# Package: NVCSSL (via r-universe)

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| Description Fits Bayesian regularized varying coefficient models with the Nonparametric Varying Coefficient Spike-and-Slab Lasso (NVC-SSL) introduced by Bai et al. (2023) <arxiv:1907.06477>.  Functions to fit frequentist penalized varying coefficients are also provided, with the option of employing the group lasso penalty of Yuan and Lin (2006)  <doi:10.1111 j.1467-9868.2005.00532.x="">, the group minimax concave penalty (MCP) of Breheny and Huang  <doi:10.1007 s11222-013-9424-2="">, or the group smoothly clipped absolute deviation (SCAD) penalty of Breheny and Huang (2015)  <doi:10.1007 s11222-013-9424-2="">.</doi:10.1007></doi:10.1007></doi:10.1111></arxiv:1907.06477> |  |  |  |  |
| License GPL-3  |  |  |  |  |
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NVC\_frequentist

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| NVC_frequentist | Fits frequentist penalized nonparametric varying coefficient (NVC) models |
|-----------------|---|
|                 |   |

## **Description**

This function implements frequentist penalized nonparametric varying coefficient (NVC) models. It supports the following penalty functions: the group lasso penalty of Yuan and Lin (2006), the group minimax concave penalty (MCP) of Breheny and Huang (2015), and the group smoothly clipped absolute deviation (SCAD) penalty of Breheny and Huang (2015). This function solves a penalized regression problem of the form,

$$argmax_{\gamma} \frac{1}{N} \ell(\gamma) + pen_{\lambda}(\gamma),$$

where N is the total number of observations,  $\ell(\gamma)$  is the loss function, and  $pen_{\lambda}(\cdot)$  is a penalty function with regularization parameter  $\lambda>0$ . Since the objective function is rescaled by 1/N, the penalty  $\lambda$  is typically smaller than the spike hyperparameter  $\lambda_0$  used by the NVC\_SSL function. The BIC criterion is used to select the optimal tuning parameter  $\lambda$ .

## Usage

## Arguments

| У       | $N \times 1$ vector of response observations $y_{11},, y_{1m_1},, y_{n1},, y_{nm_n}$  |
|---------|---|
| t       | $N \times 1$ vector of observation times $t_{11},, t_{1m_1},, t_{n1},, t_{nm_n}$  |
| X       | $N \times p$ design matrix with columns $[X_1,,X_p]$ , where the $k$ th column contains the entries $x_{ik}(t_{ij})$ 's   |
| n_basis | number of basis functions to use. Default is n_basis=8.   |
| penalty | string specifying which penalty function to use. Specify "gLASSO" for group lasso, "gSCAD" for group SCAD, or "gMCP" for group MCP.   |
| lambda  | grid of tuning parameters. If lambda is not specified (i.e. lambda=NULL), then the program automatically chooses a grid for lambda. Note that since the objective function is scaled by $1/N$ , the automatically chosen grid for lambda typically consists of smaller values than the default grid for lambda0 used by the function NVC_SSL. |

include\_intercept

Boolean variable for whether or not to include an intercept function  $\beta_0(t)$  in the estimation. Default is include\_intercept=TRUE.

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## Value

The function returns a list containing the following components:

t\_ordered all N time points ordered from smallest to largest. Needed for plotting.

classifications

 $p \times 1$  vector of indicator variables, where "1" indicates that the covariate is selected and "0" indicates that it is not selected. These classifications are determined by the optimal lambda chosen from BIC. Note that this vector does not include an intercept function.

beta\_hat  $N \times p$  matrix of the estimates for varying coefficient functions  $\beta_k(t), k = 1, ..., p$ , using the optimal lambda chosen from BIC. The kth column in the matrix is the kth estimated function at the observation times in t\_ordered.

beta0\_hat estmate of the intercept function  $\beta_0(t)$  at the observation times in t\_ordered for the optimal lambda chosen from BIC. This is not returned if include\_intercept = FALSE.

gamma\_hat estimated basis coefficients (needed for prediction) for the optimal lambda.

lambda\_min the individual lambda which minimizes the BIC. If only one value was originally passed for lambda, then this just returns that lambda.

lambda0\_all grid of all L regularization parameters in lambda. Note that since the objective function is scaled by 1/N for the penalized frequentist methods in the NVC\_frequentist function, the lambda\_all grid that is chosen automatically by NVC\_frequentist typically consists of smaller values than the default values in the lambda0\_all grid for NVC\_SSL.

