cpr: An R Package For Finding Parsimonious B-Spline Regression Models via Control Polygon Reduction and Control Net Reduction

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Abstract

The R package cpr provides tools for selection of parsimonious B-spline regression models via algorithms coined ‘control polygon reduction’ (CPR) and ‘control net reduction’ (CNR). B-Splines are commonly used in regression models to smooth data and approximate unknown functional forms. B-Splines are defined by a polynomial order and a knot sequence. Defining the knot sequence is non-trivial, but is critical with respect to the quality of the regression models. The focus of the CPR and CNR algorithms is to reduce a large knot sequence down to a parsimonious collection of elements while maintaining a high quality of fit. The algorithms are quick to implement and are flexible enough to support many types of data and regression approaches. The cpr package provides the end user collections of tools for the construction of B-spline basis matrices, construction of control polygons and control nets, and the use of diagnostics of the CPR and CNR algorithms.

Keywords: uni-variable b-splines, control polygons, multi-variable b-splines, control nets, knot selection, parsimony, tensor products, regression.

1. Introduction

Since their formal definition by Curry and Schoenberg (1947), B-splines have become a common tool for approximating functions and surfaces with piece-wise polynomials. The fields of numeric analysis, computer aided graphics and design, and statistics, to name only a few, have all benefited from B-splines. The richness of the B-spline literature is partially due to the lack of an analytic solution for optimal specification of the knot sequence defining the B-splines and the resulting spline functions Jupp (1978).

Methods for knot sequence specification vary based on secondary objectives. Controlling the wiggliness of the spline function has been done by using knot sequences of large cardinality and maximizing a penalized objective function (see O’Sullivan et al. (1986) and penalized B-splines of Eilers and Marx (1996), and Eilers and Marx (2010)). Estimation of the target function via the (regression) coefficients instead of the spline function results in a larger knot sequences (Lyche and Mørken 1988). If we allow the location of the knots to be free then there are many different adaptive methods (Biller 2000; Bakin et al. 1997; Friedman and Roosen...
1995; Miyata and Shen 2003; Ruppert and Carroll 2000; Richardson et al. 2008; Zhou and Shen 2001) for knot sequences specification.

What we found to be lacking from the literature was a method for knot sequences specification which was able to provide regression models with a high quality of fit with a small number of degrees of freedom. Further, we desired a model selection approach that was computationally efficient for B-spline models of uni-variable functions and extendible to multi-variable functions via tensor products of B-splines. For selection of such models, we developed the Control Polygon Reduction (CPR) (DeWitt 2017), a backward-step selection process based on the geometry of the control polygons about B-splines. Computational efficiency is gained by operating on sparse low-rank matrices instead of a dense high-rank design matrix.

cpr\(^1\) is an R (R Core Team 2016) package developed to provide extended functions for B-splines, tensor products, control polygons, control nets, and the model selection algorithms CPR and CNR.

This manuscript will focus on CPR and is structured as follows: Section 2 provides a brief overview of B-splines, control polygons, and the assessment of the influence of a knot on a spline function. The CPR algorithm is defined in Section 3. Section 4 has detailed examples of the use of the functions provided by cpr along with explanations for modeling functions of one continuous predictor. A brief overview of the CNR algorithm as associated tools is provided in Section 5.

## 2. Background

Consider the following general model

\[
y = f(x) + Z_1\beta + Z_2b + \epsilon,
\]  

(1)

where \(y\) is a \(n \times 1\) vector of responses and \(x\), another \(n \times 1\) vector, is a continuous predictor. The \(Z_1\beta\) denotes the \(n \times p\) design matrix and \(p \times 1\) coefficients vector for (optional) fixed effects, \(Z_2b\) the design matrix and coefficients for (optional) random effects, and \(\epsilon\) the model, or measurement, error. The function \(f\) is the primary focus of our work, we aim to model this function with parsimonious B-splines.

The control polygon reduction (CPR) model selection approach is a backward-step selection process. By starting with a large number of knots, CPR omits the least influential knot at each step, between regression fits.

In this section we present an overview of B-splines, control polygons, and introduce our metric for assessing the relative influence of an internal knot. Additional detail on B-splines can be found in de Boor (2001) and Prautzsch et al. (2002).

### 2.1. Uni-variable B-splines and Control Polygons

A B-spline basis matrix is defined by a polynomial order \(k\) and knot sequence \(\xi\) with the common construction of \(k\)-fold knots on the boundaries, set to the minimum and maximum

\(^1\)Released Version: https://cran.r-project.org/package=cpr; Developmental Version: https://github.com/dewittpe/cpr
of the support, \( l \geq 0 \) interior knots, and sorted in a non-decreasing order. The matrix,

\[
B_{k,\xi}(x) = \begin{pmatrix}
B_{1,k,\xi}(x_1) & B_{2,k,\xi}(x_1) & \cdots & B_{k+l,k,\xi}(x_1) \\
B_{1,k,\xi}(x_2) & B_{2,k,\xi}(x_2) & \cdots & B_{k+l,k,\xi}(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
B_{1,k,\xi}(x_n) & B_{2,k,\xi}(x_n) & \cdots & B_{k+l,k,\xi}(x_n)
\end{pmatrix},
\]

is constructed via de Boor’s recursive formula:

\[
B_{j,k,\xi}(x) = \omega_{j,k,\xi}(x) B_{j,k−1,\xi}(x) + (1 − \omega_{j+1,k,\xi}) B_{j+1,k−1,\xi}(x),
\]

with

\[
B_{j,k,\xi}(x) = 0 \text{ for } x \notin [\xi_j, \xi_{j+k}], \quad B_{j,1,\xi}(x) = \begin{cases} 1 & x \in [\xi_j, \xi_{j+1}) \\ 0 & \text{otherwise}, \end{cases}
\]

and

\[
\omega_{j,k,\xi}(x) = \begin{cases} 0 & x \leq \xi_j \\ \frac{x−\xi_j}{\xi_{j+k−1}−\xi_j} & \xi_j < x < \xi_{j+k−1} \\ 1 & \xi_{j+k−1} \leq x \end{cases}.
\]

The basis matrix \( B_{k,\xi}(x) \) provides a partition of unity over the support of \( x \), i.e., all rows sum to one, and defines a spline space \( S_{k,\xi} = \text{span} \ B_{k,\xi} \). The spline function, \( f(x) \in S_{k,\xi} \), is a convex sum the coefficients \( \theta_\xi \),

\[
f(x) = B_{k,\xi}(x) \theta_\xi = \sum_{j=1}^{k+l} B_{j,k,\xi}(x) \theta_{j,\xi}.
\]

