varycoef: An R Package for Gaussian Process-based Spatially Varying Coefficient Models

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Abstract

Gaussian processes (GPs) are well-known tools for modeling dependent data with applications in spatial statistics, time series analysis, or econometrics. In this article, we present the R package **varycoef** that implements estimation, prediction, and variable selection of linear models with spatially varying coefficients (SVC) defined by GPs, so called GP-based SVC models. Such models offer a high degree of flexibility while being relatively easy to interpret. Using **varycoef**, we show versatile applications of (spatially) varying coefficient models on spatial and time series data. This includes model and coefficient estimation with predictions and variable selection. The package uses state-of-the-art computational statistics techniques like parallelization, model-based optimization, and covariance tapering. This allows the user to work with (S)VC models in a computationally efficient manner, i.e., model estimation on large data sets is possible in a feasible amount of time.

Keywords: covariance tapering, dependent data, model-based optimization, spatial statistics, (penalized) maximum likelihood estimation, variable selection.

1. Introduction

Spatially varying coefficients (SVC) provide a flexible and interpretable approach to extend linear models to spatial data. There are various methodologies on how to estimate and make predictions for SVC models. To name a few, geographically weighted regression (GWR) introduced by Brunsdon, Fotheringham, and Charlton (1998) or Bayesian SVC processes by Gelfand, Kim, Sirmans, and Banerjee (2003) are popular examples. Today, there are several R packages and other software implementations for SVC modeling available; each with individual focuses in their respective framework. A thorough comparison between all

of them is beyond the scope of this work. Instead, we provide a rough outline of existing software implementations.

In R (R Core Team 2021), GWR has been implemented in packages like **GWmodel** (Gollini, Lu, Charlton, Brunsdon, and Harris 2015), **spgwr** (Bivand and Yu 2017), and **gwrr** (Wheeler 2013). A detailed comparison between those packages can be found in Gollini *et al.* (2015). Bayesian SVC modeling is implemented in the R packages **spTDyn** (Bakar, Kokic, and Jin 2016) and **spBayes** (Finley, Banerjee, and Gelfand 2015; Finley and Banerjee 2020). Both packages use Markov chain Monte Carlo (MCMC) sampling algorithms and are rather restricted in the number of observation locations. Another Bayesian method to estimate SVC models uses the explicit stochastic partial differential equation (SPDE, Lindgren, Rue, and Lindström 2011) link between Gaussian fields and Gaussian Markov random fields (GMRF, Rue and Held 2005). Using integrated nested Laplace approximation (INLA) implemented in the R package **INLA** (Lindgren and Rue 2015), one can estimate SVC models for data sets with a large number of observations. However, the number of hyper parameters and therefore varying coefficients is limited (Rue, Riebler, Sørbye, Illian, Simpson, and Lindgren 2017). Finally, spatially varying coefficients can be modeled using splines. Available options include the packages **mgcv** (Wood 2017) and **mboost** (Hothorn, Bühlmann, Kneib, Schmid, and Hofner 2021). In other programming languages some of the above mentioned methodologies are available, too. For instance, the Python spatial analysis library **PySAL** (Rey and Anselin 2010) implements Bayesian SVC processes by Gelfand *et al.* (2003). GWR is also available in **PySAL** and geographic information system (GIS) software like ArcGIS or GRASS.

This article discusses SVC models where each coefficient is defined by a Gaussian process (GP, Rasmussen and Williams 2005), so called GP-based SVC models. The proposed model is similar to Bayesian SVC processes by Gelfand *et al.* (2003), but with some specific assumptions on the model, we can provide a computationally efficient way of estimating GP-based SVC models using a classical maximum likelihood estimation (MLE) approach (Dambon, Sigrist, and Furrer 2021b). Therefore, in contrast to all of the methodologies and software implementations above, the R package **varycoef** implements a frequentist approach for SVC modeling using Gaussian processes. Additionally, while all of the above SVC modeling implementations from above are either limited in the number of observations or spatially varying coefficients, **varycoef** has been developed for to work well with large data sets or a moderate number of varying coefficients. Over time, the methodology as well as the corresponding R package **varycoef** have been augmented continuously. For instance, the package now implements a joint variable selection procedure for GP-based SVC models (Dambon, Sigrist, and Furrer 2021a) using penalized maximum likelihood estimation (PMLE). Another new feature of **varycoef** is the support of different types of covariance functions and the idea of SVC models has been generalized to work different types of dependent data such as time series. The goal of this article is to present the current state of the package **varycoef** with its versatile applications.

The rest of this article is structured as follows. In Section 2 we introduce GP-based SVC models in their original form to be used by **varycoef**. Section 3 covers the MLE of GP-based SVC models including prediction methods. The variable selection using PMLE is discussed and showcased in Section 4. In particular, we move from a classical application using spatial data and show an application on time series data. Section 5 summarizes this work.

2. GP-based SVC Models

We commence with a formal introduction of Gaussian processes before extending the linear regression models to GP-based SVC models.

2.1. Gaussian Processes

Gaussian processes are widely used for modeling dependency structures. Applications can be found in – but are not limited to – spatial statistics (Gelfand and Schliep 2016; Banerjee, Gelfand, Finley, and Sang 2008; Datta, Banerjee, Finley, and Gelfand 2016), econometrics (Wu, Lobato, and Ghahramani 2014), and time series modeling (Roberts, Osborne, Ebden, Reece, Gibson, and Aigrain 2013). Similarly to a normal distribution, a GP is defined as an infinite-dimensional process with a mean function $\boldsymbol{\mu}$ and a covariance function c,

$$\boldsymbol{\mu}(\cdot) : D \to \mathbb{R},$$
$$c(\cdot, \cdot; \boldsymbol{\theta}) : D \times D \to [0, \infty),$$

for some domain $D \subset \mathbb{R}^d, d \geq 1$, and covariance parameters $\boldsymbol{\theta}$. In this work, we restrict ourselves to constant mean functions and isotropic covariance functions. That is, the covariance function is only depending on the distance of its arguments $u = \|\boldsymbol{s} - \boldsymbol{s}'\|$, where $\| \cdot \|$ denotes the Euclidean distance and $\boldsymbol{s}, \boldsymbol{s}' \in D$.

Popular examples of covariance functions are given by the Matérn or generalized Wendland covariance class. In the isotropic case, former one is defined as

$$c : [0, \infty) \to [0, \infty),$$
$$u \mapsto \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\sqrt{2\nu} \frac{u}{\rho} \right)^\nu K_\nu \left(\sqrt{2\nu} \frac{u}{\rho} \right), \tag{1}$$

where $\sigma^2 \geq 0$ is the variance, $\rho > 0$ is the range, $\nu > 0$ is the smoothness, and K_ν is the modified Bessel function of second kind and order ν. Setting the smoothness ν to some specific values simplifies the bulky formula of (1) to simple functions like the exponential $c(u) = \sigma^2 \exp(-u/\rho)$ for $\nu = 1/2$ or the squared exponential $c(u) = \sigma^2 \exp(-u^2/\rho)$ for $\nu = \infty$. We let the definition of the covariance function up to the user and only assume that the covariance parameters $\boldsymbol{\theta} := (\rho, \sigma^2)$ are unknown. Both are essential to interpret the estimated Gaussian process as the range ρ provides a measure of spatial dependence and the variance σ^2 gives the volatility of the Gaussian process. We provide examples of Gaussian processes defined by zero-means and different covariance functions of Matérn class. They are given on $[0, 10] \subset \mathbb{R}$, i.e., in $d = 1$ dimension. Throughout this article as well as in **varycoef**, we use the package **RandomFields** (Schlather, Malinowski, Menck, Oesting, and Strokorb 2015) to sample Gaussian processes. The two sampled processes are depicted in Figure 1.

2.2. Spatially Varying Coefficient Models

Let n be the number of observations and let p be the number covariates given by $\boldsymbol{x}^{(j)} := (x_1^{(j)}, ..., x_n^{(j)}) \in \mathbb{R}^n, j = 1, ..., p$. With the responses $\boldsymbol{y} = (y_1, ..., y_n) \in \mathbb{R}^n$, errors $\boldsymbol{\varepsilon} := (\varepsilon_1, ..., \varepsilon_n) \sim \mathcal{N}_n(\boldsymbol{0}, \tau^2 \mathbf{I}_n)$ where $\tau > 0$, and coefficients $\boldsymbol{\beta} = (\beta_1, ..., \beta_p) \in \mathbb{R}^p$ the linear model is given by:

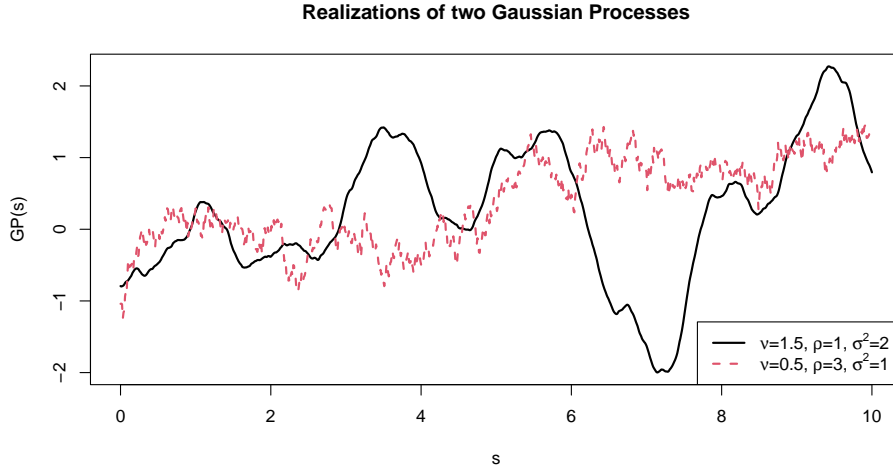$$y_i = \beta_1 x_i^{(1)} + ... + \beta_p x_i^{(p)} + \varepsilon_i.$$

Figure 1: Two zero-mean Gaussian processes with Matérn covariance functions and distinct parametrizations. The observation location s_i are defined equidistantly on $[0, 10] \subset \mathbb{R}$ with distance 0.01, i.e., $n = 1001$. One can clearly see the effects of the parameters ν, ρ, and σ^2 on the smoothness, the range of dependence, and the variance of the curves, respectively.

Spatially varying coefficient models generalize the linear model. In a classical context of regressing spatial data sets, one considers the observation locations $s_i \in D$ that are associated to each observed sample i. Here, one usually assumes $d = 2$ and that the observation locations s_i do not necessarily have to be distinct. A general SVC model is then given by:

$$y_i = \beta_1(s_i)x_i^{(1)} + ... + \beta_p(s_i)x_i^{(p)} + \varepsilon_i.$$

It is a this point where the above mentioned methodologies to estimate the SVC model differ depending on the assumption of the coefficients $\boldsymbol{\beta}_j(\cdot)$. In our case, we assume fixed effects μ_j and random effects $\boldsymbol{\eta}_j(\cdot)$ defined by zero-mean Gaussian processes with an isotropic covariance function $c_j(\cdot; \boldsymbol{\theta}_j)$ to model the spatial structures of the coefficients, i.e, we have $\boldsymbol{\beta}_j(\cdot) \approx \mu_j + \boldsymbol{\eta}_j(\cdot)$. Additionally, we assume prior mutual independence between all $\boldsymbol{\eta}_j(\cdot)$.