BIC\_all  $L \times 1$  vector of BIC values corresponding to all L entries in lambda\_all. The lth entry corresponds to the lth entry in lambda\_all.

beta\_est\_all\_lambda

list of length L of the estimated varying coefficients  $\beta_k(t)$ , k=1,...,p, corresponding to all L lambdas in lambda\_all. The lth entry corresponds to the lth entry in lambda\_all.

beta0\_est\_all\_lambda

 $N \times L$  matrix of estimated intercept function  $\beta_0(t)$  corresponding to all L entries in lambda\_all. The lth column corresponds to the lth entry in lambda\_all. This is not returned if include\_intercept=FALSE.

gamma\_est\_all\_lambda

 $dp \times L$  matrix of estimated basis coefficients corresponding to all entries in lambda\_all. The lth column corresponds to the lth entry in lambda\_all.

classifications\_all\_lambda

 $p \times L$  matrix of classifications corresponding to all the entries in lambda\_all. The lth column corresponds to the lth entry in lambda\_all.

iters\_to\_converge

number of iterations it took for the group ascent algorithm to converge for each entry in lambda\_all. The *l*th entry corresponds to the *l*th entry in lambda\_all.

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#### References

Bai, R., Boland, M. R., and Chen, Y. (2023). "Scalable high-dimensional Bayesian varying coefficient models with unknown within-subject covariance." *arXiv pre-print arXiv:arXiv:1907.06477*.

Breheny, P. and Huang, J. (2015). "Group descent algorithms for nonconvex penalized linear and logistic regression models with grouped predictors." *Statistics and Computing*, **25**:173-187.

Wei, F., Huang, J., and Li, H. (2011). "Variable selection and estimation in high-dimensional varying coefficient models." *Statistica Sinica*, **21**:1515-1540.

Yuan, M. and Lin, Y. (2006). "Model selection and estimation in regression with grouped variables." *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, **68**:49-67.

## **Examples**

```
## Load data
data(SimulatedData)
attach(SimulatedData)
v = SimulatedData$v
t = SimulatedData$t
id = SimulatedData$id
X = SimulatedData[,4:103]
## Fit frequentist penalized NVC model with the SCAD penalty.
## Can set penalty as "gLASSO", "gSCAD", or "gMCP".
## No need to specify an 'id' argument when using NVC_frequentist() function
NVC_gSCAD_mod = NVC_frequentist(y, t, X, penalty="gSCAD")
## Classifications. First varying coefficients are selected as nonzero
NVC_gSCAD_mod$classifications
## Optimal lambda chosen from BIC
NVC_gSCAD_mod$lambda_min
## Plot first estimated varying coefficient function
t_ordered = NVC_gSCAD_mod$t_ordered
beta_hat= NVC_gSCAD_mod$beta_hat
plot(t_ordered, beta_hat[,1], lwd=3, type='l', col='blue',
     xlab="Time", ylim = c(-12,12), ylab=expression(beta[1])
## Plot third estimated varying coefficient function
plot(t_ordered, beta_hat[,3], lwd=3, type='1', col='blue',
     xlab="Time", ylim = c(-4,2), ylab=expression(beta[3]))
## Plot fifth estimated varying coefficient function
plot(t_ordered, beta_hat[,5], lwd=3, type='1', col='blue',
     xlab="Time", ylim = c(0,15), ylab=expression(beta[5]))
```

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## **Description**

This is a function to predict the responses  $y(t_{new})$  for new subjects at new time points  $t_{new}$  with new covariates  $X_{new}$ . The function accepts an estimated NVC model that was fit using either the NVC\_SSL or NVC\_frequentist functions and returns the predicted y(t)'s. This function can be used for either out-of-sample predictions or for in-sample predictions if the "new" subjects are the same as the ones used to obtain the fitted NVC model.