There is no one-to-one association between the elements of the knot sequence, cardinality \( n(\xi) = 2k+l \) and the coefficients, \( n(\theta_\xi) = k+l \). However, a meaningful geometric relationship between \( \xi \) and \( \theta_\xi \) does exist in the form of a control polygon, \( CP_{k,\xi,\theta_\xi} \), a strong convex hull for \( B_{k,\xi}(x) \theta_\xi \),

\[
CP_{k,\xi,\theta_\xi} = \left\{ \left( \xi_j^*, \theta_{j,\xi}^* \right) \right\}_{j=1}^{k+l}; \quad \xi_j^* = \frac{1}{k−1} \sum_{i=1}^{k−1} \xi_{j+i}.
\]

\( CP_{k,\xi,\theta_\xi} \) is a sequence of \( k+l \) control vertices. We may interpret the control polygons as a piecewise linear function approximating the spline function \( B_{k,\xi}(x) \theta_\xi \). Changes in convexity and other subtle characteristics of the spline function are exaggerated by the control polygon. An example basis, spline function, and control polygon are shown in Figure 1. The control polygons are helpful for illustrating the relationship between two splines with \( \xi_1 \subset \xi_2 \).

### 2.2. Relationship Between Splines of Different Dimensions

Consider two knot sequences \( \xi \) and \( \xi' \). Then, for a given polynomial order \( k \), \( S_{k,\xi} \subset S_{k,\xi' \cup \xi'} \) (de Boor 2001, pg 135). Given this relationship between spline spaces, and the convex sums generating spline functions, Bohm (1980) presented a method for refining \( \xi \) without affecting the spline function. Specifically, for \( \xi \) and \( \xi' \) with \( n(\xi') = \sum_{x \in \xi'} 1_{(\min(\xi), \max(\xi))}(x) \), there exists an \( \theta_{\xi' \cup \xi} \) such that \( B_{k,\xi' \cup \xi}(x) \theta_{\xi' \cup \xi} = B_{k,\xi}(x) \theta_\xi \), for all \( x \in [\min(\xi), \max(\xi)] \).
From (9) we know that if \( \xi_j \in \xi \) has no influence on \( B_{k,\xi} (x) \theta_\xi \) then the regression coefficients \( \theta_{\xi \setminus \xi_j} \) are such that
\[
B_{k,\xi} (x) \theta_\xi = B_{k,\xi \setminus \xi_j} (x) \theta_{\xi \setminus \xi_j} \quad \text{with} \quad \theta_\xi = W_{k,\xi \setminus \xi_j} (\xi_j) \theta_{\xi \setminus \xi_j}.
\]
In practice we do not expect this equality to hold. Instead, we expect to observe, under the assumption that $\xi_j$ has no influence,

$$\theta_\xi = W_{k,\xi \setminus \xi_j} (\xi_j) \theta_{\xi \setminus \xi_j} + \epsilon$$

for some deviations $\epsilon$. As $\theta_{\xi \setminus \xi_j}$ is unknown, we may estimate it via least squares, i.e.,

$$\theta_{\xi \setminus \xi_j} = \left(W_{k,\xi \setminus \xi_j}^T (\xi_j) W_{k,\xi \setminus \xi_j} (\xi_j)\right)^{-1} W_{k,\xi \setminus \xi_j}^T (\xi_j) \theta_{\xi}.$$  \hspace{1cm} (12)

As illustrated in Figure 2 the spline initial spline $B_{k,\xi} (x) \theta_{\xi}$ and $B_{k,\xi \setminus \xi_j} (x) \theta_{\xi \setminus \xi_j}$ will differ. The control polygons help to elucidate the differences between these two splines. A measure of the difference between the two splines or between the two control polygons is needed to assess the influence of $\xi_j$. If we ‘reinsert’ $\xi_j$ into $\xi \setminus \xi_j$ then we can get a vector of ordinates $\theta_{(\xi \setminus \xi_j) \cup \xi_j}$ to approximate $\theta_{\xi}$. Again using (9) we find the values of $\theta_{(\xi \setminus \xi_j) \cup \xi_j}$,

$$\theta_{(\xi \setminus \xi_j) \cup \xi_j} = W_{k,\xi \setminus \xi_j} (\xi_j) \theta_{\xi \setminus \xi_j}$$

$$= W_{k,\xi \setminus \xi_j} (\xi_j) \left(W_{k,\xi \setminus \xi_j}^T (\xi_j) W_{k,\xi \setminus \xi_j} (\xi_j)\right)^{-1} W_{k,\xi \setminus \xi_j}^T (\xi_j) \theta_{\xi}.$$  \hspace{1cm} (13)

By this construction, $B_{k,\xi \setminus \xi_j} (x) \theta_{\xi \setminus \xi_j} = B_{k,(\xi \setminus \xi_j) \cup \xi_j} (x) \theta_{(\xi \setminus \xi_j) \cup \xi_j}$. The control polygons $CP_{k,\xi \setminus \xi_j}$ and $CP_{k,(\xi \setminus \xi_j) \cup \xi_j}$ have the same abscissae but differ in their ordinates. The squared length of the residual vector, i.e., the squared Euclidean distance between the ordinates $\theta_{\xi}$ and $\theta_{(\xi \setminus \xi_j) \cup \xi_j}$ is the influence weight for $\xi_j$. That is, the influence weight of $\xi_j \in \xi$ for $CP$ is

$$w_j = \left\| \theta_{\xi} - \theta_{(\xi \setminus \xi_j) \cup \xi_j} \right\|_2^2$$

$$= \left\| \left(1 - W_{k,\xi \setminus \xi_j} (\xi_j) \left(W_{k,\xi \setminus \xi_j}^T (\xi_j) W_{k,\xi \setminus \xi_j} (\xi_j)\right)^{-1} W_{k,\xi \setminus \xi_j}^T (\xi_j) \right) \theta_{\xi} \right\|_2.$$  \hspace{1cm} (14)

The influence weights $w_j$ are non-negative and provide a relative measure of the influence of knots with in a sequence. See Figure 2 to compare the relative influence of $\xi_6$ and $\xi_8$ on the spline. Knot $\xi_6$ has a smaller influence weight, $w_6 = 0.278$, than $\xi_6$, $w_6 = 0.539$. As such, if we were required to reduce the cardinality of $\xi$ by one, then omission of $\xi_8$ would be preferable to the omission of $\xi_6$ because $\xi_8$ has a lower influence on the spline function than $\xi_6$.

