An R Package for Spatio-Temporal Change of Support

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Abstract

Spatio-temporal change of support (STCOS) methods are designed for statistical inference and prediction on spatial and/or temporal domains which differ from the domains on which the data were observed. Bradley, Wikle, and Holan (2015; Stat) introduced a parsimonious class of Bayesian hierarchical spatio-temporal models for STCOS for Gaussian data through a motivating application involving the American Community Survey (ACS), an ongoing survey administered by the U.S. Census Bureau that measures key socioeconomic and demographic variables for various populations in the United States. Importantly, their methodology provides ACS data-users a principled approach to estimating variables of interest, along with associated measures of uncertainty, on customized geographies and/or time periods. In this work, we develop an R package to make the methodology broadly accessible to federal statistical agencies, such as the Census Bureau, the ACS data-user community, and to the general R-user community. The package is illustrated through a detailed case-study based on real data.

Keywords: American Community Survey, Basis Functions, Bayesian, Change of Support, Spatio-Temporal.

1. Introduction

The American Community Survey (ACS) is an ongoing survey administered by the U.S. Census Bureau for the purpose of measuring key socioeconomic and demographic variables for the U.S. population. Public-use ACS data are available through the American FactFinder website [http://factfinder.census.gov] dating back to the year 2005. Estimates have historically been released for 1-year, 3-year, or 5-year periods; 3-year period estimates were discontinued after 2013. The Census Bureau releases annual ACS period estimates for a variety of geographies including states, counties, census tracts, and school districts. At their finest geography, ACS data are released at the census block-group level; however, estimates for an area are suppressed unless the area meets certain criteria. For example, an area must typically have a population of at least 65,000 for 1-year estimates to be released, but there is no population requirement for 5-year estimates [U.S. Census Bureau 2016].
Because statistical agencies like the Census Bureau have direct access to the confidential microdata, special tabulations for new geographies or period lengths can be prepared internally as needed. However, data users outside of the Census Bureau may be interested in custom geographies and/or nonstandard time periods which are not provided by the agency. Spatio-temporal change of support (STCOS) methodology enables such users to compute model-based estimates for custom geographies and time periods using public-use ACS releases. Providing ACS data-users the tools to engage in STCOS has recently been identified as an important problem by a National Academy of Sciences (NAS) panel (National Academy of Sciences 2015). The STCOS methodology developed in Bradley, Wikle, and Holan (2015) makes use of spatio-temporal dependencies in the direct survey estimates (and also incorporates associated direct survey variance estimates) through a Bayesian hierarchical model. Estimates, predictions, and appropriate measures of uncertainty can be extracted from the fitted model.

STCOS methodology is not limited to applications involving ACS data, but was developed specifically with the ACS in mind. Other domain specific areas often encounter a need for prediction and/or inference on spatial and/or temporal supports that differ from the observed data. For example, spatial change of support (COS) arises in atmospheric science and oceanography (Wikle and Berliner 2005), water quality modeling (Rode et al. 2010), environmental health (Fuentes et al. 2006), and remote sensing (Nguyen, Cressie, and Braverman 2012), among others. See Gotway and Young (2002), Bradley et al. (2015), and the references therein for a review of the change of support literature.

The STCOS problem can be motivated by an illustration. We will take median household income as our variable of interest throughout this article. Suppose we would like to produce 3-year model-based estimates in Missouri congressional districts for the year 2015. Congressional districts are geographic regions which receive representation by an elected official in the U.S. House of Representatives and are determined by the redistricting process which is based on data from each decennial census. Geographies on which we want to produce estimates and predictions are referred to as target supports. Figure 1 displays the eight designated congressional districts in Missouri for the year 2015. Geographies on which direct estimates are available are used to fit the STCOS model and are referred to as source supports. For this illustration, we could take the source supports to be all 1-year, 3-year, and 5-year ACS releases for the counties within Missouri. Including available periods over a number of years allows the STCOS model, in this case, to find trends in both time and space, and make use of estimates which represent varying levels of granularity and sparseness. Figure 2 shows both direct estimates and associated variance estimates for Missouri in the year 2013. We notice that 1-year and 3-year period estimates have been suppressed for many counties. We emphasize that counties and congressional districts do not necessarily align, and the crux of the STCOS problem is to “translate” between the county-level observations and the congressional districts. The third type of support which must be discussed is the fine-level support; for this example we could consider the counties in Missouri, as defined in 2015, which are shown in Figure 1. The STCOS methodology works by translating each of the source supports to the fine-level support during the model fitting process. Once the model has been fit, estimates and predictions on target supports of interest are obtained by translating from the fine-level support.

The Census Bureau does release ACS estimates on congressional districts, but releases of 3-year estimates for all geographies were discontinued after 2013.
The STCOS model has been fully specified by Bradley et al. (2015). However, many potential users, both subject-domain scientists and ACS data-users, will not have both the expertise and time to program the methodology for their use; e.g., see Weinberg et al. (2018). For this reason, we have developed the stcos package, a user-friendly and efficient R implementation of the STCOS model. The software takes source and fine-level supports as inputs, fits the STCOS Bayesian hierarchical model via Markov chain Monte Carlo (MCMC; Gibbs sampling), and produces estimates and predictions on target supports of interest.

The remainder of the article proceeds as follows. Section 2 reviews the STCOS model of Bradley et al. (2015). Note that some additional details are provided here, and some small variations have been made from the original formulation. Section 3 discusses the design of the stcos package at a high-level. Section 4 describes basic use of the package and introduces its main functions. Section 5 presents a small case study to produce model-based estimates of median household income for several neighborhoods in the City of Columbia in Boone County, Missouri; R code to carry out the analysis is shown in detail. Finally, Section 6 concludes the article. This article is intended to be largely self-contained for a wide range of readers; those eager to begin using the package can focus primarily on Sections 4 and 5. Readers interested in a larger-scale application of stcos may refer to Raim et al. (2017), which presents a model selection study using an earlier prototype version of the software. There, county-level ACS estimates are used to produce model-based estimates on congressional districts for the continental U.S. The stcos package itself is available on the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/package=stcos. The complete code for the City of Columbia analysis is provided in the inst/columbia/ directory of the stcos package sources.

2. The STCOS model

Let \( T = \{1, \ldots, T\} \) index the times for which direct estimates are available and \( L \) denote the set of all possible time periods. We will take \( T \) to consist of the years 2005 through 2017, corresponding to the ACS releases available during the preparation of this article, and \( L = \{1, 3, 5\} \) to denote 1-year, 3-year, and 5-year period releases. Data may not be released for all \((t, \ell) \in T \times L\); for example, ACS 3-year estimates were discontinued after 2013. Let \((T \times L)^*\) denote the subset of \( T \times L \) that corresponds to a data release. For each \((t, \ell) \in (T \times L)^*\), the associated source support \( D_{t\ell} \) is a collection of areal units whose estimates are included in the release. For each areal unit \( A \in D_{t\ell} \), \( z_{t\ell}(A) \) is the direct survey estimate for one survey variable of interest and \( \sigma_{t\ell}(A) \) is the corresponding variance estimate. We will write \( Z_{t\ell}(A) \) when considering the direct survey estimate as a random variable. The fine level support will be denoted \( D_B = \{B_1, \ldots, B_{n_B}\} \). The total surface area of a given areal unit \( A \) will be denoted \( |A| \).