## Usage

```
NVC_predict(NVC_mod, t_new, id_new, X_new)
```

## **Arguments**

| NVC mod     | an object with a fitted NVC model returned by the NVC SSL or NVC  | : frequentist |
|-------------|---|---------------|
| ITT C_IIIOU | an object with a litted in a confidence of the inverse of inverse |               |

function

t\_new vector of new observation times

id\_new vector of new labels, where a label corresponds to one of the new subjects

X\_new new design matrix with columns  $[X_1, \ldots, X_p]$  where the kth column corre-

sponds to the kth covariate. X\_new must have the p columns, i.e. the same

number of varying coefficients estimated by NVC\_mod.

## Value

The function returns a list containing the following components:

id vector of each *i*th subject's label

time vector of each jth observation time for each ith subject

 $y_pred$  vector of predicted responses corresponding to each jth observation time for

each ith subject

#### References

Bai, R., Boland, M. R., and Chen, Y. (2023). "Scalable high-dimensional Bayesian varying coefficient models with unknown within-subject covariance." *arXiv pre-print arXiv:arXiv:1907.06477*.

## Examples

```
## Load simulated data
data(SimulatedData)
attach(SimulatedData)
y = SimulatedData$y
t = SimulatedData$t
id = SimulatedData$id
```

```
X = SimulatedData[,4:103]
## Fit frequentist penalized NVC model with the group lasso penalty.
## No need to specify an 'id' argument when using NVC_frequentist() function.
NVC_gLASSO_mod = NVC_frequentist(y=y, t=t, X=X, penalty="gLASSO")
## Make in-sample predictions. Here, we DO need to specify 'id' argument
NVC_gLASSO_predictions = NVC_predict(NVC_gLASSO_mod, t_new=t, id_new=id, X_new=X)
## Subjects
NVC_gLASSO_predictions$id
## Observation times
NVC_gLASSO_predictions$time
## Predicted responses
NVC_gLASSO_predictions$y_pred
## Fit NVC-SSL model to the data instead. Here, we do need to specify id
NVC_SSL_mod = NVC_SSL(y=y, t=t, id=id, X=X)
NVC_SSL_predictions = NVC_predict(NVC_SSL_mod, t_new = t, id_new=id, X_new=X)
## Subjects
NVC_SSL_predictions$id
## Observation times
NVC_SSL_predictions$time
## Predicted responses
NVC_SSL_predictions$y_pred
```

NVC\_SSL

Nonparametric Varying Coefficient Spike-and-Slab Lasso (NVC-SSL)

## **Description**

This function implements the Nonparametric Varying Coefficient Spike-and-Slab Lasso (NVC-SSL) model of Bai et al. (2023) for high-dimensional NVC models. The function returns the MAP estimator for the varying coefficients  $\beta_k(t), k = 1, ..., p$ , obtained from the ECM algorithm described in Bai et al. (2023). The BIC criterion is used to select the optimal spike hyperparameter  $lambda_0$ .

If the user specifies return\_CI=TRUE, then this function will also return the 95 percent pointwise posterior credible intervals for the varying coefficients  $\beta_k(t), k = 1, ..., p$ , obtained from Gibbs

sampling. If the number of covariates p is large, then the user can additionally use the approximate MCMC algorithm introduced in Bai et al. (2023) (approx\_MCMC=TRUE) which is much faster than the exact Gibbs sampler and gives higher simultaneous coverage.

Finally, this function returns the number of iterations and the runtime for the ECM algorithms and MCMC algorithms which can be used for benchmarking and timing comparisons.