For a finite set of observations $\boldsymbol{s} = (\boldsymbol{s}_1, ..., \boldsymbol{s}_n)$ the Gaussian processes $\boldsymbol{\eta}_j(\cdot)$ from above reduce to zero-mean normal distributions. Therefore, we can write the GP-based SVC model as a linear mixed model:

$$\boldsymbol{y} = \mathbf{X}\boldsymbol{\mu} + \mathbf{W}\boldsymbol{\eta}(\boldsymbol{s}) + \boldsymbol{\varepsilon}. \tag{2}$$

The full derivation of (2) is given in Dambon *et al.* (2021b). In the resulting model, the first term on the right hand side is the data matrix $\mathbf{X} = (\boldsymbol{x}^{(1)}|...|\boldsymbol{x}^{(p)}) \in \mathbb{R}^{n \times p}$ associated with the fixed effects $\boldsymbol{\mu} = (\mu_1, ..., \mu_p)$. The random effects and its corresponding covariates are given in the second term. Not every fixed effect covariate $\boldsymbol{x}^{(j)}$ has to be associated with a random effect or vice versa. Therefore, we denote the q random effect covariates by $\boldsymbol{w}^{(k)} \in \mathbb{R}^n$ for $k = 1, ..., q$ and the data matrix $\mathbf{W} = (\text{diag }\boldsymbol{w}^{(1)}|...|\text{diag }\boldsymbol{w}^{(q)}) \in \mathbb{R}^{q \times nq}$. The random effects are contained in $\boldsymbol{\eta}(\boldsymbol{s}) \in \mathbb{R}^{nq}$ which is the sole component modeling the spatially varying relationship depending on the locations $\boldsymbol{s}$. Individual zero-mean spatially varying coefficients are defined as $\boldsymbol{\eta}_k(\cdot) \sim \mathcal{GP}(0, c_k(\cdot; \boldsymbol{\theta}_k))$. For observation locations $\boldsymbol{s}$, they reduce to a normal
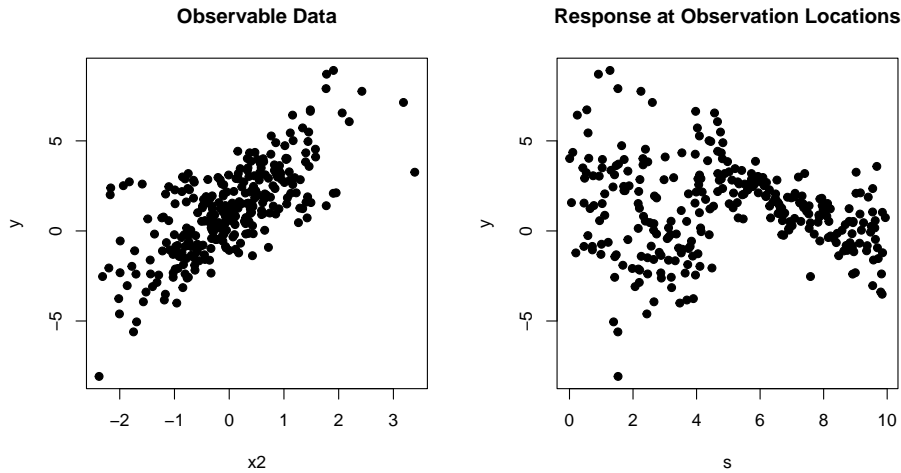
Figure 2: Sampled data using function `sample_fullSVC()` with spatially varying coefficients for the intercept $x^{(1)}$ and covariate $x^{(2)}$, respectively. Here, we only display the data without the true coefficients as latter ones are unknown in real world applications, too.

distribution with $\eta_k(s) \sim \mathcal{N}_n(\mathbf{0}, \Sigma_k)$, where $(\Sigma_k)_{lm} := c_k(\|s_l - s_m\|; \theta_k)$. The random effect $\eta(s)$ is the joint effect over all individual Gaussian processes, i.e., $\eta(s) = (\eta_1(s), ..., \eta_q(s)) \sim \mathcal{N}_{nq}(\mathbf{0}, \Sigma)$ with joint block covariance matrix $\Sigma = \text{diag}(\Sigma_1, ..., \Sigma_q)$. Finally, we add the errors ε, also called the nugget in spatial modeling.

Inspired by the example in Figure 1, we sample data under the assumption of an GP-based SVC model. The package **varycoef** provides the function `sample_fullSVC()` to sample data from a GP-based SVC model with observations on the real line, i.e., $d = 1$. In total we consider $n = 300$ observations with i.i.d. locations $s_i \sim \mathcal{U}([0, 10])$. It is called a full SVC model since each covariate is associated with a spatially varying coefficient, i.e., $p = q$ and $x^{(j)} = w^{(j)}$. Here, `sample_fullSVC()` gives an intercept $x^{(1)} = \mathbf{1}_n$ and $x^{(2)} \sim \mathcal{N}_n(\mathbf{0}_n, \mathbf{I}_{n \times n})$. The mean and covariance parameters are provided in the code below. The resulting data, i.e., the response y and the covariate $x^{(2)}$ are depicted in Figure 2.

```
R> library(varycoef)
R> set.seed(123)
R> # SVC parameters
R> df.pars <- data.frame(var = c(2, 1), scale = c(0.5, 1), mean = c(1, 2))
R> # nugget standard deviation
R> tau <- 0.5
R> # sample locations
R> n <- 300
R> s <- sort(runif(n, min = 0, max = 10))
R> # sample SVCs and data
R> SVCdata <- sample_fullSVC(
+    df.pars = df.pars, nugget.sd = tau, locs = s, cov.name = "mat32")
```

2.3. Optimization of Likelihood

Our goal is to estimate the parameters of interest $\boldsymbol{\omega} := (\boldsymbol{\theta}, \boldsymbol{\mu})$ with all covariance parameters given by $\boldsymbol{\theta} = (\rho_1, \sigma_1^2, ..., \rho_q, \sigma_q^2, \tau^2)$. We rely on maximum likelihood estimation, where the multivariate normal distribution and corresponding log-likelihood of the GP-based SVC model (2) is given by:

$$\mathbf{Y} \sim \mathcal{N}_n \left(\mathbf{X}\boldsymbol{\mu}, \boldsymbol{\Sigma}_\mathbf{Y}(\boldsymbol{\theta}) := \sum_{k=1}^{q} \left(\boldsymbol{w}^{(k)}\boldsymbol{w}^{(k)\top} \right) \odot \boldsymbol{\Sigma}_k + \tau^2 \mathbf{I}_{n\times n} \right), \tag{3}$$

$$\ell(\boldsymbol{\omega}) = -\frac{1}{2} \left(n \log(2\pi) + \log\det \boldsymbol{\Sigma}_\mathbf{Y}(\boldsymbol{\theta}) + (\boldsymbol{y} - \mathbf{X}\boldsymbol{\mu})^\top \boldsymbol{\Sigma}_\mathbf{Y}(\boldsymbol{\theta})^{-1} (\boldsymbol{y} - \mathbf{X}\boldsymbol{\mu}) \right). \tag{4}$$

3. Implementation of MLE

3.1. Control Parameters

Due to their high modularity, there are several components to define a GP-based SVC model as well as the respective MLE. Here, the function `SVC_mle_control()` sets several control parameters, which we go through step by step.

Covariance Function

The covariance functions c_k used to define $\boldsymbol{\Sigma}_k$ play a major role in the definition of the likelihood, i.e., the objective function. The argument `cov.name` takes a string to define the covariance function c_k. The list of supported covariance functions is given in Table 1. Note that we assume the same covariance function for each Gaussian process and that the covariance function can be written as $c(u; \boldsymbol{\theta}) = \sigma^2 r(u/\rho)$, i.e., it is given by a correlation function $r(h)$ and only has the range ρ and variance (also called partial sill) σ^2 as parameters.

```
R> # setting covariance function to Matern with smoothness nu = 3/2
R> SVC_mle_control(cov.name = "mat32")
```

Profile Likelihood

The parameter of interest $\boldsymbol{\omega}$ is of dimension $p + 2q + 1$. For numeric optimization, such a high dimensional parameter space tends to have numerical instabilities. In order to reduce the computational burden, one can concentrate the log likelihood and optimize on the profile likelihood. From (3), we can see that $\mathbf{Y}$ has the form of a generalized linear model. The mean effect parameter $\boldsymbol{\mu}$ is a nuisance parameter, which can explicitly be defined by the covariance parameter $\boldsymbol{\theta}$, i.e.:

$$\boldsymbol{\mu}(\boldsymbol{\theta}) = \left(\mathbf{X}^\top \boldsymbol{\Sigma}_\mathbf{Y}^{-1}(\boldsymbol{\theta})\mathbf{X} \right)^{-1} \mathbf{X}^\top \boldsymbol{\Sigma}_\mathbf{Y}^{-1}(\boldsymbol{\theta})\boldsymbol{y}.$$

Therefore, the optimization can be expressed as only depending on the covariance parameter $\boldsymbol{\theta}$ or, in other words, being expressed by an isometric profile of the full likelihood. The binary

cov.name	**Name**	**Family**	**Compact**	**Correlation function $r(h)$**
`"exp"`	Exponential	Matérn ($\nu = 1/2$)	FALSE	$\exp(-h)$
`"mat32"`		Matérn ($\nu = 3/2$)	FALSE	$(1 + \sqrt{3}h)\exp(-\sqrt{3}h)$
`"mat52"`		Matérn ($\nu = 5/2$)	FALSE	$(1 + \sqrt{5}h + 5h^2/3)\exp(-\sqrt{5}h)$
`"sph"`	Spherical	–	TRUE	$\left[1 - 3h/2 + h^3/2\right]_+$
`"wend1"`		Wendland ($\kappa = 1$)	TRUE	$[1 - h]_+^4(4h + 1)$
`"wend2"`		Wendland ($\kappa = 2$)	TRUE	$[1 - h]_+^6(35h^2/3 + 6h + 1)$

Table 1: Supported covariance functions $c(u; \boldsymbol{\theta})$ defined by their respective correlation functions $r(h)$, such that $c(u; \boldsymbol{\theta}) = \sigma^2 r(u/\rho)$. Compactly supported correlation functions are defined using the shorthand $[x]_+$, i.e., the positive part of x and 0 otherwise.
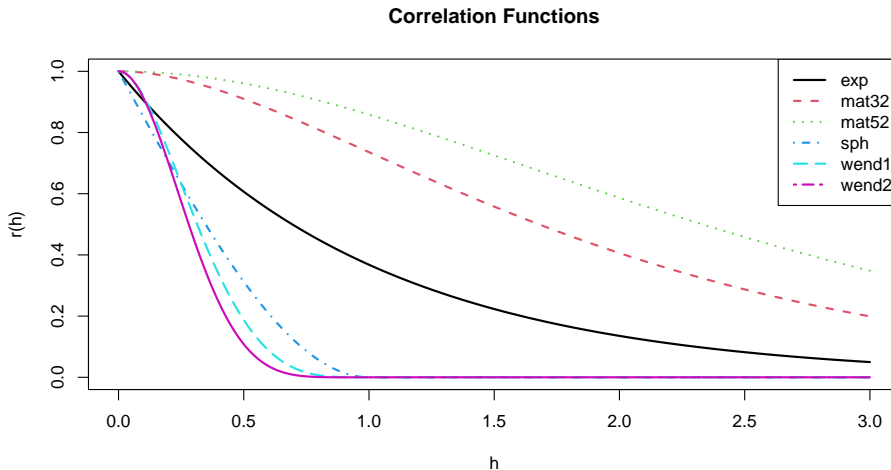

Figure 3: Correlation functions $r(h)$ as defined in Table 1.

argument `profileLik` of `SVC_mle_control()` toggles if the optimization is to be computed on the profile likelihood, or not.