The STCOS model is a Bayesian Hierarchical Model (Cressie and Wikle 2011) which can be described at a high level in three parts. Let \( N(\mu, \Sigma) \) denote a normal distribution with mean \( \mu \) and covariance matrix \( \Sigma \), and \( IG(a, b) \) denote an Inverse Gamma distribution with density \( f(x \mid a, b) = b^a x^{-a-1} e^{-b/x} / \Gamma(a) \). First, the data model is

\[
Z_{t\ell}(A) = Y_{t\ell}(A) + \varepsilon_{t\ell}(A),
\]

\( \varepsilon_{t\ell}(A) \) ind \( \sim \) \( N(0, \sigma_{t\ell}^2(A)) \),
for $A \in D_\ell$ and $(t, \ell) \in (\mathcal{T} \times \mathcal{L})^*$. Second, the process model is
\[ Y_{1t}^{(\ell)}(A) = h(A)\top \mu_B + \psi_{1t}^{(\ell)}(A)\top \eta + \xi_{1t}^{(\ell)}(A), \]
\[ \eta \mid \sigma_K^2 \sim \text{N}\left(0, \sigma_K^2 K\right), \]
\[ \xi_{1t}^{(\ell)}(A) \mid \sigma_\xi^2 \overset{\text{iid}}{\sim} \text{N}\left(0, \sigma_\xi^2\right), \]
for $A \in D_\ell$ and $(t, \ell) \in (\mathcal{T} \times \mathcal{L})^*$. Finally, the parameter model is
\[ \mu_B \sim \text{N}\left(0, \sigma_\mu^2 I\right), \]
\[ \sigma_\mu^2 \sim \text{IG}(a_\mu, b_\mu), \]
\[ \sigma_K^2 \sim \text{IG}(a_K, b_K), \]
\[ \sigma_\xi^2 \sim \text{IG}(a_\xi, b_\xi). \]

The STCOS model assumes that direct estimates $Z_{1t}^{(\ell)}(A)$ constitute a noisy observation of an underlying latent process $Y_{1t}^{(\ell)}(A)$. The variance of the noise $\varepsilon_{1t}^{(\ell)}(A)$ is assumed known and fixed as $\sigma^2_{1t}(A)$, the variance of the direct estimate. The mean of the latent process $Y_{1t}^{(\ell)}(A)$ consists of a coarse spatial trend $h(A)\top \mu_B$ and a spatio-temporal random process $\psi_{1t}^{(\ell)}(A)\top \eta$. Conjugate priors are assumed for the coefficients and variance parameters from the previous two stages. The matrix $K$, which provides the covariance structure for the random coefficient of $\eta$, is assumed to be known and is computable from the fine-level support. More explanation for each of these terms is given below.

The latent process model is motivated by the following construction. Define a continuous-space discrete-time process,
\[ Y(u; t) = \delta(u) + \sum_{j=1}^{\infty} \psi_j(u; t) \cdot \eta_j, \quad \text{for } u \in \bigcup_{i=1}^{n_B} B_i \text{ and } t \in \mathcal{T}, \]
where $\delta(u)$ is a large-scale spatial trend process and $\{\psi_j(u, t)\}_{j=1}^\infty$ is a prespecified set of spatio-temporal basis functions. Integrating $Y(u; t)$ uniformly over $u \in A$ and an $\ell$-year period,
\[ Y_{1t}^{(\ell)}(A) = \frac{1}{|A|} \int_A \delta(u) \, du + \frac{1}{|A|} \sum_{k=t-\ell+1}^t \sum_{j=1}^r \sum_{r=1}^\infty \int_A \psi_j(u; k) \cdot \eta_j \, du \]
\[ + \frac{1}{|A|} \sum_{k=t-\ell+1}^t \sum_{j=1}^r \sum_{r=1}^\infty \int_A \psi_j(u; k) \cdot \eta_j \, du \]
\[ = \mu(A) + \psi_{1t}^{(\ell)}(A)\top \eta + \xi_{1t}^{(\ell)}(A). \tag{2.1} \]

In (2.1), we have used the notation
\[ \mu(A) = \frac{1}{|A|} \int_A \delta(u) \, du, \tag{2.2} \]
\[ \psi_{1t}^{(\ell)}(A)\top \eta = \frac{1}{|A|} \sum_{k=t-\ell+1}^t \sum_{j=1}^r \sum_{r=1}^\infty \int_A \psi_j(u; k) \cdot \eta_j \, du, \tag{2.3} \]
\[ \xi_{1t}^{(\ell)}(A) = \frac{1}{|A|} \sum_{k=t-\ell+1}^t \sum_{j=1}^r \sum_{r=1}^\infty \int_A \psi_j(u; k) \cdot \eta_j \, du, \tag{2.4} \]
so that (2.2) represents a large-scale spatial trend, (2.3) is a spatio-temporal random process, and (2.4) is the remainder. We assume that \( \xi(A) \) is \( \sigma^2 \text{id} \sim N(0, \sigma^2) \), and make use of local bisquare basis functions for the small-scale spatio-temporal trend, which are of the form

\[
\psi_j(u, t) = \left[ 2 - \frac{\|u - c_j\|^2}{w_s^2} - \frac{|t - g_t|^2}{w_t^2} \right] \cdot I(\|u - c_j\| \leq \tilde{w}_s) \cdot I(|t - g_t| \leq w_t).
\]

These functions require specification of the number and location of spatial knot points \( c_j \), \( j = 1, \ldots, r_{\text{space}} \), the number and location of temporal knot points \( g_t \), \( t = 1, \ldots, r_{\text{time}} \), the spatial radius \( \tilde{w}_s \), and the temporal radius \( w_t \). We assume evenly spaced temporal knot points, and spatial knot points which are selected according to a space-filling design (Nychka and Saltzman 1998). It can be difficult to choose \( \tilde{w}_s \) directly; for example, the influence of \( \tilde{w}_s \) depends on the geographic units on which the supports are given. We therefore take \( \tilde{w}_s = w_s \cdot Q_{0.05} \), where \( Q_{0.05} \) is the 0.05 quantile of all nonzero pairwise distances between spatial cutpoints and \( w_s \) is a parameter to be selected by the user. See Raim et al. (2017) for a model selection study varying several factors in this model such as the number of knot points and the selection of \( w_s \) and \( w_t \).

Once the point-level basis functions are fully specified, we must evaluate the basis functions at the area level. For area \( A \) and an \( \ell \)-year period, we take a Monte Carlo approximation

\[
\psi_j^{(\ell)}(A) \approx \frac{1}{\ell Q} \sum_{k=\ell-\ell+1}^\ell \sum_{q=1}^Q \psi_j(u_q, k),
\]

using a random sample of locations \( u_1, \ldots, u_Q \) from a uniform distribution on the region \( A \). Next, for the large-scale spatial trend process, we make the simplifying assumption that

\[
\delta(u) = \sum_{i=1}^{n_B} \mu_i I(u \in A \cap B_i),
\]

for an area \( A \). Then, \( \delta(u) \) takes on a constant value on each overlap \( A \cap B_i \) for \( B_i \in D_B \).

Define

\[
h(A) = \left( \frac{|A \cap B_1|}{|A|}, \ldots, \frac{|A \cap B_{n_B}|}{|A|} \right)^\top
\]

as the vector of proportions in which \( A \) overlaps with each area \( B_i \) in the fine-level support; this is based on the geography, and is therefore a known quantity in the analysis. Geographies will be specified using shapefiles, as will be discussed in Sections 3 and 5. Modern software libraries, such as those available in R, can readily compute overlaps between areas represented in shapefiles. Now, integrating over \( u \in A \),

\[
\mu(A) = \frac{1}{|A|} \sum_{i=1}^{n_B} \int_{A \cap B_i} \delta(u) du = \frac{1}{|A|} \sum_{i=1}^{n_B} \mu_i \int_{A \cap B_i} du = \sum_{i=1}^{n_B} \mu_i \frac{|A \cap B_i|}{|A|} = h(A)^\top \mu_B.
\]

The coefficient \( \mu_B = (\mu_1, \ldots, \mu_{n_B})^\top \) represents the change-of-support coefficient between the fine-level support and all other supports, and is the primary quantity of interest in the model. To simplify the remaining presentation, we may now write the model in vector form. Suppose there are \( N \) total observations, indexed \( i = 1, \ldots, N \), in all of the source supports combined.
Let $\mathbf{H}$ be the mapping from each index $i$ to a triple $(A, t, \ell)$ consisting of the area $A$, time $t$, and period $\ell$ for the $i$th observation. Let vec$(S)$ denote that a vector is constructed from the elements of the ordered set $S$, Diag$(S)$ represent a diagonal matrix whose elements consist of $S$, and rbind$(S)$ represent a matrix with the elements of $S$ as rows. We may then write

$$ Z = \text{vec} \left( Z_i^{(t)}(A) : (A, t, \ell) = \mathcal{H}(i), \ i = 1, \ldots, N \right), $$

$$ H = \text{rbind} \left( h_i^{(t)}(A)^\top : (A, t, \ell) = \mathcal{H}(i), \ i = 1, \ldots, N \right), $$

$$ S = \text{rbind} \left( \psi_i^{(t)}(A)^\top : (A, t, \ell) = \mathcal{H}(i), \ i = 1, \ldots, N \right), $$

$$ \xi = \text{vec} \left( \xi_i^{(t)}(A) : (A, t, \ell) = \mathcal{H}(i), \ i = 1, \ldots, N \right), $$

$$ \varepsilon = \text{vec} \left( \varepsilon_i^{(t)}(A) : (A, t, \ell) = \mathcal{H}(i), \ i = 1, \ldots, N \right), $$

$$ V = \text{Diag} \left( \sigma_{\eta_i}^2(A) : (A, t, \ell) = \mathcal{H}(i), \ i = 1, \ldots, N \right), $$

