDate(new_t)
R> # Get obs data
R> obs_s <- setdiff(unlist(spa_df$location), new_s)
R> obs_t <- setdiff(unlist(tem_df$time), new_t)
R> obs_data_df <- data_df[data_df[, .I[
+    location %in% obs_s & time %in% obs_t]], ]
R> obs_spa_df <- spa_df[spa_df[, .I[location %in% obs_s]], ]
R> obs_tem_df <- tem_df[tem_df[,.I[time %in% obs_t]], ]
R> # Get new data
R> new_data_df <- data_df[data_df[, .I[
+    location %in% new_s | time %in% new_t]], ]
R> new_spa_df <- spa_df[spa_df[, .I[location %in% new_s]], ]
```

```
R> new_tem_df <- tem_df[tem_df[, .I[time %in% new_t]], ]
```

Subsequently, we train the BKTR model on the observed data to predict the new unobserved datasets. As a last step, we compare the interpolation results with the real observed response values when they are not missing with the usual error metrics.

```
R> # Train and predict
R> bktr_regressor <- BKTRRegressor$new(
+    data_df = obs_data_df,
+    spatial_positions_df = obs_spa_df,
+    temporal_positions_df = obs_tem_df,
+    #... other parameters like section 6.1)
R> preds <- bktr_regressor$predict(
+    new_data_df, new_spa_df, new_tem_df)
R> # Sort data for comparison and remove na values
R> new_data_df <- data_df[
+    data_df[, .I[location %in% new_s | time %in% new_t]],
+    c('location', 'time', 'nb_departure')]
R> pred_y_df <- preds$new_y_df
R> setkey(new_data_df, location, time)
R> setkey(pred_y_df, location, time)
R> non_na_indices <- which(!is.na(new_data_df$nb_departure))
R> # Compare predictions
R> y_err <- (new_data_df$nb_departure[non_na_indices]
+    - pred_y_df$y_est[non_na_indices])
R> sprintf('Predicting %d y values || MAE: %.4f || RMSE: %.4f',
+    length(non_na_indices), mean(abs(y_err)), sqrt(mean(y_err ^ 2)))
```

```
[1] "Predicting 1664 y values || MAE: 0.0878 || RMSE: 0.1278"
```

We can perceive that once the data is sorted and split into training and prediction, the other commands related to predictions are fairly easy to use. Also, since the $\boldsymbol{Y}$ values had some missing data points, we needed to remove them from the evaluated vector to calculate the error metrics properly. Nonetheless, we can see that the results of interpolation on BIXI data are convincing. Obtaining values of $\text{RMSE}_{\boldsymbol{Y}} = 0.088$ and a $\text{MAE}_{\boldsymbol{Y}} = 0.128$, which are higher than the in-sample errors, but still showcase decent prediction capabilities on a real set of data.

7. Summary and discussion

The **BKTR** (Bayesian Kernelized Tensor Regression) packages, presented through this work, introduce a compelling tool for local spatiotemporal regression analysis in both R and Python. This framework offers a user-friendly endpoint, while also focusing on flexibility and computational performance. Leveraging a library specific for tensor computation like Falbel and Luraschi (2023) allows this package to be extremely efficient and to also harness the computing speed of dedicated floating point operation hardware like GPUs. The sensible default values and choices used in **BKTR** allows for a low friction starting point for the majority of users, while enabling complex fine-tuning for the more advanced one through composed kernels and access to multiple regression parameters. This library, implemented in two of the most prominent statistical programming languages, makes the work realized by Lei *et al.* (2023) available to the research community. The **BKTR** packages also bring to life a new feature that is the capacity to do predictions on unobserved time points and locations, called interpolation. We show, through extensive testing, the important capabilities of **BKTR** in regression, imputation and interpolation. Since it is one of the very first package enabling local regressions to fit coefficients for every location and time points combinations of very large dataset, we think that this breakthrough will greatly improve the modelling process of a vast amount of spatiotemporal analysis.