Initial Values and Boundary Conditions

The numeric optimization – both over the profile likelihood and the full likelihood – requires providing initial values $\boldsymbol{\omega}^{(init)} \in \boldsymbol{\Omega}$. If not otherwise specified, we provide the following initial values. With respect to the mean parameters, we use the results from an ordinary least squares $\hat{\boldsymbol{\mu}}$(OLS) of the linear model $\boldsymbol{y} = \mathbf{X}\boldsymbol{\mu} + \boldsymbol{\varepsilon}$. Concerning the covariance parameters, we use the median recorded distance between observations δ and the empirical variance of the response $\boldsymbol{y}$ denoted by $s_{\boldsymbol{y}}^2$. In particular, we set the initial values for the range to $\delta/4$ and for the variance of the Gaussian processes (including the nugget) to $s_{\boldsymbol{y}}^2/(q + 1)$. Another possibility to set the initial values of the latent Gaussian processes is to first apply a GWR. With the estimated coefficients we are able to compute the semivariograms and to deduct the respective covariance parameters. Latter method is currently not implemented.

Parameter type	Lower bound l_j	Initial value $\omega_j^{(init)}$	Upper bound u_j
Range	$10^{-3}\delta$	$\delta/4$	10δ
Variance	0	$s_{\boldsymbol{y}}^2/(q+1)$	$10s_{\boldsymbol{y}}^2$
Nugget Variance	10^{-6}	$s_{\boldsymbol{y}}^2/(q+1)$	$10s_{\boldsymbol{y}}^2$
Mean	`-Inf`	$\hat{\mu}_j(\text{OLS})$	`Inf`

Table 2: Default parameter settings, i.e., if no other arguments for `lower`, `init`, or `upper` of `SVC_mle_control()` are provided, respectively. The settings for the mean parameters are only required for an optimization over the full likelihood.

To ensure that the covariance matrix $\boldsymbol{\Sigma_Y}(\boldsymbol{\theta})$ is well-defined and positive-definite, we require and check that $\sigma_k^2 \geq 0, \rho_k > 0$, and $\tau^2 > 0$ for all $k = 1, ..., q$. Additionally, the "L-BFGS-B" optimization by Byrd, Lu, Nocedal, and Zhu (1995) allows lower bounds $\boldsymbol{l} \in \boldsymbol{\Omega}$ and upper bounds $\boldsymbol{u} \in \boldsymbol{\Omega}$ on the parameter of interest $\boldsymbol{\omega} \in \boldsymbol{\Omega}$, i.e., $\boldsymbol{l} \leq \boldsymbol{\omega} \leq \boldsymbol{u}$. These bounds can benefit the stability of the numeric optimization, but have to be chosen carefully. For instance, if the range parameter ρ_k of a covariance function is much larger than the diameter of the (observed) domain D, there is little to say about the corresponding Gaussian process. In fact, one could consider the coefficient to be non varying at all. On the other hand, if such upper bound is set too low, it hinders the optimization to obtain the best estimate. We can argue similarly for the lower bound. If a range parameter ρ_k becomes too small, the estimated Gaussian process starts to behave like a nugget and an appropriately chosen lower bound $\boldsymbol{l}$ could prevent this. To summarize, we give the default initial values and boundaries for each type of parameter in Table 2.

```
R> # covariance parameter length: 2 GPs with each 2 parameters + nugget
R> P <- 2*2+1
R> # setting bounds and initial values (overwriting the default values)
R> SVC_mle_control(
+    lower = c(rep(c(0.1, 0), 2), 1e-6),
+    init = rep(1, P),
+    upper = rep(Inf, P)
+  )
```

Covariance Tapering

Introduced by Furrer, Genton, and Nychka (2006), covariance tapering is a technique to tackle the "big n problem", which arises from a large number of observations n (Heaton, Datta, Finley, Furrer, Guinness, Guhaniyogi, Gerber, Gramacy, Hammerling, Katzfuss, Lindgren, Nychka, Sun, and Zammit-Mangion 2019; Lasinio, Mastrantonio, and Pollice 2013). In particular, for $n > 10'000$ computers struggle to calculate the determinant or solving a linear system of $\boldsymbol{\Sigma_Y}$ in a feasible time. Here, covariance tapering is a pragmatic approach which makes the evaluation of such calculations – and therefore of the log likelihood (4) – time efficient by inducing a sparse matrix structure.

Therefore, the original covariance function c is multiplied with another, suitable covariance function $c^\star$ with a sufficiently small support, i.e., $c^\star(u) = 0$ for all u greater than some taper

distance $\rho_\star > 0$. The covariance function $c^\star$ has to be chosen in accordance with the original covariance function c, see Furrer *et al.* (2006) for details. The tapered covariance function $c^{(tap)}(u) := c(u)c^\star(u)$ maintains most of its original characteristics, like the order of differentiability at the origin. Due to the small support of $c^{(tap)}(u)$, the induced covariance matrix becomes sparse and can be stored efficiently. Further, there exist optimized algorithms to take advantage of the sparse matrix structure, e.g., the Cholesky decomposition by Ng and Peyton (1993) implemented in the R package **spam** (Furrer and Sain 2010). The optimization of the likelihood is either executed on matrices without covariance tapering or on sparse matrices of class 'spam', where covariance tapering has been applied. Here, the `SVC_mle_control()` argument `tapering` triggers covariance tapering. By default, it is set to `NULL` and no covariance tapering is applied. If a positive scalar is provided, it defines the taper range $\rho_\star$ and therefore the sparsity structure of the covariance matrix.

```
R> # setting the taper range to distance 5 in the units of the locations
R> SVC_mle_control(tapering = 5)
```

Parallelized Optimization

The optimization of the log likelihood function (4) is implemented with the R function `optim()`, specifically the "L-BFGS-B" quasi-Newton gradient method (Byrd *et al.* 1995). In each iteration step ι, `optim()` sequentially evaluates the objective function fn several times. Let $\boldsymbol{\omega}^{(\iota)} \in \boldsymbol{\Omega}$ be the current parameter value. First `optim()` evaluates $fn(\boldsymbol{\omega}^{(\iota)})$ and then approximates its gradient gr at $\boldsymbol{\omega}^{(\iota)}$ by evaluating $fn(\boldsymbol{\omega}^{(\iota)} + \boldsymbol{\epsilon}_p)$ for some $\boldsymbol{\epsilon}_p \in \mathbb{R}^{|\boldsymbol{\Omega}|}, p = 1, ..., P$. The number of evaluations P to approximate the gradient generally increases with the dimension of the parameter space $\boldsymbol{\Omega}$, i.e., $|\boldsymbol{\Omega}| := \dim \boldsymbol{\Omega}$. However, all of the above mentioned evaluations of fn are independent of each other and we can take advantage of a parallel computing. It is implemented with the package **optimParallel** (Gerber and Furrer 2019), where we only have to provide an initialized cluster as part of a 'list' object in the argument `parallel`. In the documentation of `SVC_mle_control()` we give the following code to initialize parallel computing.

```
R> # Code for setting up parallel computing
R> require(parallel)
R> # exchange number of nodes (1) for detectCores()-1 or appropriate number
R> cl <- makeCluster(1)
R> clusterEvalQ(
+     cl = cl,
+     {
+       library(spam)
+       library(varycoef)
+     })
R> # use this list for parallel argument in SVC_mle_control
R> parallel.control <- list(cl = cl, forward = TRUE, loginfo = TRUE)
R> # SVC_mle goes here ...
R> # DO NOT FORGET TO STOP THE CLUSTER!
R> stopCluster(cl); rm(cl)
```

3.2. Maximum Likelihood Estimation

Once the control parameters have been set, the subsequent maximum likelihood estimation is straight forward. The corresponding function is `SVC_mle()`, where one has to provide the before mentioned control settings from `SVC_mle_control()` and data. In particular, the function requires a numeric vector `y` of length `n` as the response, the fixed effects data `X` as a matrix with dimension (`n, p`) and the locations `locs`. The latter should be provided as a matrix of dimension (`n, d`), where `d` is the dimension of the domain D. In contrast to most methodologies for SVC models, the domain D does not have to be a subset of $\mathbb{R}^2$, i.e., with $d = 2$. If the matrix `W` is not defined, all covariates provided for the fixed effects will be used to model random effects, i.e., SVCs, too. Otherwise, the matrix `W` of dimension (`n, q`) explicitly defines the covariates $\boldsymbol{w}^{(k)}$. The estimated parameter of interest by maximizing the likelihood is denoted $\hat{\boldsymbol{\omega}}(\text{MLE})$. We give two examples. The first one is the sampled data set with $d = 1$ from above. The second one is a real data set of approximately 25'000 observations with $d = 2$.

Simple SVC Model

We use the data generated with `sample_fullSVC()` and displayed in Figure 2, i.e., we take the data contained in `SVCdata`. We optimize over the profile likelihood and set the covariance function to be a Matérn with $\nu = 3/2$. All other control parameters are the default ones.

```
R> # set control parameters
R> crtl <- SVC_mle_control(cov.name = "mat32", profileLik = TRUE)
R> # Run MLE (takes approximately one minute)
R> fit <- with(SVCdata, SVC_mle(y = y, X = X, locs = locs, control = crtl))
R> summary(fit)


Call:
SVC_mle.default(y = y, X = X, locs = locs, control = crtl)


Fitting a GP-based SVC model with 2 fixed effect(s) and 2 SVC(s)
using 300 observations at 300 different locations / coordinates.


Residuals:
     Min.    1st Qu.     Median    3rd Qu.       Max.
-1.334351  -0.318621   0.003409   0.315742   1.272693


Residual standard error: 0.489
Multiple R-squared: 0.9599, BIC: 657.7



Coefficients of fixed effect(s):
     Estimate Std. Error Z value Pr(>|Z|)
Var1   1.1799     0.3820   3.089  0.00201 **
Var2   2.2225     0.6675   3.329  0.00087 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Covariance parameters of the SVC(s):
           Estimate Std. Error W value Pr(>W)
SVC1.range  0.32576    0.07048      NA     NA
SVC1.var    1.22053    0.47731   6.539 0.0106 *
SVC2.range  0.85962    0.26378      NA     NA
SVC2.var    1.63277    1.02824   2.522 0.1123
nugget.var  0.29060    0.02708      NA     NA
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1


The covariance parameters were estimated using
Matern (nu = 3/2) covariance functions.
No covariance tapering applied.


MLE:
The MLE terminated after 69 function evaluations with convergence code 0
(0 meaning that the optimization was succesful).
The final profile log likelihood value is -317.4.
```

The summary output of the function `SVC_mle()` provides an overview of the data and model, the estimated parameters for the fixed and random effects, as well as the summary of the optimization. If possible, the estimates' standard errors are approximated using the Hessian of the optimization. Further, we use a Z test on the fixed effects (H_0: $\mu_j = 0$) and a Wald test on the Gaussian process variances (H_0: $\sigma_k^2 = 0$). The other covariance parameters, i.e., the ranges ρ_k and the nugget variance τ^2, are defined to be strictly positive. Therefore no Wald test is conducted and the corresponding test statistics and p-values for these parameters are always set to `NA`.