(2.6)

where $h_i^{(t)}(A) = h(A)$ does not vary with $t$ or $\ell$. The STCOS model can now be written

$$ Z = H\mu_B + S\eta + \xi + \varepsilon, $$

$$ \varepsilon \sim N(0, V), \ \eta \mid \sigma_K^2 \sim N(0, \sigma_K^2 K), \ \xi \mid \sigma_\xi^2 \sim N(0, \sigma_\xi^2 I), $$

$$ \mu_B \mid \sigma_\mu^2 \sim N(0, \sigma_\mu^2 I), \ \sigma_\mu^2 \sim \text{IG}(a_\mu, b_\mu), \ \sigma_K^2 \sim \text{IG}(a_K, b_K), \ \sigma_\xi^2 \sim \text{IG}(a_\xi, b_\xi). $$

(2.7)

We now discuss specification of the matrix $K$. Let $I(\cdot)$ be the indicator function and $A \sim B$ be the predicate that area $A$ is adjacent to area $B$; $A \sim A$ is taken to be false by definition. We take $W = (w_{ij})$ to be a weight matrix based on adjacencies in $D_B$, with

$$ w_{ij} = \frac{I(A_i = A_j)}{\sum_{l=1}^{n_B} I(A_i = A_l)}, \ i, j \in \{1, \ldots, n_B\}. $$

The matrix $Q = I - \tau W$ corresponds to the precision matrix of a particular class of conditional autoregressive (CAR) process. We take $\tau \in (0, 1)$ to be known, for simplicity, to ensure that $Q$ is nonsingular. Other choices of $W$ and $Q$ can be considered to obtain other classes of CAR precision matrices as well (see Cressie and Wikle 2011, Carlin, Gelfand, and Banerjee 2014, and the references therein). For the purpose of specifying a spatio-temporal variance, suppose the fine-level support behaves according to the process

$$ Y^*_t = \mu_B + X\beta + \nu_t, $$

$$ \nu_t = M\nu_{t-1} + b_t, $$

$$ b_t \mid \sigma_K^2 \overset{iid}{\sim} N(0, \sigma_K^2 Q^{-1}), $$

(2.8)

for $t \in \mathcal{T}$. That is, $\{Y^*_t\}$ is a vector autoregressive (VAR) process in time and a CAR process in space. The matrix $X$ is only utilized in certain covariance structures, to be discussed shortly. Let $\Sigma_{y^*}$ denote the covariance matrix of $(Y^*_t : t \in \mathcal{T})$ under model (2.8). We take $K$ to be the minimizer of

$$ \| \Sigma_{y^*} - S^* CS^{*\top} \|_F, \text{ such that } C \text{ is an } r \times r \text{ positive semidefinite matrix,} $$

(2.9)

under the Frobenius norm $\| \cdot \|_F$, where $S^* = \text{rbind} \left( \psi_i^{(t)}(A)^\top : A \in D_B, t \in \mathcal{T}, \ell \in \mathcal{L} \right)$ is the basis function expansion on the fine-level geography. In (2.9), $\Sigma_{y^*}$ represents the desired
covariance structure under model (2.8), while \( S^*CS^*\top \) represents the covariance contribution of \( S\eta \) in the actual model (2.7), where
\[
\text{Var}(Y \mid \mu_B, \sigma^2_{\mu}, \sigma^2_\xi, \sigma^2_K) = \sigma^2_K S K S^\top + \sigma^2_\xi I,
\]
conditioning on random variables in the parameter model. The solution to (2.9),
\[
C^* = (S^*\top S^*)^{-1} S^*\top \Sigma_y^* S^* (S^*\top S^*)^{-1},
\]
provides the best positive approximant to \( \Sigma_y^* \); details are given in Appendix A. For the remainder of the article, we will take \( \Sigma_y^* \) to be positive definite and \( S^* \) to be full rank so that \( K \) is positive definite. Bradley et al. (2015) further discuss this approach within the context of the present model, and Higham (1988) discusses the positive approximant problem in the general setting. We may write \( \Sigma_y^* = \sigma^2_K \tilde{\Sigma}_y^* \) so that
\[
C^* = \sigma^2_K K,
\]
\( K = (S^*\top S^*)^{-1} S^*\top \tilde{\Sigma}_y^* S^* (S^*\top S^*)^{-1} \).

Notice that \( \tilde{\Sigma}_y^* \) and \( K \) are free of unknown parameters, and (2.9) does not need to be recomputed within MCMC iterations as parameter values are updated. We consider several possible structures for \( K \):

1. **Independence**: Take \( K = I \) to assume no spatial or temporal covariance in \( \eta \).

2. **Spatial-only**: Let \( \Sigma_y^* = \sigma^2_K Q^{-1} \otimes I_T \), where \( \otimes \) represents the Kronecker product, so that no temporal covariance is assumed. With \( \Sigma_y^* = Q^{-1} \otimes I_T \), we proceed with \( K \) as in (2.10).

3. **Random Walk**: Take \( M = I \) so that the fine-level process defined in (2.8) is a vector random walk with nonstationary autocovariance function
\[
\Gamma(t + h, t) = \begin{cases} t\sigma^2_K Q^{-1} & \text{if } h \geq 0, \\ (t - |h|)\sigma^2_K Q^{-1} & \text{if } -t < h < 0. \end{cases}
\]
Letting \( \tilde{\Gamma}(t + h, t) = \sigma^{-2}_K \Gamma(t + h, t) \), which is free of \( \sigma^2_K \), and choosing
\[
\tilde{\Sigma}_y^* = \begin{bmatrix} \tilde{\Gamma}(1, 1) & \cdots & \tilde{\Gamma}(1, T) \\ \vdots & \ddots & \vdots \\ \tilde{\Gamma}(T, 1) & \cdots & \tilde{\Gamma}(T, T) \end{bmatrix}
\]
as the covariance of \( \{Y_t^*\} \), \( K \) is obtained from (2.10) to be
\[
K = (S^*\top S^*)^{-1} \sum_{i=1}^T \sum_{j=1}^T \min(i, j) S_i^*\top Q^{-1} S_j^* (S^*\top S^*)^{-1},
\]
where we define \( S_t^* = \text{rbind} \left( \psi_t^{(\ell)}(A)^\top : A \in D_B, \ell \in \mathcal{L} \right) \) for each \( t \in \mathcal{T} \).
4. Moran’s I Basis: Appendix A of [Bradley et al., 2015] suggests computing the propagator matrix \( M \) using a Moran’s I basis. Let \( \Theta \) be a given real-valued \( r \times r \) matrix and \( P_\perp^X = I - X(X^T X)^{-1} X^T \) be a projection to the space orthogonal to the column space of \( X \). A Moran’s I basis can be constructed using

\[
G_{\Theta}(X) = P_\perp^X \Theta P_\perp^X.
\]

We take \( \Theta = I \) for the stcos package, as suggested by Bradley et al. (2015), to obtain \( G_{\Theta}(X) = P_\perp^X \). With this choice, the columns of \( M \) are taken to be the eigenvectors of \( G_{\Theta}(X) \). Now (2.8) is a VAR(1) process, whose autocovariance function is

\[
\Gamma(h) = \begin{cases} 
M^h \Gamma(0) & \text{if } h \geq 0 \\
(M^{-h} \Gamma(0))^\top & \text{otherwise.}
\end{cases}
\]

Our solution (2.10) to minimization problem (2.9) becomes

\[
K = (S^* S)^{-1} \left( \begin{array}{ccc}
\Gamma(0) & \cdots & \Gamma(1-T)
\end{array} \right) \left( \begin{array}{c}
S_1^*
\end{array} \right) \\
\vdots & \ddots & \vdots \\
\Gamma(T-1) & \cdots & \Gamma(T-1)
\end{array} \right) (S^* S)^{-1}
\]

\[
= (S^* S)^{-1} \left[ \sum_{i=1}^T \sum_{j=1}^T S_i^T \Gamma(i-j) S_j^* \right] (S^* S)^{-1}.
\]

Appendix A discusses efficient computation of \( \Gamma(0) \) when its dimension is large.

