

**center():**

This module uses the linear constraints to generate the transformation matrix,  $\mathbf{Z}$ .

Typically, the linear constraints can be written in the form of  $\mathbf{A}\boldsymbol{\beta} = \mathbf{0}$ , where  $\boldsymbol{\beta}$  is a  $K \times 1$  vector of parameters to be estimated, and  $\mathbf{A}$  is a  $L \times K$  matrix of linear constraints. So there are  $L$  linear constraints and each constraint is a linear combination of the  $K$  parameters.

With the  $L$  constraints in effect, we are only left with  $K - L$  parameters to estimate. So it is desirable to come up with a  $K \times (K - L)$  transformation matrix  $\mathbf{Z}$  that lets  $\boldsymbol{\beta} = \mathbf{Z}\boldsymbol{\beta}_z$ , where  $\boldsymbol{\beta}_z$  is a  $(K - L) \times 1$  vector of parameters and  $\mathbf{A}\boldsymbol{\beta} = \mathbf{0}$  for any  $\boldsymbol{\beta}_z$ .

In this way, we can simply replace  $\boldsymbol{\beta}$  with  $\mathbf{Z}\boldsymbol{\beta}_z$  in the estimating equation and then solve  $\boldsymbol{\beta}_z$ . Usually  $\mathbf{Z}$  is incorporated into the design matrix and the form of solution is preserved.

The  $\mathbf{Z}$  matrix can be obtained from QR decomposition of  $\mathbf{A}^T$ , which gives a  $K \times K$  orthogonal matrix  $\mathbf{Q}$ . The last  $K - L$  columns provide an orthonormal basis for the null space of  $\mathbf{A}^T$ , and we can use them as the  $\mathbf{Z}$  matrix, because  $\mathbf{Z}^T \mathbf{A}^T = \mathbf{0}$ . In this way, with any  $\boldsymbol{\beta}_z$ ,  $\mathbf{A}\boldsymbol{\beta} = \mathbf{A}\mathbf{Z}\boldsymbol{\beta}_z = \mathbf{0}\boldsymbol{\beta}_z = \mathbf{0}$ .

The design matrix under the reduced parameter vector  $\boldsymbol{\beta}_z$  is  $\mathbf{X}\mathbf{Z}$ , where  $\mathbf{X}$  is the original design matrix.

**Arguments:**

- (1) **c**: input to the QR decomposition,  $\mathbf{A}^T$ .
- (2) **nr, nc**:  $K$  and  $L$ , respectively.
- (3) **z**: the matrix  $\mathbf{Z}$ , as the output.

**penalty():**

This module constructs the ‘half’ penalty matrix,  $\mathbf{B}$ , of a first order difference penalty matrix.

It has the following form,

$$\mathbf{B} = \begin{pmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -1 \end{pmatrix}.$$

In this way,  $\mathbf{B}\boldsymbol{\beta}$  is a column vector of the first order difference between adjacent parameter values in  $\boldsymbol{\beta}$ , and  $\boldsymbol{\beta}^T \mathbf{B}^T \mathbf{B} \boldsymbol{\beta}$  is the sum of squared differences. **Note that  $\mathbf{B}$  is not a square matrix, but adding a row of zeros at the end will make it a square matrix. However, this does not change the calculation. So we do not add the row of zeros here.**

The first order difference penalty matrix sums up the squared difference between adjacent parameter values in a spline coefficient vector.

**Arguments:**

- (1) **d**: the dimension of  $\boldsymbol{\beta}$ .