Lucas County House Price Data

A real, larger data set is given by the Lucas County (OH) from the R package **spData** (Bivand, Nowosad, and Lovelace 2020). This data set is available as a 'data.frame' in **varycoef** using `data("house")`. We use a subset of covariates in our model and give a brief overview thereof in Table 3. The continuous covariates were transformed to account skewness and to increase numeric stability. We denote these transformed variables on the covariates using the prefix `Z` for a standardization and `l` for a logarithmic transformation using $\log(x + 1)$. The SVC model also contains the transformed year of construction as a quadratic effect to account for a potential vintage effect (see Dambon, Fahrländer, Karlen, Lehner, Schlesinger, Sigrist, and Zimmermann 2020). This results in a model with six varying coefficients and 20 fixed effects including the mean.

Due to the large observation size ($n = 25'353$ not counting the observations with 2.5 and 3 stories) and the relatively large number of SVCs ($q = 6$), we apply covariance tapering with a taper distance of 1 kilometer, optimize over the profile likelihood, and use parallel computing. The parameter estimates are given in Table 4. In Figure 4 we present two estimated SVC with

(a) Continuous Variables

	Variable	Description	Summary Statistics			
			Min.	Mean	SD	Max.
y	`price`	transaction price in USD	2000	79018	59655	875000
x	`yrbuilt`	building year	1835	1945	28	1998
	`TLA`	total living area in square feet	120	1462	613	7616
	`lotsize`	lot size in square feet	702	13332	28941	429100
	`garagesqft`	garage area in square feet	0	370	208	5755
s	`long`	longitude in meters	484575	508144	6948	538364
	`lat`	latitude in meters	195270	221710	5095	229836

(b) Factor Variables

	Variable	Levels	Frequency	
			Absolute	Relative [in %]
x	`stories`	`one`	12954	51
		`bilevel`	509	2
		`multilvl`	723	3
		`one+half`	3125	12
		`two`	8042	32
		`two+half`	2	0
		`three`	2	0
	`wall`	`stucdrvt`	204	1
		`ccbtile`	129	1
		`metlvnyl`	4235	17
		`brick`	3633	14
		`stone`	86	0
		`wood`	11174	44
		`partbrk`	5896	23
	`garage`	`no garage`	3488	14
		`basement`	78	0
		`attached`	9018	36
		`detached`	12555	50
		`carport`	218	1

Table 3: Description and summary statistics, i.e., the minimum, mean, standard deviation, and maximum of continuous and frequencies of factor variables in Lucas County house data. The respective types of data are given in the first column, where y denotes the response, x denotes explanatory variables, and s denotes the observation location in a $d = 2$ dimensional domain, i.e., Northing and Easting in Ohio North coordinate reference system (`epsg:2834`). The first listed levels of the factors are the reference levels.

the strongest spatial structure combined with their fixed effect, i.e., $\hat{\mu}_1 + \hat{\boldsymbol{\eta}}_1(\cdot)$ and $\hat{\mu}_2 + \hat{\boldsymbol{\eta}}_2(\cdot)$ respectively corresponding to the intercept and the standardized year of construction. The code for the SVC model estimation is given in the appendix (c.f. Section A.1).

Some key insights of the model can be immediately extracted. For instance, the downtown

Variable	Mean $\hat{\mu}_j$		Range $\hat{\rho}_k$		Variance $\hat{\sigma}_k^2$	
	Est.	SE	Est.	SE	Est.	SE
(Intercept)	6.130	0.064	269.202	225.676	0.09408	0.00343
Z.yrbuilt	0.163	0.007	50.795	68.081	0.01795	0.00142
Z.yrbuilt.sq	−0.026	0.004	0.011		0.01221	0.00037
l.TLA	0.499	0.007	101.474		0.00000	0.00000
l.lotsize	0.127	0.004	101.472		0.00000	0.00000
l.garagesqft	0.075	0.005	101.397	219.921	0.00010	0.00005
storiesbilevel	−0.062	0.013				
storiesmultilvl	−0.026	0.010				
storiesone+half	0.026	0.006				
storiestwo	0.056	0.005				
wallccbtile	−0.171	0.025				
wallmetlvnyl	0.037	0.016				
wallbrick	0.063	0.016				
wallstone	0.016	0.027				
wallwood	−0.007	0.016				
wallpartbrk	0.033	0.016				
garagebasement	−0.256	0.041				
garageattached	−0.271	0.032				
garagedetached	−0.300	0.032				
garagecarport	−0.345	0.033				
Nugget					0.03143	0.00046

Table 4: Parameter estimates (Est.) and corresponding standard errors (SE) of GP-based SVC model for Lucas county data. If no corresponding standard error is given, then it could not be retrieved from the Hessian.

area of Toledo has the lowest mean pricing, while house prices are highest along the shore line of the Maumee River close to Perrysburg. Northwest and West of Toledo are a couple of local, high pricing areas. These features can also be obtained from classical geo-statistical models where we model a spatially varying intercept. For the effect of the year of construction yrbuilt we observe some interesting behavior. For a majority of locations the coefficient is clearly positive. The strongest, positive effect is present at the downtown area. Over all, we interpret these results as high desirability of newly built houses. However, in the suburbs of Toledo and along the Maumee River, we clearly see a deviation of this behavior as there are some locations where the yrbuilt coefficient is close to zero, or even negative. This hints at a vintage effect being present. We refer to Dambon *et al.* (2020) where an similar analysis for single family houses in the Canton of Zurich (Switzerland) is conducted. The remaining estimated spatially varying coefficients are given in the appendix (c.f. Section A.2).

3.3. Prediction

Once the parameter of interest $\hat{\omega}$(MLE) has been found, we can calculate (spatial) predictions using the empirical best linear unbiased predictor (EBLUP). In **varycoef**, a predict() method for the class 'SVC_mle', i.e., the model output of SVC_mle(), has been implemented. The ar-
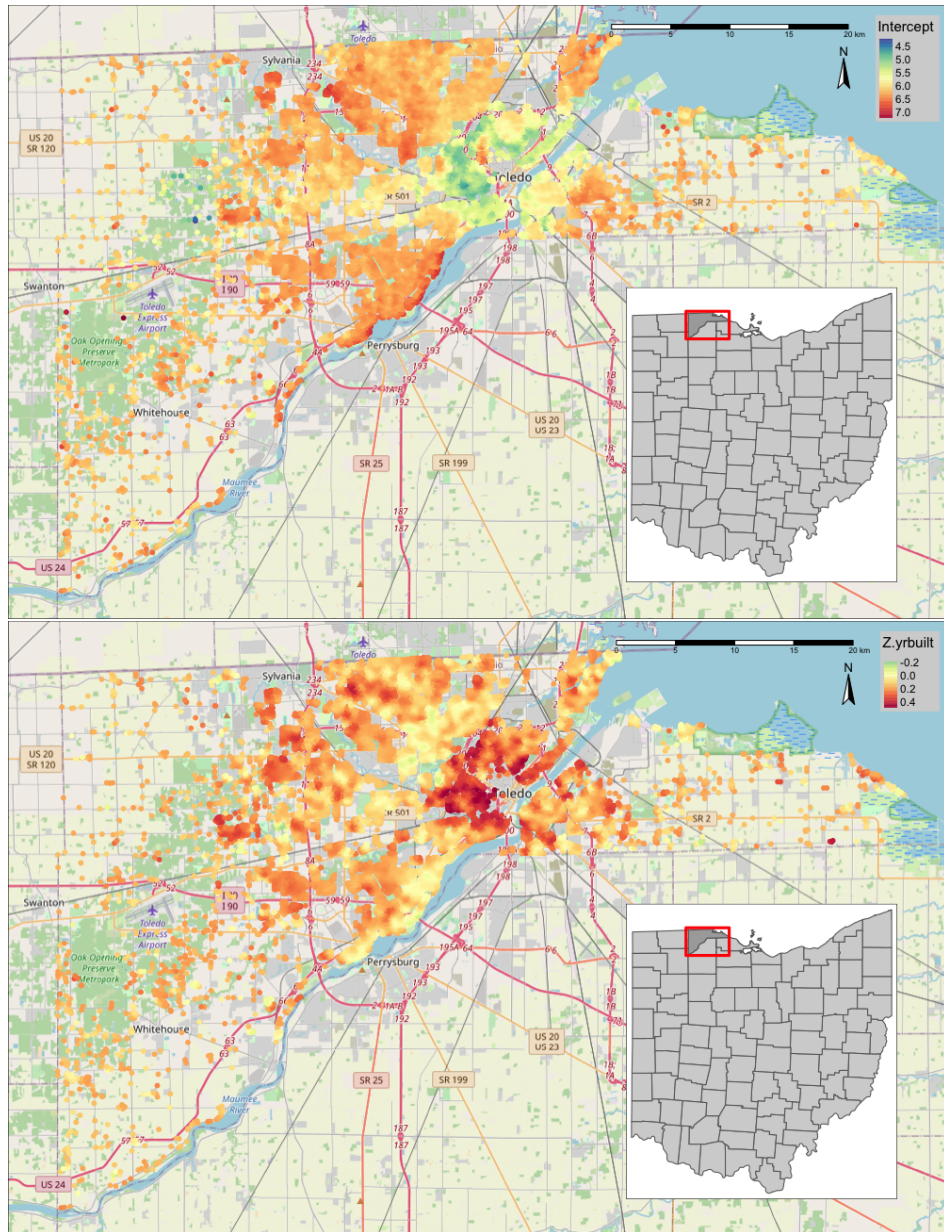
Figure 4:   Two estimated spatially varying coefficients for the intercept (upper panel) and the standardized year of construction (lower panel). The inset maps shows the State of Ohio with Lucas county filled in dark grey.
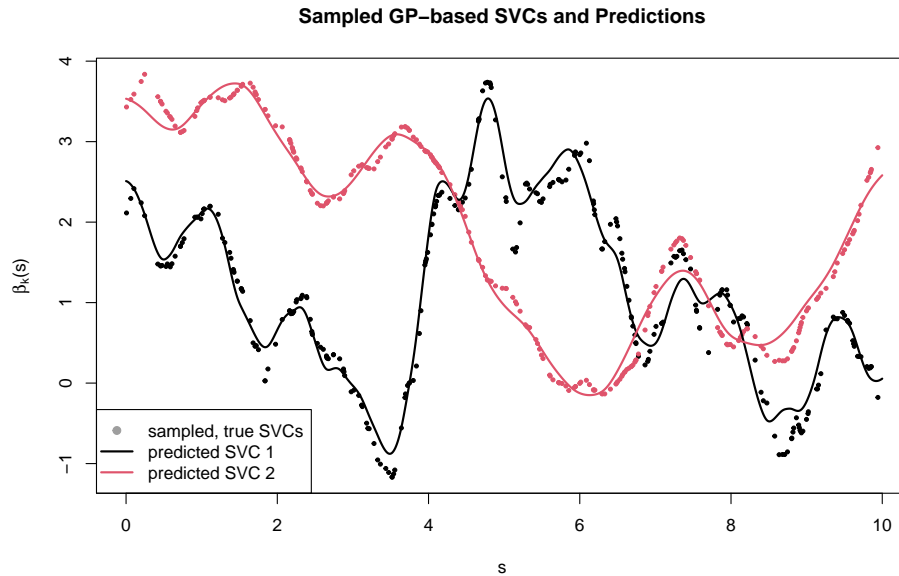
Sampled GP–based SVCs and Predictions