We aim to continuously improve and expand the functionalities of the **BKTR** packages that we hereby presented. We will do so by actively monitoring the user issues and requests that will be provided to the respective GitHub of each package. By having developed the package in both languages, we also commit to continue developing features in a way that will be accessible for R and Python developers. Since both packages are based on **torch** and **pytorch** we will keep a close eye on both packages' advancements to be able to provide to our users the latest enhancements in tensor computation.

Computational details

Results in this paper were obtained using Google Colab instances using a type of shape that was *High-Ram* and a V100 GPU. Thus, the calculations were done with an 8 core Xeon processor, 25.5GB of total CPU Ram and 16GB of GPU Ram. We also used the default R and Python versions in Colab which were R 4.3.1 with **torch** 0.11.0 and Python 3.10.6 with **pytorch** 1.12.1.

References

Abadi M, Agarwal A, Barham P, Brevdo E, Chen Z, Citro C, Corrado GS, Davis A, Dean J, Devin M, Ghemawat S, Goodfellow I, Harp A, Irving G, Isard M, Jia Y, Jozefowicz R, Kaiser L, Kudlur M, Levenberg J, Mané D, Monga R, Moore S, Murray D, Olah C, Schuster M, Shlens J, Steiner B, Sutskever I, Talwar K, Tucker P, Vanhoucke V, Vasudevan V, Viégas F, Vinyals O, Warden P, Wattenberg M, Wicke M, Yu Y, Zheng X (2015). "**TensorFlow**: Large-Scale Machine Learning on Heterogeneous Systems." Software available from tensorflow.org, URL `https://www.tensorflow.org/`.

Baddeley A, Turner R (2005). "**spatstat**: An R Package for Analyzing Spatial Point Patterns." *Journal of Statistical Software*, **12**(6), 1–42. `doi:10.18637/jss.v012.i06`.

Bakar KS, Kokic P, Jin H (2016). "Hierarchical Spatially Varying Coefficient and Temporal Dynamic Process Models using **spTDyn**." *Journal of Statistical Computation and Simulation*, **86**(4), 820–840. URL `https://doi.org/10.1080/00949655.2015.1038267`.

Bakar KS, Sahu SK (2015). "spTimer: Spatio-Temporal Bayesian Modeling Using R." *Journal* *of Statistical Software*, **63**(15), 1–32. doi:10.18637/jss.v063.i15. URL https://www.jstatsoft.org/index.php/jss/article/view/v063i15.

BIXI Montréal (2023). "Open Data." Accessed: 2023-07-11, URL https://bixi.com/en/open-data.

Carpenter B, Gelman A, Hoffman MD, Lee D, Goodrich B, Betancourt M, Brubaker M, Guo J, Li P, Riddell A (2017). "**Stan**: A Probabilistic Programming Language." *Journal of Statistical Software*, **76**(1), 1–32. doi:10.18637/jss.v076.i01. URL https://www.jstatsoft.org/index.php/jss/article/view/v076i01.

Chang W (2021). ***R6**: Encapsulated Classes with Reference Semantics.* R package version 2.5.1, URL https://CRAN.R-project.org/package=R6.

DMTI Spatial Inc (2019). "Enhanced Point of Interest (DMTI)." URL https://www.dmtispatial.com.

Douglas Nychka, Reinhard Furrer, John Paige, Stephan Sain (2021). "**fields**: Tools for Spatial Data." R package version 15.2, URL https://github.com/dnychka/fieldsRPackage.

Dowle M, Srinivasan A (2023). ***data.table**: Extension of 'data.frame'.* R package version 1.14.8, URL https://CRAN.R-project.org/package=data.table.

Duvenaud D (2014). *Automatic Model Construction with Gaussian Processes*. Ph.D. thesis, University of Cambridge.

Falbel D, Luraschi J (2023). ***torch**: Tensors and Neural Networks with 'GPU' Acceleration.* R package version 0.9.1, URL https://CRAN.R-project.org/package=torch.