We assume by default that \( X \) is computed from a space-only bisquare basis expansion of the form

\[
\psi_j(u) = \left[ 1 - \frac{\|u - c_j\|^2}{\tilde{w}_s^2} \right] \cdot I(\|u - c_j\| \leq \tilde{w}_s),
\]

which is aggregated to the area level in a similar manner to (2.5). As with the spatio-temporal bisquare basis, we take \( \tilde{w}_s = w_s \cdot Q_{0.05} \), where \( Q_{0.05} \) is the 0.05 quantile of all nonzero pairwise distances between cutpoints and \( w_s \) is selected by the user. Alternatively, the user can directly specify a custom design matrix for \( X \), which must have the same number of rows as \( S^* \).

It is worth noting once more that descriptions such as “independence” and “spatial-only” are used to describe possible covariance structures for \( \eta \), but do not necessarily convey their covariance contribution to the model through \( Y \), which comes via \( SKS^\top \). For example, an independence assumption for \( \eta \) yields \( SKS^\top = SS^\top \), which is not a diagonal matrix because our chosen system of basis functions is not orthogonal.

We can obtain a Gibbs sampler by considering the joint distribution of (2.7):

\[
f(z, \eta, \xi, \mu_B, \sigma^2_\mu, \sigma^2_K, \sigma^2_\xi) \\
= N(z \mid H \mu_B + S \eta + \xi, V) \cdot N(\xi \mid 0, \sigma^2_\xi I) \cdot N(\eta \mid 0, \sigma^2_K I) \\
\times N(\mu_B \mid 0, \sigma^2_\mu I) \cdot IG(\sigma^2_\mu \mid a_\mu, b_\mu) \cdot IG(\sigma^2_K \mid a_K, b_K) \cdot IG(\sigma^2_\xi \mid a_\xi, b_\xi).
\]
Algorithm 2.1 Gibbs sampler steps for STCOS model.

1. Draw $[\mu_B | \--] \sim N(\vartheta_\mu, \Omega_{\mu}^{-1})$,
   \[ \vartheta_\mu = \Omega_{\mu}^{-1} H^T V^{-1} (z - S \eta - \xi), \quad \Omega_{\mu} = H^T V^{-1} H + \sigma^{-2}_\mu I. \]

2. Draw $[\eta | \--] \sim N(\vartheta_\eta, \Omega_{\eta}^{-1})$,
   \[ \vartheta_\eta = \Omega_{\eta}^{-1} S^T V^{-1} (z - H \mu_B - \xi), \quad \Omega_{\eta} = S^T V^{-1} S + \sigma_K^{-2} K^{-1}. \]

3. Draw $[\xi | \--] \sim N(\vartheta_\xi, \Omega_{\xi}^{-1})$,
   \[ \vartheta_\xi = \Omega_{\xi}^{-1} V^{-1} (z - H \mu_B - S \eta), \quad \Omega_{\xi}^{-1} = V^{-1} + \sigma^{-2}_\xi I. \]

4. Draw $[\sigma^2_\mu | \--] \sim IG(a^*_\mu, b^*_\mu)$, $a^*_\mu = a_\mu + n_B/2$ and $b^*_\mu = b_\mu + \mu_B^T \mu_B/2$.

5. Draw $[\sigma^2_K | \--] \sim IG(a^*_K, b^*_K)$, $a^*_K = a_K + r/2$ and $b^*_K = b_K + \eta^T K^{-1} \eta/2$.

6. Draw $[\sigma^2_\xi | \--] \sim IG(a^*_\xi, b^*_\xi)$, $a^*_\xi = a_\xi + N/2$ and $b^*_\xi = b_\xi + \xi^T \xi/2$.

It is routine to derive the full conditional distributions of $\mu_B$, $\eta$, $\xi$, $\sigma^2_\mu$, $\sigma^2_K$, and $\sigma^2_\xi$; details are omitted for brevity. The steps of the Gibbs sampler which result from the full conditionals are stated as Algorithm 2.1. The notation $[W | \--]$ is used to denote the distribution of the random variable $W$ conditioned on all other random quantities.

3. Package design

The stcos package serves three major roles in carrying out an STCOS data analysis. The first role is preprocessing, in which we convert spatio-temporal data into the quantities $z$, $V$, $H$, $S$, and $K^{-1}$ which are needed to fit the model. The second role is to actually fit the model by running the Gibbs sampler outlined in Algorithm 2.1. The final role is postprocessing, in which estimates and predictions are made on target supports using draws from the sampler. Preprocessing must be carried out once for a given set of source supports and a corresponding fine-level support. If multiple variables are of interest, the model must be refit for each; however, preprocessing need not be repeated so long as the geography is not changed. Postprocessing is then carried out for each target support of interest.

The stcos package benefits from a number of other R packages, most importantly the sf package by Pebesma (2018), which facilitates working with geographical data in R. Source, fine-level, and target supports are input to stcos in the form of sf objects. In this article, we assume that outputs are also desired as sf objects to facilitate plotting and further geographical processing.

Internally, the stcos package uses the R6 package (Chang 2017) to implement a stronger form of object-oriented programming than the more standard S3 or S4 methods. Users of the stcos package will interact with two major classes—SpaceTimeBisquareBasis and STCOSPrep—
which have been implemented via \texttt{R6}; these will be described in the next section. Bisquare basis function computations are carried out in \texttt{C++}, for efficiency, via the \texttt{Rcpp} and \texttt{RcppArmadillo} packages (Eddelbuettel 2013; Eddelbuettel and Sanderson 2014). Matrices such as \( H \) and \( S \) can have a large number of zeros; therefore, we use the \texttt{Matrix} package (Bates and Maechler 2017) to support operations on sparse matrices. The \texttt{fields} package (Nychka et al. 2015) provides functionality to select spatial knot points using a space-filling design. The \texttt{dplyr} package (Wickham et al. 2019) and \texttt{ggplot2} package (Wickham 2016) are not directly used by the \texttt{stcos} package, but provide convenient platforms for users to manipulate data in \texttt{sf} objects and produce high quality graphics from them, respectively.

4. Basic use of the software

We will now outline the major functions in the \texttt{stcos} package. In Section 5, we will provide a small example showing the functions in action. We will assume that the following essential packages are loaded.

\begin{verbatim}
R> library("sf")
R> library("fields")
R> library("stcos")
\end{verbatim}

Source, fine-level, and target supports must be specified as \texttt{sf} objects. Source supports should have direct estimates and their associated variance estimates embedded into them. An example of a prepared source support object is as follows:

\begin{verbatim}
R> head(acs5_2013, 3)
Simple feature collection with 3 features and 8 fields
geometry type: POLYGON
dimension: XY
bbox: xmin: -10280140 ymin: 4712766 xmax: -10277220 ymax: 4714750
epsg (SRID): 3857
proj4string: +proj=merc +a=6378137 +b=6378137 +lat_ts=0.0 +lon_0=0.0
+x_0=0.0 +y_0=0 +k=1.0 +units=m +nadgrids=@null +wktext
+no_defs
geoid state county tract blockgroup DirectEst DirectMOE DirectVar
1 290190005001 29 019 000500 1 9970 3157 3683788
2 290190005002 29 019 000500 2 12083 7048 18360194
3 290190006001 29 019 000600 1 105156 16979 106553987

geometry
1 POLYGON ((-10278231 4713772...
2 POLYGON ((-10279369 4713339...
3 POLYGON ((-10280135 4712926...
\end{verbatim}

The \texttt{epsg} and \texttt{proj4string} descriptors specify the projection of the data; e.g., see Bivand, Pebesma, and Gómez-Rubio (2013, Chapter 4). The \texttt{stcos} package requires that all supports

\footnote{We have manipulated this output and some subsequent outputs to ensure that they fit on the page.}
for an analysis have a common projection; this should not be a limitation, as the user may transform an sf object from its original projection using the function sf::st_transform. The last four lines of the previous display show a table with nine fields, where each row corresponds to an area (county) in the file. The geometry field contains details about the county’s geography, which we typically will not want to manipulate directly. The fields STATE and COUNTY represent Federal Information Processing Standards (FIPS) codes for the state and county respectively, and GEO_ID is an identifier which combines the two. The fields DirectEst, DirectMOE, and DirectVar represent direct ACS estimates of median household income and associated direct variance estimates; these columns were not present in the shapefile originally and were augmented when preparing the analysis.