Figure 5: Sampled, true SVCs from `SVCdata` (dots) and predicted SVCs (lines) using MLE of GP-based SVC model.

gument `newlocs` takes the new locations to spatially predict the random effects. If arguments `newX` and `newW` are provided, the response and predicitive variance are also calculated. Note that the predicted random effects only contain $\hat{\boldsymbol{\eta}}_k$, i.e., the zero-mean Gaussian processes. If a corresponding mean effect is associated to the same covariate, it can be retrieved by the `coef()` method and added to the predicted Gaussian process, similar to Figure 4. Finally, we visualize the true and predicted varying coefficients by our MLE approach in Figure 5.

```
R> # Predict SVCs on whole interval
R> newlocs <- seq(0, 10, by = 0.01)
R> SVCpred <- predict(fit, newlocs = newlocs)
R> # Combine random effects from GPs
R> SVCpredbeta <- as.matrix(SVCpred[, 1:2]) +
+    # and fix effects
+    matrix(coef(fit), nrow = length(newlocs), ncol = 2, byrow = TRUE)
R> head(SVCpredbeta)


        SVC_1    SVC_2
[1,] 2.509802 3.533227
[2,] 2.506545 3.530252
[3,] 2.501862 3.527029
[4,] 2.495821 3.523557
[5,] 2.488497 3.519835
[6,] 2.479956 3.515861
```

4. Variable Selection

4.1. Introduction

Due to the flexible nature of a GP-based SVC models, some natural questions arise when defining the model or interpreting the results of an estimated model: *Which covariates should be defined with spatially varying coefficients? Is a constant coefficient sufficient? Did the estimated model overfit the data due to its high flexibility?* To address these questions, we introduced a joint variable selection method for the fixed and random effects of the GP-based SVC model (Dambon *et al.* 2021a).

4.2. Optimization of the Penalized Likelihood

The penalized likelihood is defined by the likelihood ℓ (4) and L_1 penalties (Tibshirani 1996) on the fixed effects μ_j and the variance σ_k^2, i.e.,

$$p\ell(\boldsymbol{\omega}) = \ell(\boldsymbol{\omega}) + n \sum_{j=1}^{p} \lambda_j |\mu_j| + \sum_{k=1}^{q} \lambda_{p+k} |\sigma_k^2| \tag{5}$$

The optimization problem is related to variable selection of linear mixed models (for an overview, see Müller, Scealy, and Welsh 2013) and, in particular, the works of Bondell, Krishna, and Ghosh (2010) and Ibrahim, Zhu, Garcia, and Guo (2011). We assume that the shrinkage parameters of the penalized likelihood (5) are defined like in an adaptive Lasso (Zou 2006). However, we account for their inherit difference as the parameters shrink the fixed and random effects, respectively. For the unknown shrinkage parameters $(\lambda_{\boldsymbol{\mu}}, \lambda_{\boldsymbol{\theta}}) \in (\mathbb{R}_{>0})^2$, we have:

$$\lambda_j := \frac{\lambda_{\boldsymbol{\mu}}}{\hat{\mu}_j}, \quad \lambda_{p+k} := \frac{\lambda_{\boldsymbol{\theta}}}{\hat{\sigma}_k^2}. \tag{6}$$

For now, we assume that $(\lambda_{\boldsymbol{\mu}}, \lambda_{\boldsymbol{\theta}})$ are fixed and known. The objective function of the optimization is defined as $-2p\ell(\boldsymbol{\omega})$. Its optimization is achieved by a coordinate descent where we cyclically iterate between the optimization of the fixed effects $\boldsymbol{\mu}$ and the covariance parameters $\boldsymbol{\theta}$, i.e.,

$$\boldsymbol{\mu}^{(t+1)} = \underset{\boldsymbol{\mu} \in \mathbb{R}^p}{\operatorname{argmin}} -2p\ell(\boldsymbol{\mu}|\boldsymbol{\theta}^{(t)}),$$

$$\boldsymbol{\theta}^{(t+1)} = \underset{\boldsymbol{\theta} \in \boldsymbol{\Theta}}{\operatorname{argmin}} -2p\ell(\boldsymbol{\theta}|\boldsymbol{\mu}^{(t+1)}),$$

for $t \geq 0$, where the initial value is given by $\boldsymbol{\theta}^{(0)} = \hat{\boldsymbol{\theta}}(\text{MLE})$. While the first step is implemented by the **glmnet** package (Friedman, Hastie, and Tibshirani 2010), the second step requires more effort. We refer to Dambon *et al.* (2021a) for more details. Under convergence, the coordinate descent approach returns the penalized maximum likelihood estimates denoted $\hat{\boldsymbol{\omega}}(\text{PMLE})$.

4.3. Selection of Shrinkage Parameters

In the last section, we assumed the shrinkage parameters $(\lambda_{\boldsymbol{\mu}}, \lambda_{\boldsymbol{\theta}})$ to be known. Here, we focus on their selection by optimizing an information criterion. For some shrinkage parameters

IC.type	Name	Model complexity penalty $\alpha(\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}})$
`"cAIC_VB"`	cond. Akaike IC	$\frac{2n}{n-p-2}\big(df(\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}}) + 1 - \frac{df(\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}})-p}{n-p}\big)$
`"BIC"`	Bayesian IC	$log(n)(\|\boldsymbol{\mu}_{\boldsymbol{\lambda}}\|_0 + \|\sigma^2_{\boldsymbol{\lambda}}\|_0)$

Table 5: Supported information criterion. The provided estimates $\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}}$ are obtained from a PMLE depending on the shrinkage parameters $\lambda_{\boldsymbol{\mu}}, \lambda_{\boldsymbol{\theta}}$, c.f. Figure 6. The norm $\|\cdot\|_0$ is the number of non-zero elements.

$(\lambda_{\boldsymbol{\mu}}, \lambda_{\boldsymbol{\theta}})$, we call the coordinate descent which computes $\hat{\boldsymbol{\omega}}(\lambda_{\boldsymbol{\mu}}, \lambda_{\boldsymbol{\theta}})$ for respective shrinkage parameters, which we abbreviate with $\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}}$. For the estimated model with parameters $\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}}$ we can calculate an information criterion.

Currently, there are two information criteria implemented in **varycoef**: a conditional Akaike (cAIC) introduced by Vaida and Blanchard (2005) and a Bayesian (BIC) information criterion. For parameter estimates $\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}}$, both information criteria are defined as the sum of the goodness of fit given with $-2\ell(\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}})$ (also called deviance) and a specific model complexity penalty $\alpha(\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}})$. For the cAIC's penalty we require the effective degrees of freedom $df(\cdot)$ which are defined as the trace of the hat matrix $\mathbf{H}$:

$$df(\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}}) = \operatorname{tr}\mathbf{H}(\hat{\boldsymbol{\theta}}_{\boldsymbol{\lambda}})$$
$$= \hat{\tau}^2_{\boldsymbol{\lambda}} \operatorname{tr}\left[(\mathbf{X}^\top\boldsymbol{\Sigma}^{-1}\mathbf{X})^{-1}\mathbf{X}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\Sigma}^{-1}\mathbf{X}\right] + n - \hat{\tau}^2_{\boldsymbol{\lambda}} \operatorname{tr}\left[\boldsymbol{\Sigma}^{-1}\right],$$

where $\boldsymbol{\Sigma}^{-1} = \left[\boldsymbol{\Sigma}(\hat{\boldsymbol{\theta}}_{\boldsymbol{\lambda}})\right]^{-1}$. The respective definitions of $\alpha(\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}})$ are given in Table 5.

We provide an overview of the variable selection scheme in Figure 6. Starting with the data and some model specification, we receive a first estimate via MLE, in particular using `optim()`. The estimate $\hat{\boldsymbol{\omega}}(\text{MLE})$ is then used in the PMLE. Hence, for a given shrinkage parameter $\boldsymbol{\lambda}$ an estimate $\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}}$ is returned. For such estimate we can calculate the respective information criterion. The whole procedure beginning with an input of a shrinkage parameter $\boldsymbol{\lambda}$ over the PML-estimate $\hat{\omega}_{\boldsymbol{\lambda}}$ to an information criterion output can be expressed as a function $IC(\cdot)$. Therefore, an information criterion optimization over corresponding objective function $IC(\cdot)$ selects a shrinkage parameter by minimizing $IC(\cdot)$. The back and forth between coordinate descent for a penalized likelihood optimization and the selection of the next shrinkage parameter is also visible in Figure 6. If a required stopping condition is met, the final PML-estimate is returned. Keep in mind that the evaluation of $IC(\cdot)$ is computationally expensive and complex. The information criterion optimization is therefore an optimization of an expensive (black-box) objective function over two parameters. We offer two methods on how to optimize the function:

- The first method is a brute force grid approach by providing pairs of shrinkage parameters and computing it for all given combinations. Once the information criterion has been evaluated for each shrinkage parameter, the stopping condition is met.

- The second method is a much more sophisticated model-based optimization (MBO) which we briefly describe in the next section.
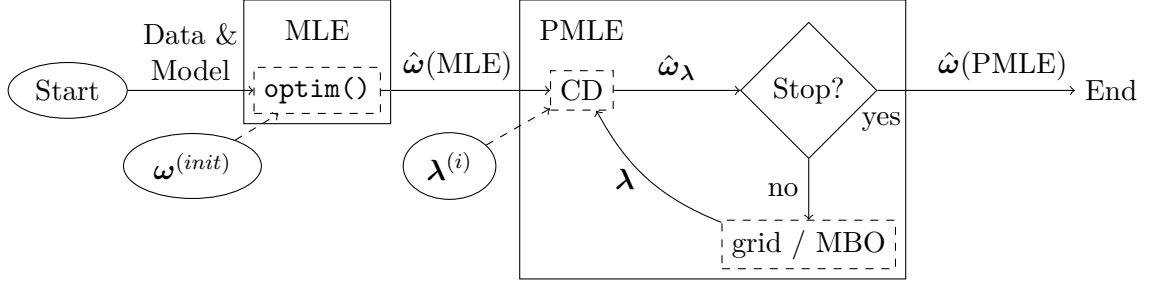
Figure 6: Variable selection scheme. The inputs are given by ellipses. Optional inputs are indicated by dashed arrows. The optimization routines are given in solid rectangles, where the algorithmic sub-routines are given in dashed rectangles, i.e., the quasi-Newton gradient method implemented in the `optim()` function, the coordinate descent (CD) algorithm, and the grid or MBO method. The stopping criterion within the PMLE depends on the optimization method. Latter method then provides the next $\boldsymbol{\lambda}$ to estimate $\hat{\boldsymbol{\omega}}_{\boldsymbol{\lambda}}$ by a coordinate descent.