## Usage

## **Arguments**

| <b>-</b>          |  |  |  |  |
|-------------------|--|--|--|--|
| У                 | $N \times 1$ vector of response observations $y_{11},,y_{1m_1},,y_{n1},,y_{nm_n}$  |  |  |  |
| t                 | $N \times 1$ vector of observation times $t_{11},, t_{1m_1},, t_{n1},, t_{nm_n}$   |  |  |  |
| id                | $N\times 1$ vector of labels, where each unique label corresponds to one of the subjects   |  |  |  |
| X                 | $N \times p$ design matrix with columns $[X_1,,X_p]$ , where the $k$ th column contains the entries $x_{ik}(t_{ij})$ 's                            |  |  |  |
| n_basis           | number of basis functions to use. Default is n_basis=8.  |  |  |  |
| lambda0           | grid of spike hyperparameters. Default is to tune lambda0 from the grid of decreasing values $(300,290,,20,10)$ .                                  |  |  |  |
| lambda1           | slab hyperparameter. Default is lambda1=1.   |  |  |  |
| а                 | hyperparameter in $B(a,b)$ prior on mixing proportion $\theta$ . Default is $a=1$ .  |  |  |  |
| b                 | hyperparameter in $B(a,b)$ prior on mixing proportion $\theta$ . Default is $b=p$ .  |  |  |  |
| c0                | hyperparameter in Inverse-Gamma $(c_0/2,d_0/2)$ prior on measurement error variance $\sigma^2$ . Default is $c_0=1$ .                              |  |  |  |
| d0                | hyperparameter in Inverse-Gamma $(c_0/2,d_0/2)$ prior on measurement error variance $\sigma^2$ . Default is $d_0=1$ .                              |  |  |  |
| nu                | degrees of freedom for Inverse-Wishart prior on $\Omega$ . Default is n_basis+2.   |  |  |  |
| Phi               | scale matrix in the Inverse-Wishart prior on $\Omega$ . Default is the identity matrix.  |  |  |  |
| include_intercept |  |  |  |  |
|                   | Boolean variable for whether or not to include an intercept function $\beta_0(t)$ in the estimation. Default is include_intercept=TRUE.            |  |  |  |
| tol               | convergence criteria for the ECM algorithm. Default is tol=1e-6.   |  |  |  |
| max_iter          | maximum number of iterations to run ECM algorithm. Default is $max\_iter=100$ .  |  |  |  |
| return_CI         | Boolean variable for whether or not to return the 95 percent pointwise credible bands. Set return_CI=TRUE if posterior credible bands are desired. |  |  |  |

Value

The function returns a list containing the following components:

fault is print\_iter=TRUE.

 ${\sf t\_ordered}$  all N time points ordered from smallest to largest. Needed for plotting classifications

 $p \times 1$  vector of indicator variables, where "1" indicates that the covariate is selected and "0" indicates that it is not selected. These classifications are determined by the optimal lambda0 chosen from BIC. Note that this vector does not include an intercept function.

beta\_hat  $N \times p$  matrix of the MAP estimates for varying coefficient functions  $\beta_k(t), k = 1$ 

1,...,p, using the optimal lambda0 chosen from BIC. The kth column in the matrix is the kth estimated function at the observation times in t\_ordered.

beta0\_hat MAP estimate of the intercept function  $\beta_0(t)$  at the observation times in t\_ordered

for the optimal lambda0 chosen from BIC. This is not returned if  $include\_intercept$ 

= FALSE.

gamma\_hat MAP estimates of the basis coefficients (needed for prediction) for the optimal

lambda0.

beta\_post\_mean  $N \times p$  matrix of the posterior mean estimates of the varying coefficient functions.

The kth column in the matrix is the kth posterior mean estimate for  $\beta_k(t)$  at the observation times in t\_ordered. This is not returned if return\_CI=FALSE.

beta\_CI\_lower  $N \times p$  matrix of the lower endpoints of the 95 percent pointwise posterior cred-

ible interval (CI) for the varying coefficient functions. The kth column in the matrix is the lower endpoint for the CI of  $\beta_k(t)$  at the observation times in

t\_ordered. This is not returned if return\_CI=FALSE.

beta\_CI\_upper  $N \times p$  matrix of the upper endpoints of the 95 percent pointwise posterior cred-

ible interval (CI) for the varying coefficient functions. The kth column in the matrix is the upper endpoint for the CI of  $\beta_k(t)$  at the observation times in

t\_ordered. This is not returned if return\_CI=FALSE.

beta0\_post\_mean

Posterior mean estimate of the intercept function  $\beta_0(t)$  at the observation times

in t\_ordered. This is not returned if return\_CI=FALSE.

beta0\_CI\_lower Lower endpoints of the 95 percent pointwise posterior credible intervals (CIs)

for the intercept function  $\beta_0(t)$  at the observation times in t\_ordered. This is

not returned if return\_CI=FALSE.