The R6 class SpaceTimeBisquareBasis encapsulates the local space-time bisquare basis functions discussed in Section 2.

```r
R> basis <- SpaceTimeBisquareBasis$new(knot.x, knot.y, knot.t, w.s, w.t)
```

The vectors knot.x, knot.y, and knot.t represent longitude, latitude, and time coordinates of each knot point, and w.s and w.t represent space and time radii for each of those points. Note that w.s represents \( w_s \), which is internally transformed to \( \tilde{w}_s = w_s \cdot Q_{0.05} \) as mentioned in Section 2. The new function is a constructor which creates the object basis. The basis object has a compute method which evaluates the bisquare basis function for given coordinates \((x, y, t)\), but users will typically not need to interact with it directly.

The R6 class STCOSPrep is primarily responsible for building the quantities \( z, V, H, S, \) and \( K^{-1} \) from sf objects. An STCOSPrep object is constructed with our basis object, our fine-level domain, the name of a unique identifier (the fine_domain_geo_name argument) in the fine-level domain object, and the number of Monte Carlo repetitions to use when computing the basis function at area level (the basis_mc_reps argument).

```r
R> sp <- STCOSPrep$new(fine_domain = dom.fine,  
    fine_domain_geo_name = "GEO_ID",  
    basis = basis, basis_mc_reps = 500)
```

Each source support is to be supplied to the add_obs method in the sp object. We must specify the relevant period for each source support; for example, the 2013 5-year estimates are based on the years 2009:2013. We must also specify the names of the fields which contain the direct estimates (the estimate_name argument), their associated variance estimates (the variance_name argument), and a unique identifier for geographic areas (the geo_name argument).

```r
R> sp$add_obs(acs5_2013, period = 2009:2013, estimate_name = "DirectEst",  
    variance_name = "DirectVar", geo_name = "GEO_ID")
```

Once all source supports have been added, we can retrieve quantities needed for the Gibbs sampler.

```r
z <- sp$get_z()  
v <- sp$get_v()  
H <- sp$get_H()  
S <- sp$get_S()
```
Here, $v$ is a vector which contains the diagonal elements of $V$; otherwise, $z$, $H$, and $S$ correspond directly to $z$, $H$, and $S$ from the notation. The design matrix $S$ computed from the bisquare basis function can have a large number of columns with a high degree of multicollinearity. If not addressed, this can lead to poor mixing of the Gibbs sampler and slow processing times for each step. A dimension reduction function for $S$ can be specified to the sp object via its set_basis_reduction member function.

```r
R> f <- function(S) { ... }
R> sp$set_basis_reduction(f)
R> S.reduced <- sp$get_reduced_S()
```

Here, a dimension-reduced $S$ is requested via the get_reduced_S function. Recall that the computation of $K^{-1}$ requires a similar matrix $S^*$, which should have the same dimension reduction applied to it; this is why sp requires knowledge of the reduction method.

The matrix $K^{-1}$ may be computed using one of the prescribed methods from Section 2.

```r
R> K.inv <- sp$get_Kinv(2009:2017, method = "independence") # Independence
R> K.inv <- sp$get_Kinv(2009:2017, method = "car") # Spatial only
R> K.inv <- sp$get_Kinv(2009:2017, method = "randomwalk") # Random Walk
R> K.inv <- sp$get_Kinv(2009:2017, method = "moran") # Moran's I
```

We provide a function to compute maximum likelihood estimates (MLEs), which can serve as a good initial value for the Gibbs sampler. Details are given in Appendix A; the function is invoked as follows.

```r
R> mle.out <- mle.stcos(z, v, H, S.reduced, K.inv)
R> init <- list(sig2K = mle.out$sig2K.hat, sig2xi = mle.out$sig2xi.hat, 
+ mu_B = mle.out$mu.hat)
```

The gibbs.stcos and gibbs.stcos.raw function run the Gibbs sampler; the former extracts relevant quantities from an object of the STCOSPrep class, which may be slightly more convenient, while the latter allows all quantities to be input individually.

```r
R> gibbs.out <- gibbs.stcos.raw(z, v, H, S.reduced, K.inv, 
+ R = 10000, report.period = 1000, burn = 1000, thin = 10, 
+ init = init)
R> gibbs.out <- gibbs.stcos(sp, R, report.period = 1000, 
+ burn = 1000, thin = 10)
```

When the Gibbs sampler is complete, saved draws can be accessed.

```r
R> mu_B.mcmc <- gibbs.out$mu_B.hist
R> eta.mcmc <- gibbs.out$eta.hist
R> xi.mcmc <- gibbs.out$xi.hist
R> sig2mu.mcmc <- gibbs.out$sig2mu.hist
R> sig2xi.mcmc <- gibbs.out$sig2xi.hist
R> sig2K.mcmc <- gibbs.out$sig2K.hist
```
Suppose $\tilde{H}$ and $\tilde{S}$ are versions of the overlap design matrix and (dimension-reduced) basis design matrix, respectively, computed from either the source supports or from target supports of interest. Draws of the posterior distribution of the mean function

$$E(Y \mid \mu_B, \eta) = \tilde{H}\mu_B + \tilde{S}\eta,$$

can be computed using the `fitted` function, and draws from the posterior predictive distribution of $Y$,

$$\int N(y \mid \tilde{H}\mu_B + \tilde{S}\eta, \sigma^2 I) f(\mu_B, \eta, \sigma^2_I, \mid z, V) d\mu_B d\eta d\sigma^2_I,$$

can be computed using the `predict` function.

R> E.mcmc <- fitted(gibbs.out, H.tilde, S.tilde)
R> Y.mcmc <- predict(gibbs.out, H.tilde, S.tilde)

5. Data analysis example: City of Columbia

We now demonstrate use of the `stcos` package on a small-scale but real example. Here, we are given four neighborhoods in the City of Columbia in Boone County, Missouri to use as the target support. We would like to produce model-based 5-year estimates of median household income using observed 5-year ACS estimates from recent years. Specifically, we will consider 5-year ACS estimates at the block-group level for years 2013–2017 as our source supports, and will produce 5-year ACS estimates for year 2017 on the four neighborhoods as our target support. A shapefile of the four neighborhoods has been provided by staff from the GIS Office for the City of Columbia.

5.1. Preparing the data

The purpose of this section is to prepare an `sf` object augmented with our direct estimates and associated variance estimates; this will serve as the primary source of data for the analysis. Datasets produced in this manner for the Columbia example are provided in the `stcos` package for convenience. Readers who are eager to move on to the analysis may skip to the next section.

We will make use of the `sf` and `dplyr` packages, so let us first load them.

R> library("sf")
R> library("dplyr")

We now load the shapefile representing the target support and transform it to a projection of choice.

R> neighbs <- st_read("neighborhoods.shp") %>% st_transform(crs = 3857)

To prepare the source supports, we need to obtain ACS estimates and corresponding shapefiles. For this example, ACS estimates can be requested from the Census Bureau’s Data API.

[https://www.census.gov/data/developers/guidance/api-user-guide.html](https://www.census.gov/data/developers/guidance/api-user-guide.html) Up-to-date instructions on use of the API can be found here.
Estimates for our source supports are requested from the API by constructing URLs with the following formats.

```r
R> est_url <- paste('https://api.census.gov/data/', year, 
+ '/acs/acs5?get=NAME,B19013_001E&for=block%20group:*&in=state:29+county:019', 
+ sep = '')
R> moe_url <- paste('https://api.census.gov/data/', year, 
+ '/acs/acs5?get=NAME,B19013_001M&for=block%20group:*&in=state:29+county:019', 
+ sep = '')
```

Note that the FIPS code for Missouri is 29 and the code for Boone County is 019. The variable B19013_001E represents direct estimates for “Median household income in the past 12 months”, and B19013_001M represents the corresponding margins of error (MOEs). Data on the two variables are gathered using two separate calls to the API. We can request the years of interest by taking `year` to be values 2013 through 2017. We use the `jsonlite` package \cite{ooms2014} to call the API and load the results into an R `data.frame`.

```r
R> json_data <- jsonlite::fromJSON(est_url)
R> est_dat <- data.frame(json_data[-1,])
R> colnames(est_dat) <- json_data[1,]

R> json_data <- jsonlite::fromJSON(moe_url )
R> moe_dat <- data.frame(json_data[-1,])
R> colnames(moe_dat) <- json_data[1,]
```