The PMLE has its respective control function named `SVC_selection_control()` to set all the control parameters. In the data example discussed in Section 4.4 as well as the Appendix B these control parameters are addressed.

Model-based Optimization

Model-based optimization (Jones 2001; Koch, Bischl, Flasch, Bartz-Beielstein, Weihs, and Konen 2012; Horn and Bischl 2016) offers compelling means to find a minimum of the objective function $IC(\cdot)$ by using a so called surrogate model. It relies on n_{init} initial values $\boldsymbol{\lambda}^{(1)}, ..., \boldsymbol{\lambda}^{(n_{\mathrm{init}})}$ that span the predefined parameter space Λ. By evaluating IC for these values, we receive n_{init} tuples $(\boldsymbol{\lambda}^{(i)}, \xi^{(i)})$ with $\xi^{(i)} := IC(\boldsymbol{\lambda}^{(i)})$, which we use to krige. More specifically, we assume a Gaussian surrogate model with constant mean and a Matérn covariance function of smoothness $\nu = 3/2$ and estimated covariance parameters, c.f. equation (1) and Table 1. In this case, the random variable $\Xi(\boldsymbol{\lambda})$ expressing the distribution at $\boldsymbol{\lambda}$ conditional on the n_{init} tuples is given by a normal distribution $\Xi(\boldsymbol{\lambda}) \sim \mathcal{N}\left(\hat{\mu}(\boldsymbol{\lambda}), \hat{s}^2(\boldsymbol{\lambda})\right)$. Here, $\hat{\mu}(\boldsymbol{\lambda})$ and $\hat{s}^2(\boldsymbol{\lambda})$ are the kriging surface and kriging variance, respectively, for which we use the plug-in estimates of the surrogate model. The parameters of the surrogate model are then iteratively updated for n_{iter} steps. In each step $\iota = 1, ..., n_{\mathrm{iter}}$:

1. Define the current information criterion minimum $\xi_{\mathrm{min}} := \min\{\xi^{(1)}, ..., \xi^{(n_{\mathrm{init}}+\iota-1)}\}$.

2. Compute an infill criterion from the current posterior distribution $\Xi(\boldsymbol{\lambda})$. We use the expected improvement (EI, see equation (7) below) infill criterion which can be expressed analytically for a Gaussian process surrogate model (see equation (8) below):

$$\mathrm{EI}(\boldsymbol{\lambda}) = E_{\Xi}\left(\max\{\xi_{\mathrm{min}} - \Xi(\boldsymbol{\lambda}), 0\}\right) \tag{7}$$

$$= \begin{cases} (\xi_{\mathrm{min}} - \hat{\mu}(\boldsymbol{\lambda}))\Phi\left(\frac{\xi_{\mathrm{min}}-\hat{\mu}(\boldsymbol{\lambda})}{\hat{s}(\boldsymbol{\lambda})}\right) + \hat{s}(\boldsymbol{\lambda})\phi\left(\frac{\xi_{\mathrm{min}}-\hat{\mu}(\boldsymbol{\lambda})}{\hat{s}(\boldsymbol{\lambda})}\right), & \text{if } \hat{s}(\boldsymbol{\lambda}) > 0, \\ 0, & \text{if } \hat{s}(\boldsymbol{\lambda}) = 0. \end{cases} \tag{8}$$

In the equation above Φ and ϕ denote the cumulative distribution function and the probability density function of the standard normal distribution, respectively. The next, best shrinkage parameter $\boldsymbol{\lambda}^{(n_{\mathrm{init}}+\iota)}$ is found by maximizing (8).
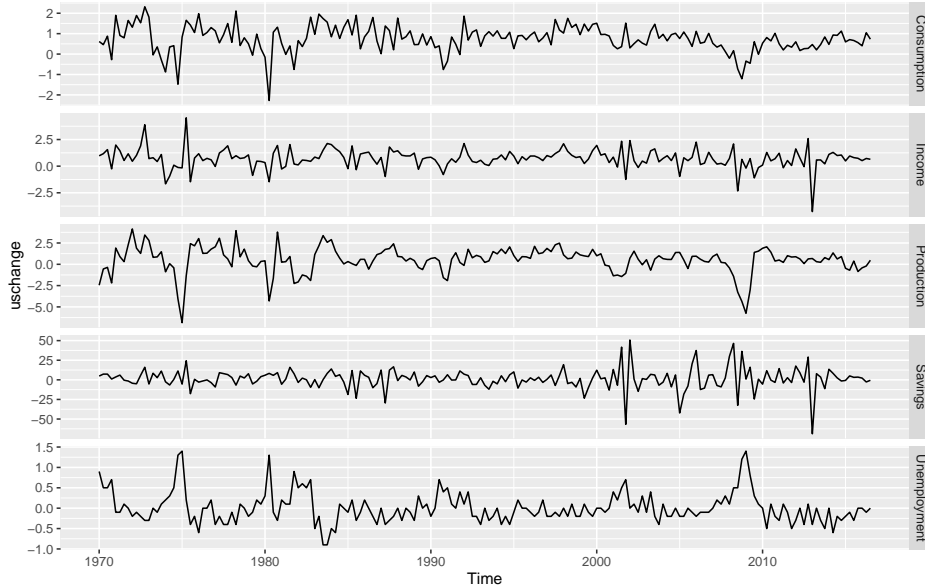
Figure 7: Time series of `uschange` data.

3. Evaluate the information criterion at respective location, i.e., $\xi^{(n_{\mathrm{init}}+\iota)} := IC(\boldsymbol{\lambda}^{(n_{\mathrm{init}}+\iota)})$, and add the tuple $(\xi^{(n_{\mathrm{init}}+\iota)}, \boldsymbol{\lambda}^{(n_{\mathrm{init}}+\iota)})$ to the existing set of tuples.

4. Update the surrogate model's parameters and the distribution of $\Xi(\boldsymbol{\lambda})$.

The n_{init} initial shrinkage parameters $\boldsymbol{\lambda}^{(i)}$ are drawn as Latin hypercube sample (LHS) from a predefined subset of the parameter space Λ using the R packages **lhs** (Carnell 2020) and **ParamHelpers** (Bischl, Lang, Richter, Bossek, Horn, and Kerschke 2020). The surrogate model is defined using the R package **mlr** (Bischl, Lang, Kotthoff, Schiffner, Richter, Studerus, Casalicchio, and Jones 2016). The MBO is implemented with the R package **mlrMBO** (Bischl, Richter, Bossek, Horn, Thomas, and Lang 2017).

4.4. A Final Example: Growth Rates in the USA

We showcase the variable selection with a small time series data set, the `uschange` data set in the R package **fpp2** (Hyndman and Athanasopoulos 2018). It contains the quarterly percentage changes of personal consumption (`Consumption`) and personal disposable income (`Income`) as well as the US production (`Production`), savings (`Savings`), and the unemployment (`Unemployment`) rates from Q1 1970 to Q3 2016.

```
R> data("uschange", package = "fpp2")
R> # divide times series into data and time points of observation
R> train_dat <- as.data.frame(uschange); train_t <- as.numeric(time(uschange))
```

In total, the data contains 187 observations of 5 variables. The dependency structure is given by the quarters on which the measurements where recorded. The goal is to regress the personal consumption change on all other 4 covariates with an additional intercept. Therefore, the full
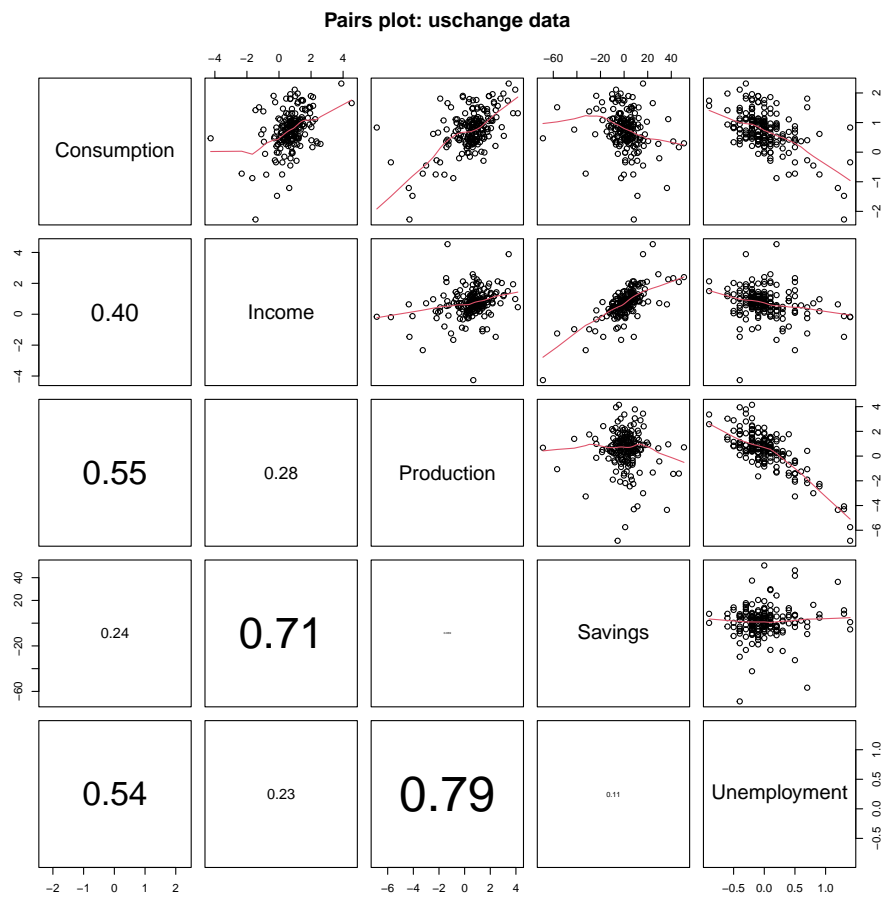
Figure 8:   Pairs plot of `uschange` data with smoothing lines and pair-wise absolute correlations.

varying coefficient model in shorthand notation is given by:

$$y_t = \beta_1(t) + \beta_2(t)\texttt{Income}_t + \beta_3(t)\texttt{Production}_t + \beta_4(t)\texttt{Savings}_t + \beta_5(t)\texttt{Unemployment}_t + \varepsilon_t, \tag{9}$$

with response $\texttt{Consumption}_t$. In this application the term *spatially* varying coefficient might be confusing and we simply refer to $\beta_j(t)$ as a varying coefficient. The model (9) is very similar to the varying-coefficient models introduced by Hastie and Tibshirani (1993). However, our model and methodology differs in the definition and estimation of $\beta_j(\cdot)$.