Finley AO, Banerjee S, EGelfand A (2015). "**spBayes** for Large Univariate and Multivariate Point-Referenced Spatio-Temporal Data Models." *Journal of Statistical Software*, **63**(13), 1–28. URL https://www.jstatsoft.org/article/view/v063i13.

Gamerman D, Lopes HF, Salazar E (2008). "Spatial Dynamic Factor Analysis." *Bayesian Analysis*, **3**(4), 759–792. doi:10.1214/08-BA329. URL https://doi.org/10.1214/08-BA329.

Gardner J, Pleiss G, Weinberger KQ, Bindel D, Wilson AG (2018). "Gpytorch: Blackbox Matrix-Matrix Gaussian Process Inference with GPU Acceleration." *Advances in neural information processing systems*, **31**.

Gelfand AE, Kim HJ, Sirmans CF, Banerjee S (2003). "Spatial Modeling With Spatially Varying Coefficient Processes." *Journal of the American Statistical Association*, **98**(462), 387–396. doi:10.1198/016214503000170. https://doi.org/10.1198/016214503000170, URL https://doi.org/10.1198/016214503000170.

Geman S, Geman D (1984). "Geman, D.: Stochastic Relaxation, Gibbs Distribution, and the Bayesian Restoration of Images. IEEE Trans. Pattern Anal. Mach. Intell. PAMI-6(6), 721-741." *IEEE Trans. Pattern Anal. Mach. Intell.*, **6**, 721–741. doi:10.1109/TPAMI.1984.4767596.

Gräler B, Pebesma E, Heuvelink G (2016). "Spatio-Temporal Interpolation Using **gstat**." *The R Journal*, **8**, 204–218. URL https://journal.r-project.org/archive/2016/RJ-2016-014/index.html.

Khatri C, Rao CR (1968). "Solutions to Some Functional Equations and their Applications to Characterization of Probability Distributions." *Sankhyā: The Indian Journal of Statistics, Series A*, pp. 167–180.

Kolda TG, Bader BW (2009). "Tensor Decompositions and Applications." *SIAM review*, **51**(3), 455–500.

Lei M, Labbe A, Sun L (2023). "Scalable Spatiotemporally Varying Coefficient Modelling with Bayesian Kernelized Tensor Regression." arXiv:2109.00046.

Lindgren F, Rue H (2015). "Bayesian Spatial Modelling with **R-INLA**." *Journal of Statistical Software*, **63**(19), 1–25. doi:10.18637/jss.v063.i19. URL https://www.jstatsoft.org/index.php/jss/article/view/v063i19.

Lunn DJ, Thomas A, Best N, Spiegelhalter D (2000). "**WinBUGS** – A Bayesian Modelling Framework: Concepts, Structure, and Extensibility." *Statistics and Computing*, **10**(4), 325–337. ISSN 0960-3174. doi:10.1023/A:1008929526011. URL https://doi.org/10.1023/A:1008929526011.

Lustiger H (2022). *Design Patterns in R*. Tidylab, Auckland, New Zealand. URL https://github.com/tidylab/R6P.

Millo G, Piras G (2012). "**splm**: Spatial Panel Data Models in R." *Journal of Statistical Software*, **47**(1), 1–38. URL https://www.jstatsoft.org/v47/i01/.

Neal RM (2003). "Slice sampling." *The Annals of Statistics*, **31**(3), 705 – 767. doi:10.1214/aos/1056562461. URL https://doi.org/10.1214/aos/1056562461.

Paszke A, Gross S, Massa F, Lerer A, Bradbury J, Chanan G, Killeen T, Lin Z, Gimelshein N, Antiga L, Desmaison A, Kopf A, Yang E, DeVito Z, Raison M, Tejani A, Chilamkurthy S, Steiner B, Fang L, Bai J, Chintala S (2019). "**PyTorch**: An Imperative Style, High-Performance Deep Learning Library." In *Advances in Neural Information Processing Systems 32*, pp. 8024–8035. Curran Associates, Inc. URL http://papers.neurips.cc/paper/9015-pytorch-an-imperative-style-high-performance-deep-learning-library.pdf.