We now merge `est_dat` and `moe_dat` into a single `data.frame`.

```r
R> my_dat <- est_dat %>%
+   inner_join(moe_dat, by = c('state' = 'state', 'county' = 'county',
+                             'tract' = 'tract', 'block group' = 'block group')) %>%
+   select(state, county, tract, blockgroup = 'block group',
+          DirectEst = B19013_001E, DirectMOE = B19013_001M) %>%
+   mutate(state = as.character(state)) %>%
+   mutate(county = as.character(county)) %>%
+   mutate(tract = as.character(tract)) %>%
+   mutate(blockgroup = as.character(blockgroup)) %>%
+   mutate(DirectEst = as.numeric(as.character(DirectEst))) %>%
+   mutate(DirectMOE = as.numeric(as.character(DirectMOE))) %>%
+   mutate(DirectEst = replace(DirectEst, DirectEst < 0, NA)) %>%
+   mutate(DirectMOE = replace(DirectMOE, DirectMOE < 0, NA)) %>%
+   mutate(DirectVar = (DirectMOE / qnorm(0.95))^2) %>%
+   arrange(tract, blockgroup)
```

There are a few details to mention in this data manipulation. We have taken some care because there is a space in the variable name `block group`, and because variables in the

\[\text{https://api.census.gov/data/2015/acs5/variables.html}\]
ACS data are interpreted as factors by default. We have transformed the MOE to a variance estimate, noting that MOEs are to be interpreted as margins of error from $\alpha = 0.90$ confidence intervals; i.e.,

$$\text{MOE} = z_{\alpha/2} \sqrt{\hat{V}} \iff \hat{V} = \left( \frac{\text{MOE}}{z_{\alpha/2}} \right)^2,$$

where $z_{\alpha/2} \approx 1.645$. We have also taken care to handle special values coded in the data; namely, large negative numbers for estimates and MOEs are returned by the API when estimates are not available, which we convert to NA. We sort the entries by tract and block group for readability. The resulting data.frame for 2017 appears as follows.

```r
R> head(my_dat)

   state county tract blockgroup DirectEst DirectMOE DirectVar
1    29    019     000200          1   41063      6512  15673799
2    29    019     000200          2   31250      6978  17997303
3    29    019     000300          1   19420      7643  21591022
4    29    019     000300          2     NA        NA        NA
5    29    019     000300          3   21369     14558  78333750
6    29    019     000500          1   10995      5563  11438356
```

The `tigris` package (Walker 2018) provides a convenient way to request shapefiles from the Census Bureau Tiger/Line database. It is necessary that all supports are projected to a common coordinate system for the `stcos` package, so we transform to match the projection we used in the target support.

```r
R> my_shp <- tigris::block_groups(state = '29', county = '019',
+   year = 2017) %>%
+   st_as_sf() %>%
+   st_transform(crs = 3857)
```

Now we augment the shapefile with the direct estimates, MOEs, and variance estimates obtained earlier.

```r
R> acs5_2017 <- my_shp %>%
+   inner_join(my_dat, by = c('STATEFP' = 'state', 'COUNTYFP' = 'county',
+     'TRACTCE' = 'tract', 'BLKGRPCE' = 'blockgroup')) %>%
+   select(geoid = GEOID, state = STATEFP, county = COUNTYFP,
+     tract = TRACTCE, blockgroup = BLKGRPCE,
+     DirectEst, DirectMOE, DirectVar) %>%
+   filter(!is.na(DirectEst))
```

---

4 [https://www.census.gov/content/dam/Census/programs-surveys/acs/guidance/training-presentations/20170419_MOE.pdf](https://www.census.gov/content/dam/Census/programs-surveys/acs/guidance/training-presentations/20170419_MOE.pdf)

5 [https://census.gov/data/developers/data-sets/acs-1year/notes-on-acs-estimate-and-annotation-values.html](https://census.gov/data/developers/data-sets/acs-1year/notes-on-acs-estimate-and-annotation-values.html)
The filter step drops several block groups where no estimates are present in the ACS data note that different block groups may be missing in different years of ACS estimates. The resulting \texttt{acs5\_2017} is an object of type \texttt{sf}, whose first few entries are as follows.

\begin{verbatim}
R> head(acs5_2017)

Simple feature collection with 6 features and 8 fields
genometry type: POLYGON
dimension: XY
bbox: xmin: -10280690 ymin: 4712766 xmax: -10256290 ymax: 4752109
epsg (SRID): 3857
proj4string: +proj=merc +a=6378137 +b=6378137 +lat_ts=0.0 +lon_0=0.0 +x_0=0.0 +y_0=0 +k=1.0 +units=m +nadgrids=@null +wktext +no_defs
gtoid state county tract blockgroup DirectEst DirectMOE DirectVar
1 290190005001 29 019 000500 1 10995 5563 11438356
2 290190005002 29 019 000500 2 13872 9503 33378510
3 290190006001 29 019 000600 1 45208 39073 564285643
4 290190006002 29 019 000600 2 107500 19868 145899495
5 290190020002 29 019 002000 2 62237 13529 6765141
6 290190020003 29 019 002000 3 51019 11166 46082999
\end{verbatim}

Finally, we must designate a fine-level support for the analysis. Here we will use the block group level geography for Boone County from 2017.

\begin{verbatim}
R> dom.fine <- tigris::block_groups(state = '29', county = '019',
+ year = 2017) %>%
+ st_as_sf() %>%
+ st_transform(crs = 3857) %>%
+ mutate(geoid = GEOID) %>%
+ select(-GEOID)
\end{verbatim}

5.2. Running the analysis

After completing the steps in the previous section, inputs are prepared as \texttt{sf} objects. Datasets for this example are provided in the \texttt{stcos} package for convenience, and are listed below.

\begin{verbatim}
R> data("acs_sf")
R> ls(pattern = "acs5\_.*")

[1] "acs5\_2013" "acs5\_2014" "acs5\_2015" "acs5\_2016" "acs5\_2017"
\end{verbatim}

\begin{verbatim}
R> data("columbia\_neighbs")
R> ls(pattern = "columbia")
\end{verbatim}

\footnote{This was done for readability in the article. The full example code, included in the supplemental materials, does not filter observations with missing estimates except during model fitting.}
To construct a bisquare basis, we must select spatio-temporal knot points. We choose the temporal knot points to be \{2009, 2009.5, \ldots, 2016.5, 2017\}, covering the years relevant to the 5-year ACS estimates for years 2013–2017.

\begin{verbatim}
R> knots.t <- seq(2009, 2017, by = 0.5)
\end{verbatim}

To select spatial knot points, we first draw a large number of points uniformly over the fine-level domain using the \texttt{st_sample} function. We then use the \texttt{cover.design} function in the \texttt{fields} package, which finds a subset of these points to fill the space.

\begin{verbatim}
R> u <- st_sample(dom.fine, size = 2000)
R> M <- matrix(unlist(u), length(u), 2, byrow = TRUE)
R> out <- fields::cover.design(M, 500)
R> knots.sp <- out$design
\end{verbatim}

Now we use the \texttt{merge} function in the \texttt{base} package to perform a Cartesian join between the spatial and temporal knots, which yields the set of spatio-temporal knots.

\begin{verbatim}
R> knots <- merge(knots.sp, knots.t)
\end{verbatim}

Finally, we create a \texttt{SpaceTimeBisquareBasis} by specifying the knots, along with the radii \(w_s = 1\) and \(w_t = 1\). This is where the \texttt{stcos} package is first used.

\begin{verbatim}
R> library("stcos")
R> basis <- SpaceTimeBisquareBasis$new(knots[,1], knots[,2], knots[,3],
+ w.s = 1, w.t = 1)
\end{verbatim}

Figure 3 illustrates the selected basis functions.

We now create an \texttt{STCOSPrep} object, which will process the supports—which we have encoded as \texttt{sf} objects—into matrices and vectors which can be used in the Gibbs sampler. The \texttt{STCOSPrep} constructor requires a fine-level domain and \texttt{SpaceTimeBisquareBasis}.