### 3. Control Polygon Reduction

CPR is based on the assumption that $f$ in (1) can be sufficiently modeled by $B_{k,\xi} (x) \theta_{\xi} \in \mathbb{S}_{k,\xi}$. If we start searching for $B_{k,\xi} (x) \theta_{\xi}$ in a larger space $\mathbb{S}_{k,\xi \cup \xi'}$, then there must be at least one internal knot within $\xi \cup \xi'$ which is unnecessary to sufficiently model $f$.

By starting with a large knot sequence, $n (\xi) - 2k = L$ internal knots, is not without precedence. Large quantities of internal knots have been used, and strongly encouraged by Edlers and Marx (1996, 2010) and Binder and Tutz (2008). While the B-spline models are sensitive to knot location, the difference between a location of $\xi_j$ and $\xi_j + \epsilon$, for some small $|\epsilon| > 0$, is negligible.
Figure 2: Two examples of omitting and reinserting a knot to determine the influence of the knot on the spline function. The original control polygon is as in Figure 1b. The top row of plots here illustrate the influence of $\xi_6$ and the bottom row illustrate the influence of $\xi_8$. In the left column we present the original control polygon $CP_{k,\xi,\theta|\xi}$ and the control polygon based on a coarsened knot sequence $CP_{k,\xi|\xi,\theta|\xi}$. The right column shows the original control polygon, the coarsened control polygon, and the control polygon after reinsertion of $\xi_j$, $CP_{k,\xi|\xi \cup \xi_j,\theta|\xi_j}$. The influence weights of $\xi_6$ and $\xi_8$ are 0.539 and 0.278 respectively.
CPR is a backward-step model selection algorithm—we start with a large degree of freedom model and reduce the degrees of freedom incrementally. Final selection of the model is not done by an automated stopping criterion. Instead, sequentially larger models, starting with the zero internal knot model, are assessed by fit statistics or visual inspection until the analyst is satisfied that an additional knot provides only negligibly better fit.

As a model selection method, CPR is preferable to likelihood based forward-step, backward-step, and grid search methods. First, a forward-step method requires placing one knot somewhere on the support, generally on the median, then placing two knots, generally on the tertiles, and so forth. The model space is limited to only one model of each dimension. Further, sequential models are not within the same spline space. This can make finding an acceptable model difficult as higher dimensional models may be selected so that a needed low dimensional knot sequence is used within the larger knot sequence. CPR allows for the location of interior knots to be selected, that is, a one knot model may have the knot at any location, depending on initial knot sequence construction. The difference computational time required to run CPR versus a forward-step process is negligible.

Using a grid search of possible knot locations is computationally impractical. For \( L \) possible initial knot locations there are \( \sum_{l=0}^{L} \binom{L}{l} = 2^L \) possible models to fit. With \( L = 20 \) possible knot locations there would be 1,048,576 regression models. Likely more models than data observations, and simply too computationally expensive to be done.

Using a backward-step likelihood based selection method requires far fewer regression model fits. For \( L \) possible knot locations there are \( L(L + 1)/2 + 1 \) regression models to fit, that is, 211 models for twenty possible locations, 1,276 models for fifty possible locations, and 5,051 models for one-hundred possible locations. The computation time can still be considerable, but at least the backward-step approach is reasonable, compared to the grid search.

CPR is similar to the backward-step likelihood based approaches, but requires only \( L + 1 \) regression models to be fitted for a set of \( L \) initial knot locations. The computation time saved by requiring only \( L + 1 \) versus \( L(L + 1)/2 + 1 \) can be considerable.

The CPR Algorithm

1. Start with a knot sequence with a sufficiently large number of interior knots, say \( L = 50 \), and set \( l = L \) to index models.

2. Use an appropriate regression modeling approach to fit a regression model for (1).

3. Construct the control polygon for the current \( \xi^{(l)} \) and \( \theta^{(l)} \) estimate.

4. Use \( CP_k, \xi^{(l)}, \theta^{(l)} \) and (14) to find the influence weight for all internal knots.

5. Coarsen the knot sequence by removing the knot with the smallest influence weight.

6. Refit the regression model using the coarsened knot sequence and index \( l = l - 1 \).

7. Repeat steps 3 through 6 until all internal knots have been removed, \( i.e., \) if \( l \geq 0 \) goto 3, else goto 8.

8. Select the preferable model by visual inspection of diagnostic graphics.
There are two diagnostic plots we suggest using for step 8. 1) Consider sequential control polygons. Starting with \( l = 0 \) internal knots, compare the control polygon for \( l \) and \( l + 1 \) internal knots. When the control polygon with \( l + 1 \) internal knots appears to be nested within the control polygon based on \( l \) internal knots, the preferable model is the one with \( l \) internal knots. 2) Plot the root mean squared error (RMSE) as a function of the number of internal knots. When there is no longer a meaningful decrease in the RMSE between models with \( l \) and \( l + 1 \) internal knots, select the model with \( l \) internal knots. These diagnostic plots will be shown in examples below.

Lyche and Mørken (1988) presented a similar grouped knot removal process when estimating a function with no noise via B-splines. CPR differs from Lyche and Mørken in four key ways: 1) CPR is applicable to noisy data with an unknown target function whereas Lyche and Mørken had a known target function. 2) The regression models selected by CPR will approximate \( f(x) \approx B_{k,\xi}(x)\theta \) whereas Lyche and Mørken made estimates of the form \( f(\xi_i^*) \approx \theta_i \). 3) CPR coarsens the knot sequence by removal of one element and then refits the regression model. Lyche and Mørken coarsen the knot sequence via removal of multiple knots before refitting the regression model. 4) Given that the target function is unknown, CPR has no automated stopping criteria.

4. The cpr Package

The objective of the cpr is to provide a simple, intuitive, and clean API for the CPR algorithm. A four-line script is the foundation of the expected use case.

```
R> initial_cp <- cp(y ~ bsplines(x), data = your_data_frame)
R> cpr_run <- cpr(initial_cp)
R> plot(cpr_run)
R> preferable_cp <- cpr_run[[4]]
```

In the first line the initial control polygon is constructed via a common regression statement. Passing the initial control polygon object to the cpr function applies the CPR algorithm and returns a list of control polygons in the cpr_run object. The plot call generates the diagnostic plots used for selecting a preferable model. Lastly, the preferable control polygon is retrieved.