beta0\_CI\_upper Upper endpoints of the 95 percent pointwise posterior credible intervals (CIs) for the intercept function  $\beta_0(t)$  at the observation times in t\_ordered. This is not returned if return\_CI=FALSE.

gamma\_post\_mean

Posterior mean estimates of all the basis coefficients. This is not returned if return\_CI=FALSE.

gamma\_CI\_lower Lower endpoints of the 95 percent posterior credible intervals for the basis coefficients. This is not returned if return\_CI=FALSE.

gamma\_CI\_upper Upper endpoints of the 95 percent posterior credible intervals for the basis coefficients. This is not returned if return\_CI=FALSE.

post\_incl  $p \times 1$  vector of estimated posterior inclusion probabilities (PIPs) for each of the varying coefficients. The kth entry in post\_incl is the PIP for  $\beta_k$ . This is not returned if return\_CI=FALSE.

lambda@\_min the individual lambda@ which minimizes the BIC. If only one value was originally passed for lambda@, then this just returns that lambda@.

lambda0\_all grid of all L regularization parameters in lambda0. Note that since the objective function is scaled by 1/N for the penalized frequentist methods in the NVC\_frequentist function, the lambda\_all grid that is chosen automatically by NVC\_frequentist typically consists of smaller values than the default values in the lambda0\_all grid for NVC\_SSL.

BIC\_all  $L \times 1$  vector of BIC values corresponding to all L entries in lambda0\_all. The lth entry corresponds to the lth entry in lambda0\_all.

beta\_est\_all\_lambda0

list of length L of the estimated varying coefficients  $\beta_k(t)$ , k=1,...,p, corresponding to all L lambdas in lambda0\_all. The lth entry corresponds to the lth entry in lambda0\_all.

beta0\_est\_all\_lambda0

 $N \times L$  matrix of estimated intercept function  $\beta_0(t)$  corresponding to all L entries in lambda0\_all. The lth column corresponds to the lth entry in lambda0\_all. This is not returned if include\_intercept=FALSE.

gamma\_est\_all\_lambda0

 $dp \times L$  matrix of estimated basis coefficients corresponding to all entries in lambda0\_all. The lth column corresponds to the lth entry in lambda0\_all.

classifications\_all\_lambda0

 $p \times L$  matrix of classifications corresponding to all the entries in lambda0\_all. The lth column corresponds to the lth entry in lambda0\_all.

ECM\_iters\_to\_converge

number of iterations it took for the ECM algorithm to converge for each entry in lambda0\_all. The *l*th entry corresponds to the *l*th entry in lambda0\_all.

ECM\_runtimes  $L \times 1$  vector of the number of seconds it took for the ECM algorithm to converge for each entry in lambda0\_all. The lth entry corresponds to the lth entry in lambda0\_all.

gibbs\_runtime number of minutes it took for the Gibbs sampling algorithm to run for the total number of MCMC iterations given in gibbs\_iters

gibbs\_iters total number of MCMC iterations run for posterior inference

#### References

Bai, R., Boland, M. R., and Chen, Y. (2023). "Scalable high-dimensional Bayesian varying coefficient models with unknown within-subject covariance." *arXiv pre-print arXiv:arXiv:1907.06477*.

Bai, R., Moran, G. E., Antonelli, J. L., Chen, Y., and Boland, M.R. (2022). "Spike-and-slab group lassos for grouped regression and sparse generalized additive models." *Journal of the American Statistical Association*, **117**:184-197.