Pebesma E (2012). "**spacetime**: Spatio-Temporal Data in R." *Journal of Statistical Software*, **51**(7), 1–30. URL https://www.jstatsoft.org/v51/i07/.

Pebesma EJ (2004). "Multivariable Geostatistics in S: the **gstat** Package." *Computers Geosciences*, **30**, 683–691.

Pebesma EJ, Bivand R (2005). "Classes and Methods for Spatial Data in R." *R News*, **5**(2), 9–13. URL https://CRAN.R-project.org/doc/Rnews/.

Pedregosa F, Varoquaux G, Gramfort A, Michel V, Thirion B, Grisel O, Blondel M, Prettenhofer P, Weiss R, Dubourg V, Vanderplas J, Passos A, Cournapeau D, Brucher M, Perrot

M, Duchesnay E (2011). "Scikit-learn: Machine Learning in Python." *Journal of Machine Learning Research*, **12**, 2825–2830.

Plotly Technologies Inc (2015). "Collaborative data science." URL `https://plot.ly`.

Plummer M (2003). "**JAGS**: A Program for Analysis of Bayesian Graphical Models using Gibbs Sampling." *3rd International Workshop on Distributed Statistical Computing (DSC 2003); Vienna, Austria*, **124**.

Plummer M (2023). ***rjags**: Bayesian Graphical Models using MCMC.* R package version 4-14, URL `https://CRAN.R-project.org/package=rjags`.

R Core Team (2023). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. URL `https://www.R-project.org/`.

Rue H, Martino S, Chopin N (2009). "Approximate Bayesian Inference for Latent Gaussian Models by Using Integrated Nested Laplace Approximations." *Journal of the Royal Statistical Society Series B: Statistical Methodology*, **71**(2), 319–392.

Sigrist F, Künsch HR, Stahel WA (2015). "**spate**: An R Package for Spatio-Temporal Modeling with a Stochastic Advection-Diffusion Process." *Journal of Statistical Software*, **63**(14), 1–23. `doi:10.1111/rssb.12061`.

Snyder JP (1987). *Map Projections–A Working Manual*, volume 1395. US Government Printing Office.

Stan Development Team (2023). "**RStan**: the R Interface to Stan." R package version 2.21.8, URL `https://mc-stan.org/`.

Sturtz S, Ligges U, Gelman A (2005). "**R2WinBUGS**: A Package for Running **WinBUGS** from R." *Journal of Statistical Software*, **12**(3), 1–16. URL `http://www.jstatsoft.org`.

Takeuchi K, Kashima H, Ueda N (2017). "Autoregressive Tensor Factorization for Spatio-Temporal Predictions." In *2017 IEEE International Conference on Data Mining (ICDM)*, pp. 1105–1110. `doi:10.1109/ICDM.2017.146`.

The Pandas Development Team (2022). "**Pandas** 1.4.2." `doi:10.5281/zenodo.6408044`. URL `https://doi.org/10.5281/zenodo.6408044`.

Venables WN, Ripley BD (2002). *Modern Applied Statistics with S*. Fourth edition. Springer, New York. ISBN 0-387-95457-0, URL `https://www.stats.ox.ac.uk/pub/MASS4/`.

Walk Score (2023). "Walk Score Methodology." Accessed: 2023-07-11, URL `https://www.walkscore.com/methodology.shtml`.

Wang X, Cheng Z, Trépanier M, Sun L (2021). "Modeling Bike-Sharing Demand Using a Regression Model With Spatially Varying Coefficients." *Journal of Transport Geography*, **93**, 103059. ISSN 0966-6923. `doi:https://doi.org/10.1016/j.jtrangeo.2021.103059`. URL `https://www.sciencedirect.com/science/article/pii/S0966692321001125`.

Wardrop M (2022). "**Formulaic**: An implementation of Wilkinson formulas." URL `https://matthewwardrop.github.io/formulaic`.