In the following subsections we will present details on the relevant calls noted above. We start with bsplines for generating B-spline bases and follow with cp for construction of control polygons. We will then illustrate the use of cpr for selecting good fitting parsimonious B-spline regression models.

cpr relies on Rcpp (Eddelbuettel et al. 2011; Eddelbuettel 2013) and RcppArmadillo (Eddelbuettel and Sanderson 2014) to gain computational efficiency for several functions and matrix arithmetic. Heavy reliance on dplyr (Wickham and Francois 2016) and tidyr (Wickham 2016) for data manipulation. Two-dimensional graphics are generated via ggplot2 (Wickham 2009). Three-dimensional graphics are generated using either rgl (Adler et al. 2016) for dynamic iterative graphics, or plot3D (Soetaert 2016) of static graphics.

4.1. B-Splines
Table 1: Comparison of the arguments, with default values, for `splines::bs` and `cpr::bsplines`. The attributes for the resulting `splines::bs` and `cpr::bsplines` objects are also reported.

| splines::bs                  | cpr::bsplines |
|-----------------------------|---------------|
| Arguments                   |               |
| x                           | x             |
| df                          | df            |
| knots                       | iknots        |
| degree = 3                  | order = 4L    |
| Boundary.knots = range(x)   | bknots = range(x) |
| intercept = FALSE           | –             |
| Attributes                  |               |
| dim                         | dim           |
| degree                      | order         |
| knots                       | iknots        |
| Boundary.knots              | bknots        |
| intercept                   | –             |
| –                           | xi            |
| –                           | xi_star       |
| class                       | class         |
| –                           | call          |
| –                           | environment   |

The standard installation of R includes the `splines` (R Core Team 2016) package and the `splines::bs` function for generating the basis matrix of B-splines, i.e. the matrix shown in (2). The `cpr` package provides an alternative function, `cpr::bsplines` for generating B-spline basis matrices with the class `cpr::bs`. The differences in the functional arguments and the attributes of the return objects between `splines::bs` and `cpr::bsplines` are listed in Table 1.

A major difference between the two functions is related to the `intercept` argument of `splines::bs`. By default, `splines::bs` will omit the first column of the basis whereas `cpr::bsplines` will return the whole basis. The omission of the first column of the basis generated by `splines::bs` allows for additive `splines::bs` calls to be used on the right-hand-side of a regression formula and generate a full rank design matrix. If additive `cpr::bsplines` calls, or additive `splines::bs` with `intercept = TRUE`, are on the right-hand-side of the regression equation the resulting design matrix will be rank deficient. This is a result of the B-splines being a partition of unity. As the CPR algorithm is based on having the whole basis, the `cpr::bsplines` function is provided to make it easy to work with the whole basis without having to remember to use non-default settings in `splines::bs`. The default call `splines::bs(x)` is replicated by `cpr::bsplines(x)[, -1]` and the default call `cpr::bsplines(x)` is replicated `splines::bs(x, intercept = TRUE)`.

Specifying the polynomial order and knot sequence between the two functions differ between `splines::bs` and `cpr::bsplines`. `splines::bs` uses the polynomial `degree` whereas `cpr::bsplines` uses the polynomial `order` (order = degree + 1) to define the splines. The default for both `splines::bs` and `cpr::bsplines` is to generate cubic B-splines.
For both `splines::bs` and `cpr::bsplines` only the degrees of freedom or the internal knots need to be specified. If the end user specifies both, the specified knots take precedence. If only `df` is specified then `df - order` internal knots will be generated. `splines::bs` and `cpr::bsplines`. For a numeric vector `x`, `splines::bs` will generate a sequence of internal knots via a call equivalent to

```r
R> knots <- df + order + (1L - intercept)
R> stats::quantile(x,
+    probs = seq(0, 1, length = length(knots) + 2L)[-c(1, length(knots) + 2L)])
```

whereas `cpr::bsplines` will generate a sequence equivalent to

```r
R> stats::quantile(unique(x)[-c(1, length(unique(x)))],
+    probs = seq(1, df - order, by = 1) / (df - order + 1))
```

The function `cpr::trimmed_quantile` is provided to generate such sequences.

The return object from both `splines::bs` and `cpr::bsplines` is a matrix. The attributes returned include the argument values used to construct the basis. The major difference in the attributes between the two objects is that `cpr::bsplines` returns the full knot sequence, $\xi$, in the `xi` element and the Greville sites, $\xi^*$ in the `xi_star` element. These attributes are used in the construction of control polygons. Lastly, the classes for the two objects differ: `splines::bs` returns a three classes, `c("bs", "basis", "matrix")` and `cpr::bsplines` returns two classes, `c("cpr_bs", "matrix")`. An example construction and structure are below.

```r
R> bmat <- bsplines(x = seq(0, 6, length = 500),
+    iknots = c(1.0, 1.5, 2.3, 4.0, 4.5))
R> bmat
```

Matrix dims: [500 x 9]

```
[,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9]
[1,] 1.000  0.0000  0.000000  0.00e+00 0  0  0  0  0
[2,] 0.964  0.0354  0.000287  5.04e-07 0  0  0  0  0
[3,] 0.930  0.0693  0.001137  4.03e-06 0  0  0  0  0
[4,] 0.896  0.1018  0.002537  1.36e-05 0  0  0  0  0
[5,] 0.863  0.1330  0.004471  3.22e-05 0  0  0  0  0
[6,] 0.830  0.1627  0.006924  6.30e-05 0  0  0  0  0
```

There is no default method for plotting `splines::bs` objects. If the numeric vector `x` is sorted, then a minimally useful basis plot can be generated via `graphics::matplot`. The `cpr` package provides a plotting method for the `cpr_bs` objects. The plotting method returns a `c("gg", "ggplot")` object and can be modified by adding additional layers as would be done for any other `ggplot` object. For example, the basis plot in Figure 1a was generated by

```r
R> plot(bmat, show_xi = TRUE, show_x = TRUE, color = TRUE, digits = 1) +
   + theme(text = element_text(family = "Times", size = 10))
```
4.2. Control Polygons

cpr_cp objects are constructed by the S3 generic function

R> methods("cp")

[1] cp.cpr_bs* cp.formula*
see '?methods' for accessing help and source code

The cpr:::cp.cpr_bs method take a cpr_bs object and a vector of ordinates to construct a control polygon as defined in (7). For example, the control polygon showing in Figure 1b is generated by the bmat above and the following ordinates.