## **Examples**

```
## Load data
data(SimulatedData)
attach(SimulatedData)
y = SimulatedData$y
t = SimulatedData$t
id = SimulatedData$id
X = SimulatedData[,4:103]
## Fit NVC-SSL model. Default implementation uses a grid of 30 lambdas.
## Below illustration uses just two well-chosen lambdas
NVC_SSL_mod = NVC_SSL(y, t, id, X, lambda0=c(60,50))
## NOTE: Should use default, which will search for lambda0 from a bigger grid
# NVC_SSL_mod = NVC_SSL(y, t, id, X)
## Classifications. First 6 varying coefficients are selected as nonzero
NVC_SSL_mod$classifications
## Optimal lambda chosen from BIC
NVC_SSL_mod$lambda0_min
## Plot first estimated varying coefficient function
t_ordered = NVC_SSL_mod$t_ordered
beta_hat= NVC_SSL_mod$beta_hat
plot(t_ordered, beta_hat[,1], lwd=3, type='l', col='blue',
     xlab="Time", ylim = c(-12,12), ylab=expression(beta[1]))
## Plot third estimated varying coefficient function
plot(t_ordered, beta_hat[,3], lwd=3, type='l', col='blue',
     xlab="Time", ylim = c(-4,2), ylab=expression(beta[3]))
## Plot fifth estimated varying coefficient function
plot(t_ordered, beta_hat[,5], lwd=3, type='1', col='blue',
     xlab="Time", ylim = c(0,15), ylab=expression(beta[5]))
## If you want credible intervals, then set return_CI=TRUE to also run Gibbs sampler.
## Below, we run a total of 1000 MCMC iterations, discarding the first 500 as burnin
## and keeping the final 500 samples for inference.
NVC_SSL_mod_2 = NVC_SSL(y, t, id, X, return_CI=TRUE, approx_MCMC=FALSE,
```

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n\_samples=500, burn=500)

```
## Note that NVC_SSL() always computes a MAP estimator first and then
## initializes the Gibbs sampler with the MAP estimator.
## Plot third varying coefficient function and its credible bands
t_ordered = NVC_SSL_mod_2$t_ordered
beta_MAP = NVC_SSL_mod_2$beta_hat
beta_mean = NVC_SSL_mod_2$beta_post_mean
beta_CI_lower = NVC_SSL_mod_2$beta_CI_lower
beta_CI_upper = NVC_SSL_mod_2$beta_CI_upper
plot(t_ordered, beta_MAP[,3], lwd=3, type='l', col='blue', xlab="Time", ylim=c(-5,3), lty=1,
     ylab=expression(beta[3]), cex.lab=1.5)
lines(t_ordered, beta_mean[,3], lwd=3, type='1', col='red', lty=4)
lines(t_ordered, beta_CI_lower[,3], lwd=4, type='l', col='purple', lty=3)
lines(t_ordered, beta_CI_upper[,3], lwd=4, type='1', col='purple', lty=3)
legend("bottomleft", c("MAP", "Mean", "95 percent CI"), lty=c(1,4,3), lwd=c(2,2,3),
      col=c("blue","red","purple"), inset=c(0,1), xpd=TRUE, horiz=TRUE, bty="n")
## Plot fifth varying coefficient function and its credible bands
plot(t_ordered, beta_MAP[,5], lwd=3, type='l', col='blue', xlab="Time", ylim=c(-1,14), lty=1,
     ylab=expression(beta[5]), cex.lab=1.5)
lines(t_ordered, beta_mean[,5], lwd=3, type='1', col='red', lty=4)
lines(t_ordered, beta_CI_lower[,5], lwd=4, type='l', col='purple', lty=3)
lines(t_ordered, beta_CI_upper[,5], lwd=4, type='1', col='purple', lty=3)
legend("bottomleft", c("MAP", "Mean", "95 percent CI"), lty=c(1,4,3), lwd=c(2,2,3),
      col=c("blue","red","purple"), inset=c(0,1), xpd=TRUE, horiz=TRUE, bty="n")
```

SimulatedData

Simulated data for illustration

#### Description

This is a simulated dataset for illustration. It contains a total of N=436 observations at irregularly spaced time points for n=50 subjects. There are p=100 covariates.

## Usage

data(SimulatedData)

#### **Details**

This simulated dataset contains N=436 observations for n=50 subjects, with p=100 covariates. The first column y gives the response variables, the second column t gives the observation times, the third column id gives the unique IDs for each of the 50 subjects, and columns 4-103 (x1, ..., x100) give the covariate values.

This synthetic dataset is a slight modification from Experiment 2 in Section 5.1 of Bai et al. (2023). We use p = 100 for illustration, instead of p = 500 as in the paper.

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## References

Bai, R., Boland, M. R., and Chen, Y. (2023). "Scalable high-dimensional Bayesian varying coefficient models with unknown within-subject covariance." *arXiv pre-print arXiv:1907.06477*.

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