

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) \mathbf{c} : input to the QR decomposition, \mathbf{A}^T .
- (2) nr, nc: K and L , respectively.
- (3) \mathbf{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,

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

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) \mathbf{d} : the dimension of $\boldsymbol{\beta}$.