R> bmat <- bsplines(x = seq(0, 6, length = 500),
+ iknots = c(1.0, 1.5, 2.3, 4.0, 4.5))
R> theta <- c(1, 0, 3.5, 4.2, 3.7, -0.5, -0.7, 2, 1.5)
R> eg_cp <- cp(bmat, theta)
R> str(eg_cp)

List of 10
$ cp :Classes 'tbl_df', 'tbl' and 'data.frame': 9 obs. of 2 variables:
..$ xi_star: num [1:9] 0 0.333 0.833 1.6 2.6 ... 
..$ theta : num [1:9] 1 0 3.5 4.2 3.7 -0.5 -0.7 2 1.5 
$ xi : num [1:13] 0 0 0 0 1 1.5 2.3 4 4.5 6 ...
$ iknots : num [1:5] 1 1.5 2.3 4 4.5
$ bknots : num [1:2] 0 6
$ order : num 4
$ call : language cp.cpr_bs(x = bmat, theta = theta)
$ keep_fit: logi NA
$ fit : logi NA
$ loglik : logi NA
$ rmse : logi NA
- attr(*, "class")= chr [1:2] "cpr_cp" "list"

The resulting cpr_cp object seems trivial. A data.frame with the Greville sites and the given ordinates, along with attributes of the B-spline basis. There are several elements related to regression model fits which are NA when a cpr.cpr.bs is used to generate the control polygon. The regression related elements of a cpr_cp object are populated when the control polygon is generated using the cpr:::cp.formula method.

The cp.formula method is one of the most useful functions provided in cpr. This method uses regression methods to determine the control vertices and is called many times when running the CPR algorithm.

R> str(cpr:::cp.formula)

function (formula, data, method = stats::lm, ..., keep_fit = FALSE, check_rank = TRUE)
The arguments for this function are

- **formula** a regression formula, sufficient for the regression method which contains one call to `bsplines` on the right-hand-side.
- **data** a required `data.frame` containing the variables noted in the `formula`.
- **method** the regression method. By default this is the `lm` call from the base `stats` package. This regression method is used to estimate the ordinates for the control polygon.
- ... additional arguments passed to `method`.
- **keep_fit** If TRUE the object returned from `method` is stored in the resulting `cpr_cp` object. When FALSE only some summary statistics are retained.
- **check_rank** checks that the design matrix for the regression model is sufficient. This is done via the `cpr::matrix_rank` function.

A simple example, fitting the sine function with a cubic B-spline with ten internal knots, is below.

```R
R> dat <- tibble::data_frame(x = seq(-pi, pi, length = 200), + y = sin(x))
R> eg_cp2 <- cp(y ~ bsplines(x = x, df = 14), data = dat)
```

A quick note about how `cp.formula` generates design matrices. By construction, full B-spline basis matrix, a partition of unity, is returned by `cpr::bsplines`. The standard intercept in a regression model, implicit in R regression formulae, would be co-linear with the basis and a rank deficient design matrix would be generated. To elevate this issue, `cp.formula` automatically prepends the right-hand-side of the formula with 0 + to omit the intercept. This is also consistent with (1), a varying means model. It is also worth noting that additional additive terms can be added to the right-hand-side of the formula. The code `cp.formula` call will correctly build design matrices for model formulae when additive continuous variables and/or categorical variables are specified.

### 4.3. Relative Influence of the Knots

Our metric for assessing the relative influence of a knot was derived via the geometry of control polygons. Thus, `cpr` provides the `cpr::influence_of` function to calculate and provide the relative influence weight for each internal knot of a given `cpr_cp` object.

```R
R> influence_of(eg_cp)
# A tibble: 5 × 4
  index iknots w  rank
     <int> <dbl> <dbl> <dbl>
1     5  1.0  1.283   5
2     6  1.5  0.539   2
3     7  2.3  0.559   3
4     8  4.0  0.278   1
5     9  4.5  0.648   4
```
The default behavior of \texttt{influence_of} is to return the influence weight of all internal knots. The end user may request only a subset of knots be evaluated by passing the \texttt{indices}² of the knot of interest as the second argument to \texttt{influence_of}. The output printed to the console gives the index of each knot, the value of the knot, weight, and rank with rank \(= 1\) given to the least influential. The structure of the returned \texttt{cpr_influence_of} object is more complex than the output belies.

\begin{verbatim}
R> str(influence_of(eg_cp), max.level = 1)

List of 5
$ weight :Classes 'tbl_df', 'tbl' and 'data.frame': 5 obs. of 4 variables:
 ..- attr(*, "class")= chr [1:2] "cpr_cp" "list"
$ indices : int [1:5] 5 6 7 8 9
$ coarsened_cp :List of 5
$ reinserted_cp:List of 5
 ..- attr(*, "class")= chr "cpr_influence_of"

The \texttt{weight data.frame} is what is shown in the console. The original control polygon and a lists of each coarsened and reinserted control polygon are also returned. These lists of control polygons are useful for plotting the results. A plot similar to the right column of Figure 2 can be generated via:

\begin{verbatim}
R> plot(influence_of(eg_cp, c(6, 8)))
\end{verbatim}

4.4. Model Selection via Control Polygon Reduction

Here we demonstrate model selection via the CPR algorithm. In the following example we will use the \texttt{spdg} data set provided in the \texttt{cpr} package to model the progesterone hormone profile expressed during a menstrual cycle. The \texttt{spdg} data set is a simulated data set based on summary statistics of a subset of the Study of Women’s Health Across the Nation (SWAN) Daily Hormone Study (DHS) (Santoro \textit{et al.} 2003). SWAN is a “multi-site longitudinal, epidemiologic study designed to examine the health of women during their middle years.” The DHS was a specific sub-study in which subject provided first evacuation urine samples every day for a full menstrual cycle. Pregnanediol glucuronide (PDG), the urine metabolite of progesterone, was one of four reproductive hormones measured from the urine samples. The summary statistics and script used to generate the simulated data set can be found in the github repository for the \texttt{cpr} package, \url{https://github.com/dewittpe/cpr/tree/master/data-raw}.

\begin{verbatim}
R> str(spdg)

Classes 'tbl_df', 'tbl' and 'data.frame': 24730 obs. of 9 variables:
$ id : int 1 1 1 1 1 1 1 1 1 1 ...