Maximum Likelihood Estimation

To determine what kind of model is suitable, i.e., which coefficients are temporally varying and which are not, we will apply the variable selection described above. To this end, we start with a classical MLE of the full varying coefficient model before applying the PMLE.

```
R> # training data
R> X_train <- as.matrix(cbind(Intercept = 1, train_dat[, -1]))
R> y_train <- train_dat$Consumption
R> # prepare cluster: see Examples in ?SVC_mle_control
R> require(parallel)
R> cl <- makeCluster(detectCores()-1, setup_strategy = "sequential")
R> invisible(clusterEvalQ(
+    cl = cl,
+    {
+      library(spam)
+      library(varycoef)
+    }
+ ))
R> # control parameters of MLE including computing cluster
R> control <- SVC_mle_control(
+    profileLik = TRUE,
+    parallel = list(cl = cl, forward = TRUE, loginfo = TRUE)
+ )
R> SVC_model_mle <- SVC_mle(
+    y = y_train, X = X_train, locs = train_t, control = control
+ )
R> # stop cluster
R> stopCluster(cl); rm(cl)
R> summary(SVC_model_mle)

Call:
SVC_mle.default(y = y_train, X = X_train, locs = train_t, control = control)

Fitting a GP-based SVC model with 5 fixed effect(s) and 5 SVC(s)
using 187 observations at 187 different locations / coordinates.

Residuals:
```

```
     Min.    1st Qu.    Median   3rd Qu.       Max.
-0.067810  -0.017306   0.002322  0.014628   0.102556


Residual standard error: 0.02525
Multiple R-squared: 0.9985, BIC: -250.1



Coefficients of fixed effect(s):
             Estimate Std. Error Z value Pr(>|Z|)
Intercept    0.130568   0.035166   3.713 0.000205 ***
Income       1.008021   0.033385  30.194 < 2e-16 ***
Production   0.001372   0.006638   0.207 0.836294
Savings     -0.088688   0.024060  -3.686 0.000228 ***
Unemployment -0.055151   0.051574  -1.069 0.284916
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1



Covariance parameters of the SVC(s):
                   Estimate Std. Error W value Pr(>W)
Intercept.range    4.448799   2.191420      NA     NA
Intercept.var      0.006576   0.002882   5.206 0.0225 *
Income.range       4.109383   1.792707      NA     NA
Income.var         0.005540   0.002877   3.708 0.0542 .
Production.range   5.028521        NaN      NA     NA
Production.var     0.000000   0.000000     NaN    NaN
Savings.range     18.008847  41.658636      NA     NA
Savings.var        0.001292   0.001761   0.538 0.4632
Unemployment.range 3.485734        NaN      NA     NA
Unemployment.var   0.013210        NaN     NaN    NaN
nugget.var         0.001781   0.001078      NA     NA
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1


The covariance parameters were estimated using
exponential covariance functions.
No covariance tapering applied.



MLE:
The MLE terminated after 71 function evaluations with convergence code 52
(0 meaning that the optimization was succesful).
The final profile log likelihood value is 148.6.
```

Maximum likelihood estimation yields a zero-estimate of the variance of the coefficient of the `Production`, i.e., $\hat{\sigma}_3^2(\text{MLE}) = 0$. The fitted varying coefficients are given in Figure 9. Further, we notice that all coefficients apart the intercept's one are sign preserving and have
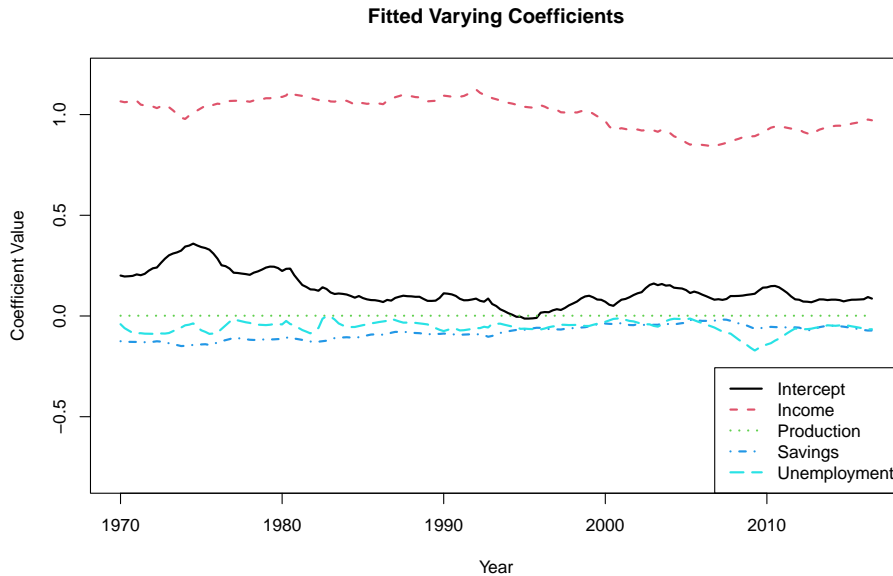
Figure 9: Temporal dependency of ML estimated varying coefficients. The estimated mean effects have been added.

a correctly associated effect. Though, it must be noted that the intercept's dip into negative values is much smaller than the intercept's mean effect standard error. Considering the fitted coefficients, we see that the `Unemployment` has some sharp peaks. For instance, $\hat{\beta}_5(t)$ has relatively large volatility in the mid 1970's as well as early 1980's and reaches its minimum for $t \approx 2008$. In all cases, the unemployment in the US reached its all-time highs (prior to the global COVID19 pandemic, c.f. Figure 7) due to great recessions like the one caused by the global financial crisis (2007-2008). Finally, we can see that the estimated model has a implausible coefficient of determination of 0.999 which hints at overfitting. Therefore, some regularization or variable selection is necessary.

Penalized Maximum Likelihood Estimation

In this section we maximize the penalized likelihood and provide respective estimates. In particular, we compare and examine both information criterion optimization methods to obtain the shrinkage parameters. The results for both methods are visualized in Figure 10. For both methods, the lower and upper bounds of both shrinkage parameters were set to 10^{-3} and 1, respectively. The grid method used a 10×10 lattice of shrinkage parameters. The MBO method used 5 initial values (squares in Figure 10) which span the shrinkage parameter space, before applying a surrogate model with a Gaussian process and updating it after each computation. Here, we used 15 further iterations using the expectation improvement infill criterion (triangles in Figure 10). The respective minimums of both methods are given by a plus sign. The selected shrinkage parameters are:

$$\hat{\boldsymbol{\lambda}}_{grid} = (0.1, 0.01)^\top, \quad \hat{\boldsymbol{\lambda}}_{MBO} = (0.3353, 0.0366)^\top,$$

with respective BIC -279.2 for the grid method and -269.8 for the MBO. The ML-estimated GP-based SVC model has a BIC of -250.1. In Figure 10 we can also see that the BIC surface
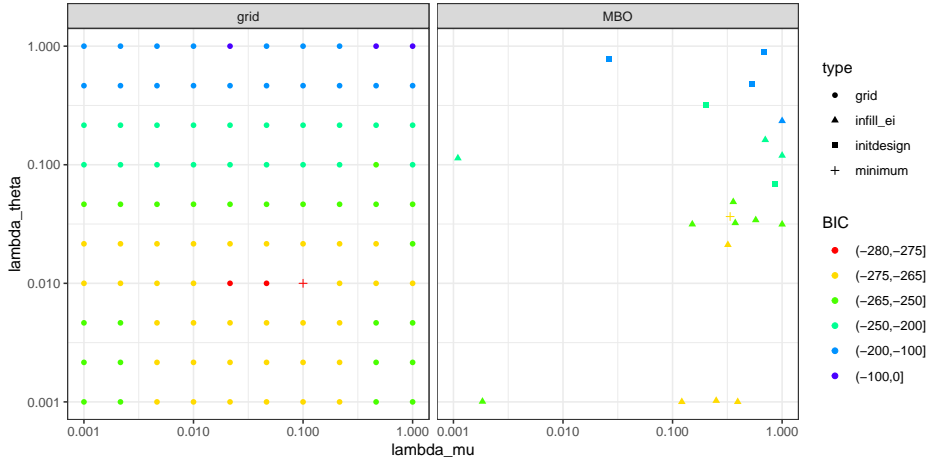
Figure 10:   Comparison of information criterion optimization methods by scatter plots for the computed pairs of $(\lambda_{\boldsymbol{\mu}}, \lambda_{\boldsymbol{\theta}})$. On the left hand side, we see the 10×10 grid structure. On the right hand side, we see the MBO. Note that both plots are on a log-log-scale. The MBO's selected shrinkage parameter is part of the initial design. Note that the color-coding for the BIC is deliberately on a non-regular basis to convey more information about the structure of the BIC.

is relatively flat in the neighborhood of the selected shrinkage parameters due to the small number of observations. In this showcase it is possible that there exist several local minima. The advantage of the MBO is the run time. While the grid method takes 15.7 minutes for the whole variable selection, the MBO requires 4.7 minutes, only 29.9% of the grid method time.

We present the ML- and PML-estimated parameters of model (9) in Table 6. In terms of variable selection, the initial MLE already has one zero-estimate of the variance for the `Production` coefficient. Both methods for optimizing the information criterion yield very similar estimates despite having slightly different selected shrinkage parameters. In both cases, PMLE further increased model sparsity by excluding `Production` entirely from the model as well as excluding the random effect for `Unemployment`. There are two possible reasons for such behavior. The model over-fitted the data or the Gaussian process was misspecified for instance in the smoothness of the covariance function. In either case the exclusion of the corresponding Gaussian process is the right step as it raises a flag. Further, one can observe that the lack of a time depending `Unemployment` coefficient is absorbed by an increase of the error variance.

5. Summary

The **varycoef** package offers user-friendly tools to model and regress dependent data using (spatially) varying coefficient models. Though the package has been developed with an application to spatial data ($d = 2$) in mind, it now supports the modeling of other types of dependent data, as long as a suitable distance measure between observations exists. The models are flexible with respect to the definition of fixed or random effects and, in particular, with respect to the covariance matrices. Several statistical and computational techniques like

Variable	Mean $\hat{\mu}_j$			Range $\hat{\rho}_k$			Variance $\hat{\sigma}_k^2$		
	MLE	grid	MBO	MLE	grid	MBO	MLE	grid	MBO
Interc.	0.131	0.126	0.124	4.45	4.73	4.76	0.0066	0.0062	0.0037
Income	1.008	1.013	1.014	4.11	5.05	5.15	0.0055	0.0031	0.0017
Produc.	0.001	0.000	0.000	5.03	5.03	5.03	0.0000	0.0000	0.0000
Savings	−0.089	−0.085	−0.080	18.01	17.55	17.48	0.0013	0.0013	0.0010
Unempl.	−0.055	−0.072	−0.063	3.49	3.24	3.24	0.0132	0.0000	0.0000
Error							0.0018	0.0025	0.0037

Table 6: Parameter estimates for varying coefficient model (9) of `uschange` data including an intercept (`Interc.`). Individual parameters are obtained by MLE and PMLE. For latter, we give parameter estimates for both information criterion optimization methods grid and MBO.

parallel computing, covariance tapering including sparse matrix algorithms, and optimization over the profile likelihood have been implemented to foster the applicability to large data sets. Besides model estimation and prediction, our R package offers a variable selection method. Model-based optimization, a powerful computational statistics algorithm, is used in **varycoef** to make the shrinkage parameter selection computationally efficient.

In this article, we gave a variety of examples that showcase the user-friendly application of **varycoef** on synthetic and real data. The gain of new insights from the estimated models is substantial and immediate. Here, our package offers a wide variety of R methods such that the usage of Gaussian process-based spatially varying coefficient models is similar to, say, linear models with `lm()` or general additive models with `gam()` from the package **mgcv**.

