Lecture_notes6

08.03-2021.

Recall Gram Schmidt and QR

The orthogonal vectors of the Q-matrix produced by the Gram-Schmidt orthogonalization process can be written in terms of projections as follows

$$\mathbf{q}_1 = \frac{1}{\|P_1\mathbf{a}_1\|}P_1\mathbf{a}_1, \mathbf{q}_2 = \frac{1}{\|P_2\mathbf{a}_2\|}P_2\mathbf{a}_2, \ \ldots\ , \mathbf{q}_n = \frac{1}{\|P_n\mathbf{a}_n\|}P_n\mathbf{a}_n,$$

where $P_1 = I_m$, $P_j = I_m - Q_{j-1}Q_{j-1}^t$ and $Q_{j-1} = [\mathbf{q}_1\ \mathbf{q}_2\ \ldots\ \mathbf{q}_{j-1}]$.

Exercise 1:
What are the Q_{j-1}-coordinates of $\hat{\mathbf{a}} = Q_{j-1}Q_{j-1}^t\mathbf{a}$?

How can we conclude the following matrix identity

$$Q_{j-1}Q_{j-1}^t = \sum_{k=1}^{j-1}\mathbf{q}_k\mathbf{q}_k^t?$$

Exercise 2:
Verify that $P_j = I_m - Q_{j-1}Q_{j-1}^t$ is a projection matrix, i.e show that $P_j^2 = P_j$ and $P_j = P_j^t$.

Exercise 3:
Recall that the orthogonal complement of a subspace $W \subseteq \mathbf{R}^m$ is defined as

$$W^{\perp} = \{\mathbf{v} \in \mathbf{R}^m | \mathbf{v}^t \mathbf{w} = 0 \text{ for all } \mathbf{w} \in W\}.$$

Verify that P_j is the projection onto $Col([\mathbf{q}_1 \ \ldots \ \mathbf{q}_{j-1}])^{\perp} = Col([\mathbf{a}_1 \ \ldots \ \mathbf{a}_{j-1}])^{\perp}$.

The modified Gram Schmidt

The modified Gram-Schmidt (MGS) algorithm works by converting the matrix A into the matrix Q. Once $\mathbf{q}_k$ is found, the remaining A-columns (of index $j > k$) are modified to be orthogonal to that $\mathbf{q}_k$. This is called a *deflation* of A w.r.t. $\mathbf{q}_k$.

Exercise 4:
Define the projection $P_{\perp \mathbf{q}_k} = I_m - \mathbf{q}_k \mathbf{q}_k^t$. Show that

$$\mathbf{q}_k^t P_{\perp \mathbf{q}_k} A = \mathbf{0},$$

and that

$$P_j = P_{\perp \mathbf{q}_{j-1}} P_{\perp \mathbf{q}_{j-2}} ... P_{\perp \mathbf{q}_2} P_{\perp \mathbf{q}_1}.$$

Exercise 5:
Make a Julia-function that does the QR-factorization according to MGS and returns the matrices Q and R.

```
function MGS(A)
```

Julia-code for QR by the CGS

```
 1 using LinearAlgebra
 2 function CGS(A)
 3 # QR-factorizarion of input-matrix A by the ...
     classical Gram Schmidt algorithm (CGS).
 4 # The function returns Q and R in the QR-factorizarion.
 5 m, n = size(A);
 6 p = min(m,n)
 7 Q = zeros(m,p);
 8 R = zeros(p,n);
 9 R[1,1] = norm(A[:,1]);
10 Q[:,1] = A[:,1]./R[1,1];
11 for i = 2:n
12     if i ≤ p
13     R[1:i-1,i] = Q[:,1:i-1]'A[:,i];
14     v = A[:,i]-Q[:,1:i-1]*R[1:i-1,i]; # ...
         Orthogonalize i-th column wrt Q[:,1:i-1].
15     R[i,i] = norm(v);
16     Q[:,i] = v./R[i,i];
17     else
18         R[:,i] = Q'A[:,i];              # Find ...
             Q-coordinates of A[:,i]
19     end
20 end
21 return Q, R;
22 end
```

Exercise 6:

Let $\epsilon = 10^{-7}$, $A = \begin{bmatrix} 1 & 1 & 1 \\ \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{bmatrix}$, $\mathbf{x} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ and $\mathbf{b} = A\mathbf{x}$.