²indices based on the full knot sequence, not just the interior knots. That is, for a fourth order spline, the first interior knot is index 5 as knots 1:4 are the left boundary knots.
The `spdg` data set contains PDG values for one full cycle from 864 subjects. Subject level variables are `age` in years, time-to-menopause, `ttm`, for years before reaching menopause, `ethnicity`, and body-mass-index, `bmi`. `day_of_cycle` are positive integers and `day_from_dlt` give the day away from the day of luteal transition (DLT). The DLT is the day between the follicular phase and luteal phase of the cycle. `day_from_dlt == 0` is the DLT, negative values are for the follicular phase, and positive values for the luteal phase. `day` is a mapping of `day_from_dlt` to $[-1, 0]$ with `day == 0` being the DLT. The follicular and luteal phases are mapped to $[-1, 0)$ and $(0, 1]$ respectively via a linear mapping. Lastly, the simulated PDG values are given in the `pdg` element. Figure 3 shows the log$_{10}$ (PDG) values by `day` for the `spdg` data set.

We will start our search for a parsimonious B-spline regression model with a high quality of fit with fourth order B-splines and fifty internal knots. We will fit a linear mixed model via `lmer` from the `lme4` package (Bates et al. 2015).

```
R> initial_cp4 <- cp(log10(pdg) ~ bsplines(day, df = 54) + (1|id),
```
Figure 4: CPR diagnostic plots. (a) show the sequential control polygons. Noticeable differences between the control polygons exist from index 1, 2, 3, and 4. The differences between \texttt{cpr\_run4[[4]]}, \texttt{cpr\_run4[[5]]}, and \texttt{cpr\_run4[[6]]} are almost indistinguishable. Ergo, \texttt{cpr\_run4[[4]]} is the preferable model. (b) show the root mean squared error (RMSE) by model index. A meaningful decrease in RMSE occurs with additional degrees of freedom until we look at the change between model index 4 and 5. Model index 4 is the preferable model.

Applying the CPR algorithm requires one call to \texttt{cpr}.

\begin{verbatim}
R> cpr_run4 <- cpr(initial_cp4)
R> cpr_run4
\end{verbatim}

A list of control polygons

\begin{verbatim}
List of 51
- attr(*, "class")= chr [1:2] "cpr_cpr" "list"
\end{verbatim}

The \texttt{cpr\_run4} object is a list of \texttt{cpr\_cp} objects. Index \texttt{i} is based on a control polygon with \texttt{i-1} internal knots. There are two plots that can be used for selection of a preferable model. The \texttt{plot} method returns a \texttt{ggplot} object and can be modified accordingly.

\begin{verbatim}
R> plot(cpr_run4, color = TRUE) + theme(legend.position = "bottom") # Figure 4a
R> plot(cpr_run4, type = "rmse", to = 10) + ylab("RMSE") +
    + scale_x_continuous(breaks = seq(1, 10, by = 2)) # Figure 4b
\end{verbatim}

Recall that if \( \xi_j \) has no influence on a spline, then the vertices of \( CP_{k, \xi_j, \theta_\xi} \) will be on the edges of \( CP_{k, \xi_j, \theta_\xi, \xi_j} \). In Figure 4a we conclude that \texttt{cpr\_run4[[4]]} is the preferable model as the
control polygons in index 4, 5, and 6 are indistinguishable. The same conclusion, based on decrease in RMSE by model index, is seen in Figure 4b.

After selecting the preferable model you can use the regression fit data provided or, easily refit and store the regression model via \texttt{stats::update}.

R> preferable_cp4 <- cpr_run4[[4]]
R> str(preferable_cp4)

List of 12
$ cp :Classes 'tbl_df', 'tbl' and 'data.frame': 7 obs. of 2 variables:
..$ xi_star: num [1:7] -1 -0.6889 -0.3703 0.0298 0.3854 ...
..$ theta : num [1:7] -0.0477 -0.4992 -0.5588 -0.1586 0.9388 ...
$ xi : num [1:11] -1 -1 -1 -1 -0.0668 ...
$ iknots : num [1:3] -0.0668 -0.0443 0.2006
$ bknots : num [1:2] -1 1
$ order : num 4
$ call : language cp(formula = log10(pdg) ~ bsplines(day, iknots = c(-0.0667568176695966, -0.0442920251104394, 0.200576701268743)) + (1 | id), data = spdg, method = lmer, check_rank = FALSE)
$ keep_fit : logi FALSE
$ fit : logi NA
$ loglik : num 8523
$ rmse : num 0.155
$ coefficients: num [1:7] -0.0477 -0.4992 -0.5588 -0.1586 0.9388 ...
$ vcov : num [1:7, 1:7] 1.23e-04 8.09e-05 1.15e-04 1.01e-04 1.08e-04 ...
- attr(*, "class")= chr [1:2] "cpr_cp" "list"

R> class(preferable_cp4$fit)

[1] "logical"

R> preferable_cp4 <- update(preferable_cp4, keep_fit = TRUE)
R> class(preferable_cp4$fit)

[1] "lmerMod"
attr(,"package")
[1] "lme4"

4.5. Exploring Additional Model Spaces

Because CPR is a relatively fast method for model selection we can explore other polynomial orders and/or knot sequences. \texttt{cpr::update_bsplines} will allow the end user to quickly modify the \texttt{cpr::bsplines} call within the \texttt{formula} element of a \texttt{cpr::cp} call. In the following, we set up \texttt{initial_cp3} and \texttt{initial_cp2} for third and second order splines. The modified \texttt{df} are such that the knot sequences between \texttt{initial_cp4}, \texttt{initial_cp3}, and \texttt{initial_cp2} are the same. The updated initial control polygons are used to seed to additional CPR runs.
Figure 5: RMSE by degrees of freedom (polynomial order plus number of internal knots) for three CPR runs. The preferable model appears to be a 3rd order B-spline with five degrees of freedom (two internal knots) as it has the lowest RMSE for the degree of freedom, and there is no noticeable decrease in RMSE for additional degrees of freedom.

```
R> initial_cp3 <- update_bsplines(initial_cp4, df = 53, order = 3)
R> initial_cp2 <- update_bsplines(initial_cp4, df = 52, order = 2)
R> cpr_run3 <- cpr(initial_cp3)
R> cpr_run2 <- cpr(initial_cp2)
```