Computational details

Most of the presented examples in this paper were generated on a MacBook Pro laptop (macOS 11.4) equipped with an Intel(R) Core(TM) i5-8259U CPU (8 logical processing cores @ 2.3 GHz) and 8 GB of RAM. Results for the Lucas County data set were generated on a Ubuntu server (Ubuntu version 16.04.7) equipped with 8 Intel Xeons E7-2850 (a total of 80 logical processing cores @ 2.0 GHz) and 2 TB of RAM. The intermediate results can be found in the GIT repository https://git.math.uzh.ch/jdambo/jss-paper-open-access.

The results in this paper were obtained using R 4.1.0 with the **varycoef** 0.3.1 package. R itself and all packages mentioned or used (except for **INLA**) are available from the Comprehensive R Archive Network (CRAN) at https://CRAN.R-project.org/. For **INLA**, please consult https://www.r-inla.org/.

Acknowledgments

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A. Lucas County Data set

A.1. Model Estimation

The initial parameters for the optimization are provided by the output of a previous optimization.

```
R> library(varycoef)
R> ## -- Prepare Data -----
R> # subset of data
R> dat <- house[, c(
+    "price", "yrbuilt", "TLA", "lotsize", "garagesqft",
+    "stories", "wall", "garage",
+    "long", "lat"
+ )]
R> # drop two levels of stories due to low frequency
R> dat <- droplevels(
+    dat[!(dat$stories == "two+half" |
+          dat$stories == "three"), ]
+ )
R> # apply log transformations and standardize
R> log.vars <- c("TLA", "lotsize", "garagesqft")
R> for (lv in log.vars) {
+    dat[[paste0("l.", lv)]] <- log(dat[[lv]]+1)
+ }
R> std.vars <- c("yrbuilt", "l.TLA", "l.lotsize", "l.garagesqft")
R> for (sv in std.vars) {
+    dat[[paste0("Z.", sv)]] <- scale(dat[[sv]])
+ }
R> ## -- Build Model, Locations and Response Matrices ------
R> # locations (now in kilometers)
R> locs <- dat[, c("long", "lat")]/1000
R> # model matrix
R> FE_formula <- log(price) ~ 1 + Z.yrbuilt + I(Z.yrbuilt^2) +
+    Z.l.TLA + Z.l.lotsize + Z.l.garagesqft +
+    stories + wall + garage
R> # - fixed effects
R> X <- as.matrix(model.matrix(
+    FE_formula, data = dat
+ ))
R> # - random effects (SVC)
R> W <- as.matrix(X[, 1:6])
R> # response
R> y <- log(dat$price)
R> ## -- initial values and boundaries -----
R> load("~/data-analysis/lucas-county/last_val.RData")
R> init <- as.numeric(last_val)
```

```
R> lower <- c(rep(c(0.01, 0), ncol(W)), 1e-6)
R> upper <- c(rep(c(300, 2), ncol(W)), 2)
R> ## -- Prepare MLE ------
R> # start cluster
R> library(parallel)
R> cl <- makeCluster(parallel::detectCores() - 1)
R> clusterEvalQ(cl, {
+    library(spam)
+    library(varycoef)
+ })
R> # control parameters
R> control <- SVC_mle_control(
+    tapering = 1,
+    profileLik = TRUE,
+    init = init, lower = lower, upper = upper,
+    parallel = list(cl = cl, forward = FALSE, loginfo = TRUE)
+ )
R> ## -- Run MLE ------
R> # takes a couple of hours
R> fit <- SVC_mle(
+    y = y, X = X, W = W,
+    locs = locs, control = control,
+    optim.control = list(
+      trace = 6,
+      parscale = abs(ifelse(init == 0, 1, init)))
+ )
R> # stop Cluster
R> stopCluster(cl); rm(cl)
```

A.2. Remaining Estimated SVCs

In Figure 11, we present the remaining estimated spatially varying coefficients of the GP-based SVC model for the Lucas County data. Note that the coefficients for the total living area and the lot size are flat.
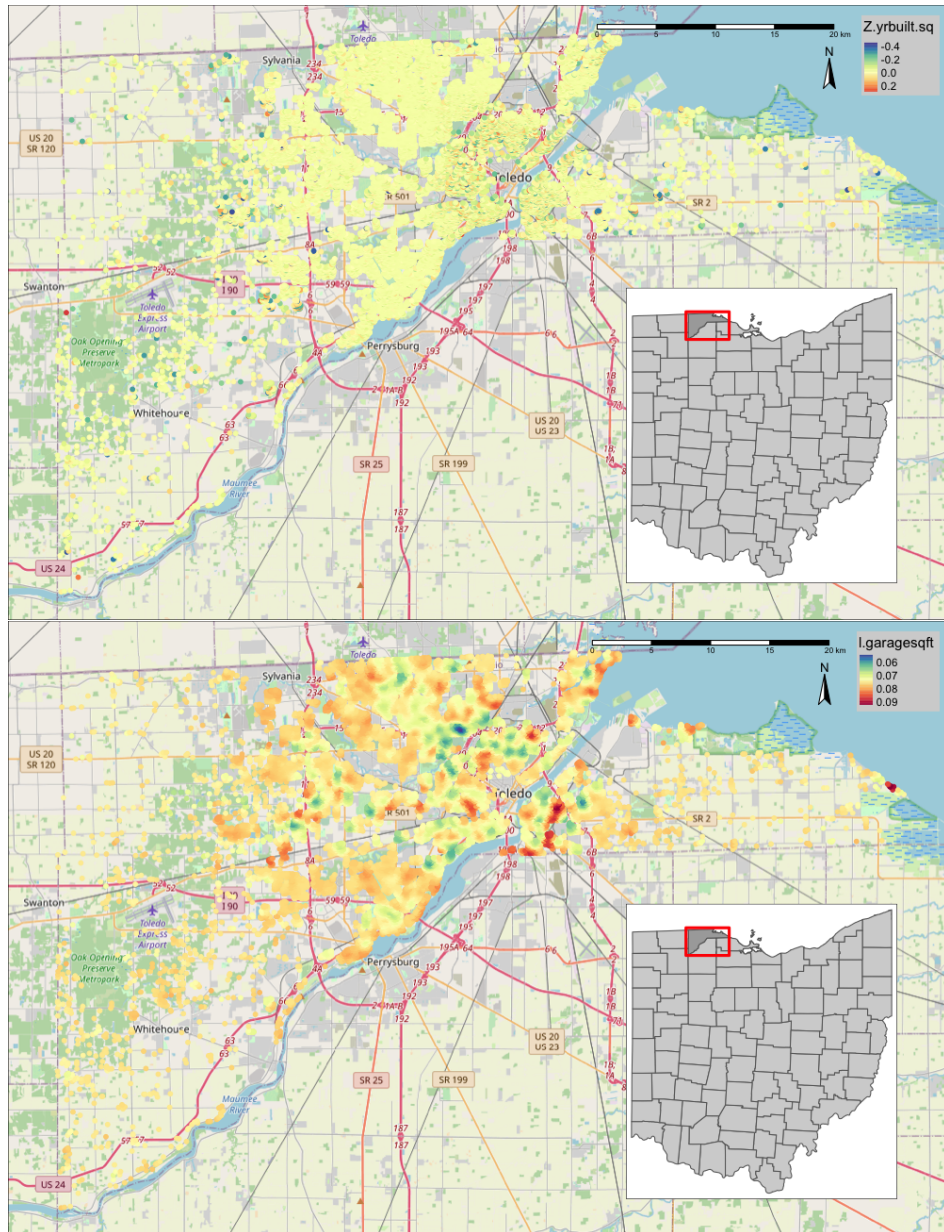
Figure 11:   Third and sixth estimated SVC.

B. US Growth Rate Data set

The code below runs the PMLE on the `uschange` data. The results were mentioned in Section 4.4.

```
R> ## -- US Change -------
R> library(fpp2)
R> data("uschange")
R> # divide times series data into...
R> str(uschange)
R> # ... variables and ...
R> train_dat <- as.data.frame(uschange)
R> # ... time points of observations
R> train_t <- as.numeric(time(uschange))
R> # visual inspection
R> autoplot(uschange, facet = TRUE)
R> pairs(train_dat)
R> # classical linear model
R> linmod <- lm(Consumption~., dat = train_dat)
R> summary(linmod)
R> ## -- MLE ------
R> # prepare for SVC model
R> X_train <- model.matrix(linmod)
R> y_train <- train_dat$Consumption
R> p <- ncol(X_train)
R> require(parallel)
R> cl <- makeCluster(detectCores()-1)
R> clusterEvalQ(
+    cl = cl,
+    {
+      library(spam)
+      library(varycoef)
+    })
R> # use this list for parallel argument in SVC_mle_control
R> parallel.control <- list(cl = cl, forward = TRUE, loginfo = TRUE)
R> # SVC Modeling
R> library(varycoef)
R> control <- SVC_mle_control(profileLik = TRUE, parallel = parallel.control)
R> SVC_model_mle <- SVC_mle(
+    y = y_train, X = X_train, locs = train_t,
+    control = control, optim.control = list(trace = 6)
+  )
R> summary(SVC_model_mle)
R> ## -- PMLE -----
R> control$extract_fun <- TRUE
R> obj_fun <- SVC_mle(
+    y = y_train,
```

```
+    X = X_train,
+    W = X_train,
+    locs = train_t,
+    control = control
+ )
R> ## grid
R> # set controls for SVC selection
R> sel_control1 <- SVC_selection_control(
+    method = "grid",
+    IC.type = "BIC",
+    r.lambda = c(1e-3, 1),
+    n.lambda = 10L,
+    CD.conv = list(N = 20, delta = 1e-8, logLik = FALSE),
+    parallel = control$parallel,
+    optim.args = list(
+      lower = SVC_model_mle$MLE$comp.args$liu$lower,
+      upper = SVC_model_mle$MLE$comp.args$liu$upper
+    ),
+    adaptive = TRUE
+ )
R> # run PMLE
R> time_start1 <- Sys.time()
R> PMLE_CD1 <- SVC_selection(
+    obj_fun, mle.par = cov_par(SVC_model_mle),
+    control = sel_control1,
+    approx = FALSE
+ )
R> time_end1 <- Sys.time()
R> ## MBO
R> sel_control2 <- SVC_selection_control(
+    method = "MBO",
+    IC.type = "BIC",
+    r.lambda = c(1e-3, 1),
+    n.init = 5L,
+    n.iter = 15L,
+    CD.conv = list(N = 20, delta = 1e-8, logLik = FALSE),
+    parallel = control$parallel,
+    optim.args = list(
+      lower = SVC_model_mle$MLE$comp.args$liu$lower,
+      upper = SVC_model_mle$MLE$comp.args$liu$upper
+    ),
+    adaptive = TRUE
+ )
R> # run PMLE
R> time_start2 <- Sys.time()
R> set.seed(1)
R> PMLE_CD2 <- SVC_selection(
```

```
+     obj_fun, mle.par = cov_par(SVC_model_mle),
+     control = sel_control2,
+     approx = FALSE
+   )
R> time_end2 <- Sys.time()
R> # timings
R> df_timings <- data.frame(
+     method = c("grid", "MBO"),
+     t_start = c(time_start1, time_start2),
+     t_end = c(time_end1, time_end2)
+   )
R> # save PMLEs
R> save(PMLE_CD1, PMLE_CD2, df_timings,
+       file = "data-analysis/uschange/sel-outcomes.RData")
```

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