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stgam: An R package for GAM-based varying coefficient models

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DOI: 10.xxxxxx/draft

Software

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Editor: Open Journals

Reviewers:

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Submitted: 01 January 1970
Published: unpublished

Summary

Very often we are interested in quantifying how and where statistical relationships vary over space, and how they change over time. Quantifying such *process heterogeneity* (spatial and or temporal) can be done using *varying coefficient* models. Our ability to undertake such space-time analyses is enhanced by the increased production and availability of data describing a wide range of phenomenon that include both spatial and temporal attributes in the form of GPS coordinates and time-stamps. The `stgam` package provides a framework for creating regression models using Generalized Additive Models (GAMs) (Hastie & Tibshirani, 1990) in which the relationships between the response (dependent) variable and individual predictor (independent) variables are allowed to vary over space, time or both, in order to create spatially, temporally or spatio-temporally varying coefficient models. However a key question is what form of space-time interaction should be specified in our statistical models? Most current approaches require this to be specified in advance, frequently randomly guessed have to be made about the form of the relationship until an effective model form and associated model fits are found. To address this the `stgam` package includes functions to create multiple models, each specifying different relationships between the response variable y and the predictor variables $x_1 \ldots x_n$. Each model is evaluated by using the Bayesian Information Criterion (BIC) (Schwarz, 1978) to approximate the likelihood (probability) of the model being the correct model given the data used in the analysis. Where multiple models are highly probable, then these can be be combined using a Bayesian Model Averaging approach (Brunsdon et al., 2023; Fragoso et al., 2018). Finally the `stgam` package contains functions for creating the spatially and / or temporally varying regression coefficient estimates, which can be mapped in the usual way to show how where and when the relationships between the response and the predictor variables vary over space and time.

Statement of need

A number approaches have been established to quantify process spatial non-stationarity or heterogeneity (Brunsdon et al., 1996; Casetti, 1972; Fotheringham et al., 2002; Gelfand et al., 2003; Griffith, 2008; Jones, 1991; McMillen, 1996) and tools also exist to quantify the *temporal* dynamics of these (Crespo et al., 2007; Di Giacinto, 2006; Elhorst, 2003; Gelfand et al., 2004; Huang et al., 2010; Pace et al., 1998, 2000). All existing models require the user to make decisions about the nature of the space-time relationships in the data and thus the model and assume the presence of latent spatial and temporal autocorrelation in variables. The most commonly used approach in geographical analyses of space-time problems is geographically and temporally weighted regression (GTWR) (Huang et al., 2010) which seeks to optimises a single space-time kernel to define the space-time relationships of all covariates with the target variable. Some recent steps in the right direction have been taken in this regard: Liu et al. (2017) developed a semi-parametric temporal extension to mixed geographically weighted

regression, in which some relationships and coefficients are assumed to be globally constant and others vary locally over time; Hong et al. (2021) used a bootstrap approach to identify global coefficients in such models, but still define the same space-time relationship for each varying covariate.

To address this gap, the `stgam` package provides a wrapper for varying coefficient modelling using the `mgcv` GAM package (S. N. Wood, 2017). GAMs are able to handle many kinds of responses (Fahrmeir et al., 2021). They generate multiple model terms which are added together and provide an intuitive approach to fit relatively complex relationships in data with complex interactions and non-linearities (S. N. Wood, 2017). The outputs of GAMs provide readily understood summaries of the relationship between predictor and response variables and how the outcome is modelled. They are able to predict well from complex systems, quantify relationships, and make inferences about these relationships, such as which variables are important and at what range of values they are most influential (Hastie & Tibshirani, 1990; S. N. Wood, 2017). GAMs can perform as well as or better than most machine learning models and they are relatively fast (Friedman, 2001; S. N. Wood, 2017). Importantly, in the context of varying coefficient modelling, GAMs combine predictive power, model accuracy and model transparency and generate "*intrinsically understandable white-box machine learning models that provide a technically equivalent, but ethically more acceptable alternative to [machine learning] black-box models*" (Zschech et al., 2022, p. p2). Through this approach one could replace a *black box* with a *glass box*. GAMs model non-linear relationships using smooths, also referred to as splines. These can be of different forms depending on the problem and data (Hastie & Tibshirani, 1990) and, as they can be represented as linear combinations of basis functions, they are sometimes referred to as Gaussian Process (GP) splines. Thus GP-splines are represented as a linear combination of non-linear *basis functions* of predictor variables, which can generate predictions of the outcome variable. Basis functions can be either single or multi-dimensional in terms of predictor variables. As a result, a GAM consists of linear sums of multi-dimensional basis functions that allow complex relationships to be modelled. The appropriate degree of "wiggliness" in each spline is determined by the smoothing parameters, which balances over-fitting versus capturing the complexity in the relationship.

GAMs with GP smooths parameterised with location and / or time can be used to construct regression models that allow coefficient estimates to vary, and thereby to capture process spatial and / or temporal heterogeneity using a varying coefficient approach. While spline-based varying coefficient models have been proposed before, for example using a generalized linear model with reduced-rank thin-plate splines (Fan & Huang, 2022), the approach used here is to consider the predictor-to-response relationship over space and time as a GP. A GP is a random process over functions, and its terms can be modelled using GP-splines within a GAM. Here low rank GP-splines parameterised with location, or with time or with both as GPs are flexible in specifying autocorrelation in spatially and / or temporally varying random functions (Williams & Rasmussen, 2006), and GP-based smoothing using observations at specific locations and time periods can identify any spatial and temporal trends in the data.

A final consideration is the need to determine model form. Consider the aim to construct a spatially and temporally varying coefficient model from a number of covariates. Standard approaches, in absence of a theoretical model, assume that some degree of spatial and temporal dependence *is* present in the data and in the relationship of each covariate with the target variable. In the GAM GP smooth approach, each covariate would be specified in a SP smooth parameterised with location and with time under the assumption that any temporal trends in coefficient estimates *will* vary with location. However, each can be specified in six different ways: it can be omitted, included as a parametric (global) term, in a smooth with location, in a smooth with time, in a smooth with location *and* time, or in two separate space and time smooths. The last five options similarly apply to the intercept.

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Package overview

The `stgam` package contains functions to support varying coefficient modelling using GAMs with GP smooths, that provide a wrapper for the GAM implementation in the `mgcv` package (S. Wood, 2015), that create, evaluate, and aggregate multiple models. It also contains two datasets that are used to illustrate the functions. These are described in Table **??**.

Table 1: Spatial models currently implemented in **geostan**.

Name	Type	Description
calculate_vcs	function	Extracts varying coefficient estimates (for SVC, TVC and STVC)
do_bma	function	Undertakes coefficient averaging using Bayesian Model Averaging (B
evaluate_models	function	Creates and evaluates multiple varying coefficient GAM GP smooth r
gam_model_probs	function	Calculates the model probabilities of the different GAM models gene
plot_1d_smooth	function	Plots a 1-Dimensional GAM smooth
plot_2d_smooth	function	Plots a 2-Dimensional GAM smooth
productivity	data	US States Economic Productivity Data (1970-1985)
us_data	data	US States boundaries

The package includes two vignettes, the first of which provides a gentle introduction to undertaking varying coefficient regression analyses with GAMs via the `mgcv` package:

```
{r eval = F, echo = T} vignette("space-time-gam-intro", package = "stgam")
```

The second vignette describes a standard `stgam` workflow to create and evaluate multiple models, and then to either select the best one or to combine competing models using Bayesian Model Averaging.

```
{r eval = F, echo = T} vignette("space-time-gam-model-probs-BMA", package =
"stgam")
```

Worked example

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