To select a preferable model we will compare the RMSE by degrees of freedom as in Figure 5.

```
R> list(cpr_run4, cpr_run3, cpr_run2) %>%
    lapply(summary) %>%
    bind_rows(.id = "order") %>%
    mutate(order = factor(order, 1:3, c("4th", "3rd", "2nd"))) %>%
    filter(index < 13) %>%
    ggplot() +
    theme_bw() +
    aes(x = dfs, y = rmse, color = order, linetype = order) +
    geom_path() +
    geom_point() +
    ylab("RMSE") +
    xlab("Degrees of Freedom")
```

The third order B-spline with five degrees of freedom, that is two internal knots, is the preferable model as it has the lowest RMSE and degrees of freedom.

```
R> # cpr_run3 with five degrees of freedom: 3rd order + 2 knots = 5 df. Model
R> # index 3 has two knots.
R> preferable_model <- cpr_run3[[3]]
```
5. Control Net Reduction

Control net reduction, CNR, is the natural extension from uni-variable B-splines to multi-variable B-splines. This section is a brief overview of the extension and tools in the \texttt{cpr} package for use in this case.

5.1. Multi-variable B-Splines

We generalize (1) to have a multi-variable function as the varying mean element, \textit{i.e.},

\[ y = f(x_1, x_2, \ldots, x_m) + Z_f \beta + Z_r b + \epsilon. \]  

Multi-variable B-spline functions are constructed by tensor products of uni-variable B-spline bases, henceforth referred to as marginal B-splines. We define the multi-variable B-spline function in terms of matrix arithmetic and as an algebraic formula, the latter will be useful in assessing the influence of a knot on a tensor product.

We denote a multi-variable \( m \)-dimensional B-spline function, built on \( m \) B-spline bases \( B_{k_1, \xi_1}(x_1), B_{k_2, \xi_2}(x_2), \ldots, B_{k_m, \xi_m}(x_m) \), as

\[ f(X) = \mathcal{B}_{K, \Xi}(X) \theta_{\Xi}, \]  

where \( K = \{k_1, k_2, \ldots, k_m\} \), denotes the set of polynomial orders, \( \Xi = \{\xi_1, \xi_2, \ldots, \xi_m\} \), is the set of knot sequences, \( \theta_{\Xi} \) is a \( \prod_{i=1}^{m} (n(\xi_i) - k_i) \times 1 \) column vector of regression coefficients, and \( X \) is the observed data

\[ X = \begin{pmatrix} x_{11} & x_{21} & \cdots & x_{m1} \\ x_{12} & x_{22} & \cdots & x_{m2} \\ \vdots & \vdots & \ddots & \vdots \\ x_{1n} & x_{2n} & \cdots & x_{mn} \end{pmatrix}. \]  

The basis for multi-variable B-splines is constructed by a recursive algorithm. The base case for \( m = 2 \) is

\[ \mathcal{B}_{\{k_1, k_2\}, \{\xi_1, \xi_2\}}(x_1, x_2) = \left( 1_{n(\xi_2) - k_2}^T \otimes B_{k_1, \xi_1}(x_1) \right) \odot \left( B_{k_2, \xi_2}(x_2) \otimes 1_{n(\xi_1) - k_1}^T \right), \]  

where \( \odot \) is the element-wise product, \( \otimes \) is a Kronecker product, and \( 1_n \) is a \( n \times 1 \) column vector of 1s. The two Kronecker products define the correct dimensions for the entry-wise product. The tensor product matrix as the same number of rows as the two input matrices and the columns are generated by all the pairwise products of the columns of the two input matrices. The general case for \( m > 2 \), the matrix \( \mathcal{B}_{K, \Xi}(X) \) is defined by

\[ \mathcal{B}_{K, \Xi}(X) = \left( 1_{n(\xi_m) - k_m}^T \otimes \mathcal{B}_{K \setminus k_m, \Xi}(X \setminus x_m) \right) \odot \left( B_{k_m, \xi_m}(x_m) \otimes 1_{\prod_{i=1}^{m-1}(n(\xi_i) - k_i)}^T \right). \]
It is possible to write (16) as a set of summations as follows:

\[ f(X) = \mathcal{B}_K \Xi (X) = \sum_{j_1=1}^{n(\xi_1) - k_1} \cdots \sum_{j_m=1}^{n(\xi_m) - k_m} B_{j_1,k_1,\xi_1}(x_1) B_{j_2,k_2,\xi_2}(x_2) \cdots B_{j_m,k_m,\xi_m}(x_m) \theta_{\Xi,j_1,j_2,\ldots,j_m} \]

\[ = \text{diag} (B_{k_1,\xi_1}(x_1) \theta_{\Xi\setminus\xi_1}(X \setminus x_1)). \]  

(20)

When the data input is a single observation, that is a tuple \((x_1, x_2, \ldots, x_m) \in \text{rows}(X)\) the last line is a singleton and the diag operation is redundant. Equation (20) is critical in the extension from the uni-variable control polygon reduction method to the multi-variable control polygon reduction method. By conditioning on \(m-1\) marginals, the multi-variable B-spline becomes a uni-variable B-spline in terms of the \(m^{th}\) marginal. Thus, the metrics and methods developed for uni-variable B-splines can be applied to multi-variable B-splines.

To simplify the explanation consider a \(m=2\) dimensional B-spline. The concepts and notation extend to \(m>2\) with ease. If we condition on \(x_2\), the two-dimensional B-spline simplifies to a uni-variable spline in \(x_1\), i.e.,

\[ \mathcal{B}_K \Xi (x_1|x_2) \theta_{\Xi} = B_{k_1,\xi_1}(x_1) \theta_{\Xi\setminus\xi_1}(x_2). \]  

(21)

In terms of the control net, the conditioning on \(x_2\) creates a slice across the net and yields the control polygon \(CP_{k_1,\xi_1,\theta_{\Xi\setminus\xi_1}}(x_2)\).