Solve the system $A\mathbf{x} = \mathbf{b}$ by

1. the normal equations $A^tA\mathbf{x} = A^t\mathbf{b}$.
2. by QR-factorization obatined from the CGS.
3. by QR-factorization obatined from the MGS.
4. by the QR-factorization in Julia.
5. by the *backslash* "$\backslash$".

‘

Compare and comment on the results.

The MGS is known to be numerically more stable than the classical Gram-Schmidt (CGS). This can be illustrated by running both algorithms on a matrix A with decreasingly small singular values.

We can design such a matrix $A = USV^t$ (say 60×60) by generating random data and extract appropriate orthogonal right and left singular vectors. As singular values we may use the values $s_i = 2^{-i}$ for $i = 1, ..., 60$.

Exercise 7:

1. Make a Julia-script that generates U, S and V to design the desired matrix $A = USV^t$.
2. Apply your Julia QR-factorization functions based on CGS and MGS to A.
3. Compare the 60 diagonal elements of the resulting R-matrices by plotting them together (use log10-scale for the plotting).

Partial Least Squares (PLS)

Partial least squares (PLS, see **Fast and stable partial least squares modelling: A benchmark study with theoretical comments, by Björck & Indahl, 2017**) is a method for computing approximate least squares solutions. It is much used in fields like **Chemometrics** and **Genomics** where prediction modelling based on high–dimensional data and "wide" datamatrices $\mathbf{X}$ ($n \gg m$) is quite common.

The idea behind PLS is to take advantage of the responses $\mathbf{y}$ to obtain projection models requiring fewer and more appropriate components than PCR to obtain good regression models for predicting $\mathbf{y}$-values from $\mathbf{X}$-data.

Most PLS-methods/algorithms have been developed "empirically" by people that were not experts in numerical linear algebra.

The Björck–Indahl collaboration was initiated as a consequence of the following two publications:

Stability of Two Direct Methods for Bidiagonalization and Partial Least Squares, by Björck (2014) presenting an investigation of the stability issues for two PLS algorithms (the *Golub-Kahan Householder bidiagonalization method* and the *NIPALS PLS*) is presented.

The geometry of PLS1 explained properly: 10 key notes on mathematical properties of and some alternative algorithmic approaches to PLS1 modelling, by Indahl (2014) focusing on understanding various aspects of the PLS-methodology in terms of elementary linear algebra.

The NIPALS PLS algorithm

The classical algorithm for PLS modelling was published by Wold et al. in 1984. $\mathbf{X}_0$ and $\mathbf{y}_0$ represent the mean–centered data (predictors) and responses.

for $a = 1 : k$ (k, # components to be extracted)

1. $\mathbf{w}_a = \mathbf{X}_{a-1}^t \mathbf{y}_{a-1}$ ($\mathbf{y}, \mathbf{X}$ inner prods $\sim$ covariances)
2. $\mathbf{w}_a = \mathbf{w}_a / \|\mathbf{w}_a\|$ (normalizing the vector from 1)
3. $\mathbf{t}_a = \mathbf{X}_{a-1} \mathbf{w}_a$ ($\mathbf{X}$-comb wrt weights from 2)
4. $\mathbf{t}_a = \mathbf{t}_a / \|\mathbf{t}_a\|$ (normalizing the vector from 3)
5. $\mathbf{p}_a = \mathbf{X}_{a-1}^t \mathbf{t}_a$ ("projection-loadings" used in 6)
6. $\mathbf{X}_a = \mathbf{X}_{a-1} - \mathbf{t}_a \mathbf{p}_a^t$ (deflate $\mathbf{X}$ to be orthogonal to $\mathbf{t}_a$)
7. $q_a = \mathbf{t}_a^t \mathbf{y}_{a-1}$ (reg. coeff wrt score vector $\mathbf{t}_a$)
8. $\mathbf{y}_a = \mathbf{y}_{a-1} - \mathbf{t}_a q_a$ (make $\mathbf{y}$ orthogonal to $\mathbf{t}_a$)

end

Organize vectors and numbers into the matrices:

$\mathbf{T}_k = [\mathbf{t}_1\ \mathbf{t}_2\ \ldots\ \mathbf{t}_k]$ (the orthonormal scores)

$\mathbf{W}_k = [\mathbf{w}_1\ \mathbf{w}_2\ \ldots\ \mathbf{w}_k]$ (the orthonormal weights)

$\mathbf{P}_k = [\mathbf{p}_1\ \mathbf{p}_2\ \ldots\ \mathbf{p}_k]$ (the $\mathbf{X}$-projection loadings)

$\mathbf{q}_k^t = [q_1\ q_2\ \ldots\ q_k]$ (the $\mathbf{T}$ regression coeffs)

Finally calculate the regression coeffs for the original $\mathbf{X}$-data by: $\boldsymbol{\beta}_k = \mathbf{W}_k (\mathbf{P}_k^t \mathbf{W}_k)^{-1} \mathbf{q}_k$ and $\beta_{0,k} = \bar{y} - \bar{\mathbf{x}} \boldsymbol{\beta}_k$, where $\bar{y}$ and $\bar{\mathbf{x}}$ denote $\mathbf{y}$ and X column means.

The NIPALS algorithm computing a k-component PLS model with orthonormal scores ($\mathbf{T}_k$) and weights ($\mathbf{W}_k$).

The above algorithm extracts weights $\mathbf{W}_k$ and scores $\mathbf{T}_k$ ($\mathbf{W}_k^t\mathbf{W}_k = \mathbf{I}_k$ and $\mathbf{T}_k^t\mathbf{T}_k = \mathbf{I}_k$) representing orthogonal bases for the so-called **Krylov subspaces** $\mathcal{K}_k(\mathbf{X}^t\mathbf{X}, \mathbf{X}^t\mathbf{y})$ and $\mathcal{K}_k(\mathbf{X}\mathbf{X}^t, \mathbf{X}\mathbf{X}^t\mathbf{y})$, respectively.

The weights $\mathbf{w}_a$ found in steps 1. and 2. of the NIPALS algorithm provide a linear combination of the $\mathbf{X}_{a-1}$-columns that maximizes the covariance with $\mathbf{y}_{a-1}$.

NOTE 1:
The Krylov subspace

$$\mathcal{K}_k(\mathbf{X}^t\mathbf{X}, \mathbf{X}^t\mathbf{y}) = Span\{\mathbf{X}'\mathbf{y}, (\mathbf{X}^t\mathbf{X})\mathbf{X}^t\mathbf{y}, \ldots, (\mathbf{X}^t\mathbf{X})^{k-1}\mathbf{X}'\mathbf{y}\}$$

$$= Col(\mathbf{W}_k)$$

is a subspace of the vector space $Col(\mathbf{X}^t)$ spanned by the rows of $\mathbf{X}$, and

$$\mathcal{K}_k(\mathbf{X}\mathbf{X}^t, \mathbf{X}\mathbf{X}^t\mathbf{y}) = Span\{(\mathbf{X}\mathbf{X}^t)\mathbf{y}, (\mathbf{X}\mathbf{X}^t)^2\mathbf{y}, \ldots, (\mathbf{X}\mathbf{X}^t)^k\mathbf{y}\}$$

$$= Col(\mathbf{T}_k).$$

is a subspace of the vector space $Col(\mathbf{X})$ spanned by the columns of $\mathbf{X}$.