Wickham H (2016). ***ggplot2**: Elegant Graphics for Data Analysis*. Springer-Verlag New York. ISBN 978-3-319-24277-4. URL `https://ggplot2.tidyverse.org`.

Wilkinson GN, Rogers CE (1973). "Symbolic Description of Factorial Models for Analysis of Variance." *Journal of the Royal Statistical Society. Series C (Applied Statistics)*, **22**(3), 392–399. ISSN 00359254, 14679876. URL `http://www.jstor.org/stable/2346786`.

A. Tensor context

In both **BKTR** packages we created modules called `tensor_ops` containing an object named `TSR`. The goal of `TSR` it to be able to centralize all tensor operations and properties in one object. This way, if in the future we needed to fix an operation or wanted to integrate another tensor operation backend like **tensorflow** (Abadi *et al.* 2015), we could do it at a central location. Since we wanted to be able to use kernels and the `BKTRRegressor` independently, we decided to set the tensor environment directly with the `TSR` object via the `set_params` method.

One of the few issue that we met with this implementation was that we were not able to use the equivalent of Python's `classmethods` and class properties with the **R6** package. Therefore, we decided to opt for a singleton design pattern to keep only one `TSR` instance with one setting alive at a time inside the R environment. To use this design pattern, we found that the **R6P** package (Lustiger 2022) was a sound implementation of it and thus decided to add it in our dependencies.

B. Covariates reshaping

With spatiotemporal data, it is not rare to observe datasets where the spatial covariates are not varying through time and where the temporal covariates are not varying through space. It is notably the case for the BIXI data of Section 6. When such a case arise, we often see that the dataset is expressed in a much more compressed manner. Effectively, when facing this setup, we can reformulate `data_df` into three matrices. The first matrix being the response variable that we call `y_df` which can be of shape $M \times N$, the spatial covariates matrix that we can call `spatial_df` having p_s spatial features and M locations with a shape of $M \times p_s$, and finally the temporal covariates with p_t temporal features and N time points with a shape of $N \times p_t$. Using those three data frames, we can create a `data_df` containing $MN \times (1 + p_s + p_t)$ and we can achieve that with few operations, repeating the matrices a certain number of times and stacking them together. However, it is possible to achieve that in a simpler manner using the `reshape_covariate_dfs` utility functions that we implemented. This function takes the three above-mentioned data frames as arguments and another argument called `y_column_name` denoting what is the desired column name for the response variable in the `y_df` data frame. With all those parameters provided, the `reshape_covariate_dfs` function will return a single data frame containing the information of the 3 data frames combined. Let see an example in action of this function using the BIXI dataset.

```
R> spatial_df <- bixi_data$spatial_features_df
R> temporal_df <- bixi_data$temporal_features_df
R> y_df <- bixi_data$departure_df
R> p_s <- ncol(spatial_df) - 1 # Not counting index column
R> p_t <- ncol(temporal_df) - 1
R> sprintf('Response M=%d and N=%d', nrow(y_df), ncol(y_df))
R> sprintf('Spatial features M=%d x p_s=%d', nrow(spatial_df), p_s)
R> sprintf('Temporal features N=%d x p_t=%d', nrow(temporal_df), p_t)
R> data_df <- reshape_covariate_dfs(spatial_df, temporal_df,
+    y_df, 'nb_departure')
```