We specify that \texttt{geoid} is the field which uniquely identifies geographic areas, and that 500 Monte Carlo repetitions are desired when computing the area level basis functions.

\begin{verbatim}
R> sp <- STCOSPrep$new(fine_domain = dom.fine, fine_domain_geo_name = "geoid",
+ basis = basis, basis_mc_reps = 500)
\end{verbatim}

We now add each of the source supports using the \texttt{add_obs} member function. For each source support, we specify the corresponding five year period, that the field \texttt{DirectEst} contains the direct estimates, that the field \texttt{DirectVar} contains the associated variance estimates, and that the field \texttt{geoid} serves as a unique identifier of geographic areas.
Some of the quantities needed to carry out the MCMC can now be retrieved.

```r
R> z <- sp$get_z()
R> v <- sp$get_v()
R> H <- sp$get_H()
R> S <- sp$get_S()
```

We take a simple principal components analysis (PCA) approach to select a small number of orthogonal columns of $S$.

```r
R> eig <- eigen(t(S) %*% S)
R> rho <- eig$values
R> idx.S <- which(cumsum(rho) / sum(rho) < 0.65)
R> Tx.S <- t(eig$vectors[idx.S,])
R> f <- function(S) { S %*% Tx.S }
R> sp$set_basis_reduction(f)
R> S.reduced <- sp$get_reduced_S()
```

For this example, we have selected the eigenvectors of $S^T S$ which contain 65% of the variability, as quantified by the eigenvalues. Figure 4 shows a plot of the eigenvalue proportions in rho.

```r
R> plot(cumsum(rho[1:200]) / sum(rho), xlab = "Dimension",
      + ylab = "Proportion of Variance")
R> abline(v = max(idx.S))
```

For this example, we will compute $K$ using the independence structure.

```r
R> K.inv <- sp$get_Kinv(2009:2017, method = "independence")
```

In our experience, standardizing the estimates in $z$ helps to improve convergence of the chains created by the Gibbs sampler. We make a corresponding transformation to the variance estimates in $v$.

```r
R> z.scaled <- (z - mean(z)) / sd(z)
R> v.scaled <- v / var(z)
```

For this example, we will provide arbitrary starting values for the Gibbs sampler.
Now we proceed to run the Gibbs sampler; we will run the sampler for 10,000 iterations, discard the first 2,000 draws, and keep one of every 10th remaining draw.

```r
R> gibbs.out <- gibbs.stcos.raw(z.scaled, v.scaled, H, S.reduced, K.inv, + R = 10000, report.period = 2000, burn = 2000, thin = 10, init = init)
R> print(gibbs.out)
```

```
2019-03-28 03:34:02 - Begin Gibbs sampler
2019-03-28 03:34:23 - Begin iteration 2000
2019-03-28 03:34:41 - Begin iteration 4000
2019-03-28 03:34:59 - Begin iteration 6000
2019-03-28 03:35:17 - Begin iteration 8000
2019-03-28 03:35:35 - Begin iteration 10000
2019-03-28 03:35:35 - Finished Gibbs sampler
> print(gibbs.out)
Fit for STCOS model
--
  Mean   SD  2.5%  25%  75%  97.5%
sig2mu 0.52405868 0.08931173 0.37494278 0.46245894 0.57491347 0.73027365
  sig2K  0.58972074 0.35955998 0.22558199 0.36080642 0.69641633 1.61360290
  sig2xi 0.04330695 0.00505916 0.03450108 0.03981828 0.04653151 0.05478935
--
Saved 800 draws
DIC: 213.127049
Elapsed time: 00:01:30
```

We use the `mcmc` construct in the `coda` package (Plummer, Best, Cowles, and Vines 2006) to help manage and plot the draws.

```r
R> library("coda")
R> sig2mu.mcmc <- mcmc(gibbs.out$sig2mu.hist)
R> sig2xi.mcmc <- mcmc(gibbs.out$sig2xi.hist)
R> sig2K.mcmc <- mcmc(gibbs.out$sig2K.hist)
```

Figure 5 displays trace and density plots of the variance components $\sigma_\mu^2$, $\sigma_\xi^2$, and $\sigma_K^2$.

### 5.3. Postprocessing the results

Using the fitted model, we can produce model-based estimates on target supports of interest. In this example, we would like to produce 5-year 2017 estimates for our four neighborhoods in Boone County: Central, East, North, and Paris. The following code computes model-based estimates for these areas and embeds them into the `neighbs` object for plotting.

```r
R> targ.neighbs <- sp$domain2model(neighbs, period = 2013:2017, + geo_name = "Region")
```
R> E.hat.scaled <- fitted(gibbs.out, targ.neighbs$H, targ.neighbs$S.reduced)
R> E.hat <- sd(z) * E.hat.scaled + mean(z)
R> neighbs$E.median <- apply(E.hat, 2, median)
R> neighbs$E.moe <- apply(E.hat, 2, sd) * qnorm(0.95)
R> neighbs$E.mean <- apply(E.hat, 2, mean)
R> neighbs$E.sd <- apply(E.hat, 2, sd)
R> neighbs$E.lo <- apply(E.hat, 2, quantile, prob = 0.05)
R> neighbs$E.hi <- apply(E.hat, 2, quantile, prob = 0.95)

The function domain2model produces \( H \) and \( S \) design matrices based on the geography of the neighbs object. The fitted function produces draws from the posterior distribution of the mean. The third line in the previous code display transforms the estimates back to the original scale—recall that the direct estimates were centered and scaled before model fitting. From the fourth line on, we summarize draws of the posterior mean in several ways, obtaining a model-based estimate of its median, mean, standard deviation, MOE (\( z_{\alpha/2} \times \) standard deviation), and a 90% credible interval. We can verify that these estimates have been augmented into the neighbs sf object.

R> print(neighbs)

Simple feature collection with 4 features and 7 fields
geometry type: POLYGON
dimension: XY
bbox: xmin: -10280270 ymin: 4715036 xmax: -10269750 ymax: 4723860
epsg (SRID): 3857
proj4string: +proj=merc +a=6378137 +b=6378137 +lat_ts=0.0 +lon_0=0.0 +x_0=0.0 +y_0=0 +k=1.0 +units=m +nadgrids=@null +wktext +no_defs

| Region  | geometry | E.mean | E.sd | E.lo |
|---------|----------|--------|------|------|
| Central | POLYGON  | 26743.07 | 1898.417 | 23599.55 |
| East    | POLYGON  | 44275.00 | 2553.565 | 40295.96 |
| North   | POLYGON  | 44545.87 | 2855.929 | 39889.87 |
| Paris   | POLYGON  | 20772.18 | 3840.388 | 14329.24 |

We are now ready to plot our estimates. The code to reproduce our plots is somewhat lengthy and therefore is included in the supplemental materials. First we compare direct and model-based estimates for 2017 source supports to assess whether the model fit is reasonable. Figures 6a and 6b show maps of the two sets of estimates. Figures 6c and 6d compare the two sets of estimates via scatter plots; year 2014 and year 2017 estimates are shown for comparison. Variation between direct and model-based estimates appears to be smaller for year 2014, with the exception of the block group with the largest direct estimate that year. Finally, Figure 7 shows the four neighborhoods of our target support in the context of the 2017
5-year direct estimates. This provides a visual aid to assess plausibility of the target support estimates. The North and East neighborhoods appear to be in the immediate vicinity of block groups with higher median household income than the West and Paris neighborhoods.

6. Conclusions

This article introduced the \texttt{stcos} R package for spatio-temporal change of support analysis, which is now available on CRAN. We worked through a small but complete example to estimate median household income in several neighborhoods in the City of Columbia in Boone County, MO. Many of the more involved aspects of STCOS methodology are encapsulated in the package, but a fair amount of programming work is still required by the end user to carry out an analysis. The R code for the City of Columbia example is provided in the supplementary materials, and should serve as a template for a complete analysis.

We hope that this software empowers users to explore official statistics on custom geographies and time periods. However, this work represents just one step in making spatial and spatio-temporal methodologies accessible to users of official statistics. Future efforts may involve improvements to the package for efficiency and usability, as well as software support for other methods in this active area.

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Figure 1: The state of Missouri in 2015. Thin lines mark boundaries between the 114 counties and one independent city. Shaded areas with thick lines mark the eight congressional districts.
Figure 2: County-level ACS data for median household income in Missouri for the year 2013. The left column shows direct estimates and the right column displays standard errors. The first, second, and third rows correspond to 1-year, 3-year, and 5-year period estimates, respectively. Public ACS estimates were not available for areas with white shading.
Figure 3: Spatial knot points selected for spatio-temporal basis function. The red dots indicate knot points and the blue circle displays the spatial radius of $w_s = 1$ at one particular knot point.