The influence weight of \(\xi_{1j} \in \xi_1\) is the Euclidean distance between the ordinates \(\theta_{\Xi\setminus\xi_1}(x_2)\) and \(\theta_{\Xi\setminus\{(\xi_1 \cup \xi_{1j})\}}(x_2)\).

\[ w_{1j|x_2} = \left\| (I - W_{k_1,\xi_1}(\xi_{1j}) (W_{k_1,\xi_1}(\xi_{1j}) W_{k_1,\xi_1}(\xi_{1j})^{-1} W_{k_1,\xi_1}(\xi_{1j})) \theta_{\Xi\setminus\xi_1}(x_2) \right\|_2. \]  

(22)

The conditional influence weight, (22), is used to get the influence weight of \(\xi_{1j}\) on \(CP_{k_1,\xi_1,\theta_{\Xi\setminus\xi_1}}(x_2)\). That is, the relative influence weight of \(\xi_{1j}\) is the maximum influence weight over a set of \(p\) values for \(x_2\).

\[ w_{1j} = \max_{x_2 \in U} w_{1j|x_2}, \]  

where

\[ U = \left\{ u : \min(x_2) + \frac{1, 2, \ldots, p}{p+1} (\max(x_2) - \min(x_2)) \right\}. \]  

(24)

We recommend and have set the default in \texttt{cpr} to use \(p = 20\) values for each marginal.

5.2. The CNR Algorithm

1. Define the initial \(K\) and \(\Xi\) set for the initial tensor product.
2. Use an appropriate regression modeling approach to fit a regression model for (15).

3. Construct the control net for the current set of knots sequences and regression coefficients.

4. Use (23) to find the influence weight for all internal knots on the marginals you are interested in reducing.

5. Coarsen the knot sequence by removing the knot with the smallest influence weight.

6. Refit the regression model using the coarsened knot sequences.

7. Repeat steps 3 through 6 until all internal knots have been removed.

8. Select the preferable model by visual inspection of diagnostic graphics.

CNR is applied to all margins of interest at once. The knot with the lowest influence weight is omitted at each step, regardless of the margin it originates from.

5.3. Implementation Issue: Dimensionality

The CNR algorithm is not immune to the curse of dimensionality. The total degrees of freedom consumed by the tensor product is the product of the degrees of freedom of each marginal B-spline. This fact needs to be considered when starting the search for a parsimonious model. Consider a two-dimensional double cubic B-spline with fifty internal knots on each marginal. This construction generates a regression model with $54 \times 54 = 2916$ regression coefficients.

This is important because a common method for solving regression problems is to use a QR decomposition of the design matrix. QR decomposition is an $O(n^3)$ algorithm where $n$ is the number of regression coefficients. It will take a considerable amount of computational resources to estimate the 2916 regression parameters, and may not be feasible for some computing environments.

The size of the initial model is even more problematic for three-dimensional B-splines. Setting up a search for a set of parsimonious knot sequences with three cubic B-splines, each with initially fifty internal knots would require 157,464 regression coefficients. This is unreasonable.

We suggest that for $m \geq 3$ to model a primary explanatory variable via uni-variable methods such as control polygon reduction, and then use the resulting uni-variable B-spline as a static marginal in the multi-variable B-spline. Example follows in the next section.

5.4. Use In The cpr Package

The use of the CNR algorithm in the cpr package is very similar to the use of the CPR algorithm. Use cpr::btensor to generate the multi-variable B-spline, cn to generate the control net, cnr to apply the CNR algorithm, and plot to see diagnostic plots. A simple example, fitting a two-dimensional B-spline over day and age, with two fourth order splines is below. The example also shows an updated version of the initial control net with a third order B-spline for day and fourth order spline for age.

```R
R> initial_cn44 <-
+   cn(log10(pdg) ~ btensor(list(day, age), df = list(24, 24)) + (1 | id),
```
As noted in the prior subsection, building $m$-dimensional B-splines, $m \geq 3$, can be difficult simply due to the number of degrees of freedom required to build the basis. For the spdg data, it might be reasonable to find a parsimonious B-spline for PDG by day via CPR, and then use that result as a foundation for the higher dimensional B-spline and CNR run. For example, build the initial knot sequences for day, age, ttm B-spline based on the preferable model from the prior section.

```
R> init_iknots <-
+     list(cpr_run3[[3]]$iknots,
+            trimmed_quantile(spdg$age, prob = 1:10/11),
+            trimmed_quantile(spdg$ttm, prob = 1:10/11))
```

Construct the initial control net, and then run CNR on only the age and ttm margins and the day margin has already been specified.

```
R> init_cn <- cn(log10(pdg) ~ btensor(list(day, age, ttm),
+                     iknots = init_iknots,
+                     order = list(3, 2, 2)) + (1 | id),
+                     data = spdg,
+                     method = lmer)
R> cnr_run <- cnr(init_cn, margin = 2:3)
```

### 6. Discussion

The cpr package provides a clean and user friendly interface for implementing our Control Polygon Reduction and Control Net Reduction algorithms for B-spline regression model selection.

The CPR and CNR algorithms take a novel approach to regression model selection. Instead of focusing on the likelihood function we focus on the geometry of the control polygons and control nets to determine the influence of any one particular knot. That said, the CPR algorithm has been shown to be able to select models with fewer degrees of freedom and with superior fit statistics compared to a forward step model selection approach. The model space searched by CPR is larger than the model space searched by a forward step model selection approach. The additional calculations for determining knot influence require few computation resources and are done quickly. Thus, CPR requires negligibly more time to run than a forward step selection approach.

Compared to a comparable likelihood based backward-step selection approach, CPR picks models which are on average equivalent to the likelihood based selected models on a degree of freedom for degree of freedom basis. The time required to run a likelihood based backward-step selection approach can be considerable, CPR is much faster.
Overall, CPR can quickly select a parsimonious model with preferable fit statistics to likelihood based model selection approaches. Further, as was demonstrated in this manuscript, since CPR requires very little time to run, exploration of B-splines or different polynomial orders is feasible. Fourth order B-splines are commonly used as they have twice differentiable and relatively smooth. However, while perhaps not as ‘smooth’, lower order splines may fit the data more efficiently than higher order splines.

CNR provides analysts many of the same benefits as CPR, fast model selection from a very large model space. The tools allow for exploration of complex non-linear multi-variable functions.

Continued development of the package can be tracked and contributed to at https://github.com/dewittp/cpr. The package is also hosted on the Comprehensive R Archive Network (CRAN) at https://cran.r-project.org/package=cpr.

7. Acknowledgements

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