```
R> sprintf('Should obtain MN=%d x P=%d', nrow(spatial_df) *
+    nrow(temporal_df), 1 + p_s + p_t)
R> sprintf('Reshaped MN=%d x P=%d', nrow(data_df), ncol(data_df) - 2)

[1] "Response M=587 and N=197"
[1] "Spatial features M=587 x p_s=13"
[1] "Temporal features N=196 x p_t=5"
[1] "Should see MN=115052 x P=19"
[1] "Reshaped MN=115052 x P=19"
```

C. Spatial coordinates projection

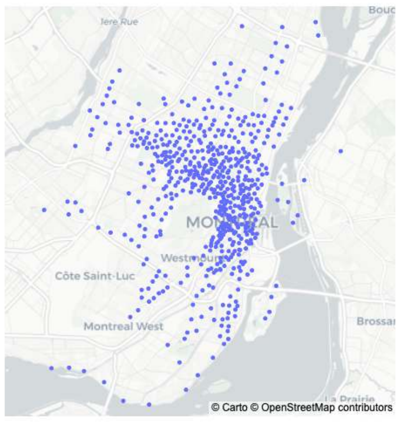
By default, a vast quantity of geographic tools use longitude and latitude measurements. Since those values represent angles on earth from the meridian and equator, we need to transform them into coordinates that can be projected in a Euclidean space. This is needed to ensure that we keep valid kernels for the MCMC sampling process. One of the simple forms of projection used on a multitude of maps is the Mercator projection (Snyder 1987). This type of projection allows to transform longitude and latitude in a 2D space by projecting them on a plane. By doing so, the coordinates become simple x and y coordinates on a map that can be drawn on a paper. This however comes with some limitations. To transform a sphere into a plane, the Mercator projection greatly distorts the size of areas that are far from the equator. To be able to do this cylindrical projection, the projection also needs to have a cutting point, which is usually the meridian. This means that even if two points are close but are located on different side of the meridian, they will appear to be extremely far on a Mercator projections.

The above-mentioned limitations can have important impacts on some datasets. However, when using coordinates that are very close to each others (e.g., at a city level) like in Section 6, those limitations become negligible. Therefore, we implemented a way to seamlessly transform by default, with a Mercator projection, all longitude and latitude coordinates provided to the `BKTRRegressor` class. When projecting the coordinates in a 2D plane, we allow the user to choose a given scale at which they want the projection to be done. This scale S^p is used to transform all provided coordinates into a square with a domain for the X and Y coordinates of $[-S^p/2, S^p/2]$. Knowing the scale in which the data was projected can help the user choosing sensible values for kernel lengthscale afterward. To help visualize the projection, we compare an example of the Mercator projected data for the BIXI dataset with a plot of the respective geographic coordinates (longitude, latitude) from Plotly Technologies Inc. (2015) using open street map. The comparison is shown is shown in Figure 9 for a scaling parameter of $S^p = 10$.

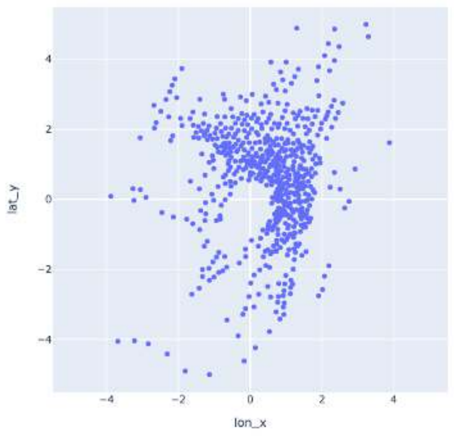
The figure show that the position property of the points are similar in both cases, but in the **BKTR** mercator's projection it is now located in on a X and Y axis having ranges of 10.

Affiliation:

Julien Lanthier, Aurélie Labbe
Department of Decision Sciences



(a) Plotly OpenStreetMap scatterbox plot on latitude and longitude



(b) Mercator projection with a scale factor of $S^p = 10$

Figure 9: Visualization comparison between Plotly OpenStreetMap scatter box plot and **BKTR** Mercator's projection for BIXI spatial locations.

HEC Montréal
3000, chemin de la Côte-Sainte-Catherine
Montréal (Québec), Canada H3T 2A7
E-mail: julien.lanthier@hec.ca, aurelie.labbe@hec.ca

Mengying Lei, Lijun Sun
Department of Civil Engineering
McGill University
817 Sherbrooke Street West, Macdonald Engineering Building
Montréal (Québec), Canada H3A 0C3
E-mail: mengying.lei@mail.mcgill.ca, lijun.sun@mcgill.ca