Figure 4: Plot of the eigenvalues of $S^T S$. The vertical line shows that 5 eigenvectors are needed to capture 65% of the variation. The y-axis has been truncated to maintain visibility for small dimensions; the total number of eigenvalues is 7,500.
Figure 5: Trace and density plots for draws of the variance components $\sigma^2_\mu$, $\sigma^2_\xi$, and $\sigma^2_K$ from the Gibbs sampler.
Figure 6: Comparison of direct and model-based ACS 5-year estimates. Figures (a) and (b) show maps based on the two estimates for year 2017. Figures (c) and (d) show scatter plots comparing the two sets of estimates for years 2014 and 2017 respectively.
Region | Median | MOE | Mean | SD | CI Lo | CI Hi
--- | --- | --- | --- | --- | --- | ---
Central | 26,791.66 | 3,122.62 | 26,743.07 | 1,898.42 | 23,599.55 | 29,909.43
East | 44,207.41 | 4,200.24 | 44,275.00 | 2,553.57 | 40,295.96 | 48,270.73
North | 44,579.62 | 4,697.59 | 44,545.87 | 2,855.93 | 39,889.87 | 49,067.62
Paris | 20,857.98 | 6,316.88 | 20,772.18 | 3,840.39 | 14,329.24 | 26,787.44

(a) Estimates based on STCOS model.

(b) Map of 2017 5-year direct estimates.

Figure 7: Model-based ACS 5-year estimates for the Central, East, North, and Paris neighborhoods in year 2017 are shown in Table 7a. Figure 7b shows the locations of the four neighborhoods (shaded in black), and year 2017 direct 5-year estimates in Boone County block groups for comparison. Direct estimates were not available for block groups marked as “Missing”, which are shaded white.
A. Computational details and proofs

We will make use of the following well-known property in several places.

**Property A.1.** If $A \in \mathbb{R}^{m \times k}$, $B \in \mathbb{R}^{k \times l}$, $C \in \mathbb{R}^{l \times n}$, then $\text{vec}(ABC) = (C^T \otimes A)\text{vec}(B)$.

The following proposition gives the explicit solution to the minimization problem stated in (2.9). See [Higham (1988)] for a more general discussion on problems involving Frobenius and 2-norm distance minimization.

**Proposition A.2 (Frobenius Norm Minimization).** Suppose $S \in \mathbb{R}^{n \times r}$ has rank $r$ and $\Sigma \in \mathbb{R}^{n \times n}$. The minimizer $X \in \mathbb{R}^{r \times r}$ of $\|\Sigma - SXS^T\|_F$ is $X = (S^T S)^{-1}S^T \Sigma S(S^T S)^{-1}$.

**Proof.** We have

$$\|\Sigma - SXS^T\|_F^2 = \text{vec}\left[(\Sigma - SXS^T)^T\right]\text{vec}\left[(\Sigma - SXS^T)\right]$$

$$= \left[\text{vec}(\Sigma) - \text{vec}(SX^T)\right]^T \left[\text{vec}(\Sigma) - \text{vec}(SX^T)\right]$$

$$= \left[\text{vec}(\Sigma) - (S \otimes S)\text{vec}(X)\right]^T \left[\text{vec}(\Sigma) - (S \otimes S)\text{vec}(X)\right]$$

$$= \|\text{vec}(\Sigma) - (S \otimes S)\text{vec}(X)\|_2^2, \quad (A.1)$$

where the norm on the last line is the usual 2-norm on $\mathbb{R}^{n^2}$. We recognize the expression in (A.1) as a standard least squares minimization whose solution is

$$\text{vec}(X) = [(S \otimes S)^T(S \otimes S)]^{-1}(S \otimes S)^T\text{vec}(\Sigma)$$

$$= [(S^T \otimes S^T)(S \otimes S)]^{-1}(S^T \otimes S^T)\text{vec}(\Sigma)$$

$$= [S^T S \otimes S^T S]^{-1}\text{vec}(S^T \Sigma S)$$

$$= [(S^T S)^{-1} \otimes (S^T S)^{-1}]\text{vec}(S^T \Sigma S)$$

$$= \text{vec}\left[(S^T S)^{-1}S^T \Sigma S(S^T S)^{-1}\right].$$

Therefore, the minimizer is $X = (S^T S)^{-1}S^T \Sigma S(S^T S)^{-1}$, as desired. 

**Remark A.3 (MLE Computation).** To compute the MLE for the STCOS model, we first note that the likelihood, excluding the parameter model, is

$$f(z \mid \mu_B, \sigma_K^2, \sigma^2_B) = \int N(z \mid H \mu_B + S\eta, \sigma^2_B I + V) \cdot N(\eta \mid 0, \sigma^2_K K) d\eta$$

$$= N(z \mid H \mu_B, \Delta)$$

$$= (2\pi)^{-N/2}|\Delta|^{-1/2}\exp\left\{-\frac{1}{2}(z - H\mu_B)^T \Delta^{-1}(z - H\mu_B)\right\},$$

where $\Delta = \sigma^2_B I + V + \sigma^2_K SKS^T$. Given $\sigma^2_K$ and $\sigma^2_B$, the likelihood is maximized by the weighted least squares estimator $\hat{\mu}_B = (H^T \Delta^{-1}H)^{-1}H^T \Delta^{-1}z$. To estimate the unknown $\sigma^2_K$ and $\sigma^2_B$, we carry out numerical maximization on the partially maximized log-likelihood

$$\ell(\sigma^2_K, \sigma^2_B) = -\frac{N}{2} \log(2\pi) - \frac{1}{2} \log |\Delta| - \frac{1}{2}(z - H\mu_B)^T \Delta^{-1}(z - H\mu_B).$$

To enforce the constraints that $\sigma^2_K > 0$ and $\sigma^2_B > 0$, we optimize over $(\phi_1, \phi_2) \in \mathbb{R}^2$ and take $\sigma^2_K = \exp(\phi_1)$, $\sigma^2_B = \exp(\phi_2)$.
Suppose now that
\[ Y_t = A Y_{t-1} + \varepsilon_t, \quad \varepsilon_t \sim N(0, \Sigma) \]
is an \( m \)-dimensional VAR(1) process. The usual computation of \( \Gamma(0) = \mathbb{E}(Y_t Y_t^\top) \),
\[
\text{vec}(\Gamma(0)) = [I - A \otimes A]^{-1} \text{vec}(\Sigma), \quad (A.2)
\]
requires the solution of an \( m^2 \times m^2 \) linear system, which is infeasible for large \( m \). The following proposition gives an equivalent expression that only requires multiplying \( m \times m \) matrices. Let \( \mathcal{M}(\cdot) \) denote the operator that rearranges an \( m^2 \times 1 \) vector \( x = (x_1^\top, \ldots, x_m^\top)^\top \) into the \( m \times m \) matrix \((x_1 \cdots x_m)^\top\). Also, let \( A \circ B \) denote the elementwise (Hadamard) product between \( m \times n \) matrices \( A \) and \( B \).

**Proposition A.4** (Computational Form for VAR(1) Autocovariance). Suppose \( A = V \text{Diag}(\lambda) V^{-1} \), where the columns of \( V \) are the eigenvectors of \( A \) and \( \lambda \) is a vector of the corresponding eigenvalues. Then the solution of
\[
\Gamma(0) - A \Gamma(0) A^\top = \Sigma \quad (A.3)
\]
is
\[
\Gamma(0) = V \cdot \mathcal{M} \left( \text{Diag}(\Omega) \circ \text{vec}(V^{-1} \Sigma V^{-\top}) \right) \cdot V^\top
\]
where \( \Omega = \text{Diag}(1 - \lambda \otimes \lambda)^{-1} \).

**Proof.** Recall that the usual solution to (A.3) is given by (A.2). Note that \( V \otimes V \) are the eigenvectors of \( A \otimes A \), with the corresponding vector of eigenvalues \( \lambda \otimes \lambda \). For any matrix \( B \) with an eigenvector \( v \), \( Bv = \theta v \) implies that \( (I - B)v = (1 - \theta)v \). Therefore, we may write
\[
\text{vec}(\Gamma(0)) = [I - A \otimes A]^{-1} \text{vec}(\Sigma) = [(V \otimes V) \text{Diag}(1 - \lambda \otimes \lambda)(V \otimes V)^{-1}]^{-1} \text{vec}(\Sigma) = (V \otimes V) \Omega \cdot \text{vec}(V^{-1} \Sigma V^{-\top}) = \text{vec} \left\{ V \left[ \text{Diag}(\Omega) \circ \text{vec}(V^{-1} \Sigma V^{-\top}) \right] V^\top \right\}.
\]
The result is obtained by applying \( \mathcal{M}(\cdot) \) to both sides. \( \square \)

Note that if \( A \) is a symmetric matrix, then \( V \) is orthogonal and the result simplifies to
\[
\Gamma(0) = V \cdot \mathcal{M} \left( \text{Diag}(\Omega) \circ \text{vec}(V^\top \Sigma V) \right) \cdot V^\top,
\]
so that no matrix inverse needs to be computed.
Spatio-Temporal Change of Support

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