After the orthogonal scores in $\mathbf{T}_k$ are calculated, the matrix of projection loadings ($\mathbf{P}_k$) satisfies the identity:

$$\mathbf{P}_k^t = \mathbf{T}_k^t\mathbf{X}.$$

The columns of $\mathbf{T}_k^\star = \mathbf{X}\mathbf{W}_k$ are often referred to at the *non-orthogonal scores*. Obviously, the columns of $\mathbf{T}_k^\star$ and $\mathbf{T}_k$ (the orthogonal scores from the NIPALS-algorithm) span the same subspace of $\mathbb{R}^m$.

NOTE 2:

Clearly (why)

$$\mathbf{T}_k^\star = \mathbf{T}_k\mathbf{T}_k^t\mathbf{T}_k^\star = \mathbf{T}_k\mathbf{P}_k^t\mathbf{W}_k.$$

The above relationship between $\mathbf{T}_k$ and $\mathbf{T}_k^\star$ corresponds to a QR-factorization of $\mathbf{T}_k^\star$ where $\mathbf{T}_k$ plays the role of $\mathbf{Q}$ and $\mathbf{B}_k$ the role of $\mathbf{R}$:

$$\mathbf{T}_k^\star = \mathbf{T}_k\mathbf{B}_k, \text{ where } \mathbf{B}_k = \mathbf{P}_k^t\mathbf{W}_k.$$

It turns out that the $k \times k$ upper triangular $\mathbf{B}_k$ matrix is actually upper bi-diagonal (only the main diagonal of $\mathbf{R}_k$ and the first super–diagonal above it are non-zero) in this case. Such bi-diagonal matrices can be inverted very effectively when neccessary.

The projection of $\mathbf{y}$ onto the column space of $\mathbf{T}_k$ is

$$\hat{\mathbf{y}} = \mathbf{T}_k\mathbf{T}_k^t\mathbf{y} = \mathbf{T}_k\mathbf{q}_k.$$

Here the $\mathbf{T}_k$-regression coeffs $\mathbf{q}_k = \mathbf{T}_k^t\mathbf{y}$ are often referred to as the $\mathbf{y}$-loadings.

Because the orthogonal scores $\mathbf{T}_k = \mathbf{X}\mathbf{W}_k(\mathbf{P}_k^t\mathbf{W}_k)^{-1}$, we therefore have

$$\hat{\mathbf{y}} = \mathbf{T}_k\mathbf{q}_k = \mathbf{X}\mathbf{W}_k(\mathbf{P}_k^t\mathbf{W}_k)^{-1}\mathbf{q}_k,$$

where the PLSR regression coeffs are directly expressed as

$$\boldsymbol{\beta}_k = \mathbf{W}_k(\mathbf{P}_k^t\mathbf{W}_k)^{-1}\mathbf{q}_k.$$

For predictions with uncentered $\mathbf{X}$-data, the associated constant term for the k-component PLS regression (PLSR) model is

$$\beta_{0,k} = \bar{\mathbf{y}} - \bar{\mathbf{x}}\boldsymbol{\beta}_k,$$

and the PLSR predictions based on k PLS-components for new data points $\mathbf{x}$ (a row-vector in $\mathbb{R}^n$) is

$$\widehat{y} = \beta_{0,k} + \mathbf{x}\boldsymbol{\beta}_k.$$

NOTE 3:

The NIPALS algorithm actually implements a Gram-Schmidt (GS) process deriving the orthogonal scores ($\mathbf{T}_k$) by starting with linear combination of $\mathbf{X}$-columns rather than just a single $\mathbf{X}$-column. The steps 5 and 6 in NIPALS represent a GS-step "deflating" the $(m \times n)$-matrix $\mathbf{X}_{a-1}$ with respect to $\mathbf{t}_a$ to assure that the subsequent scores ($\mathbf{T}_k$-columns) are orthogonal. The main difference from the MGS algorithm for QR-factorization is that each GS-step in the MGS only "deflate" a subset of the matrix columns.

NOTE 4:

From the identity $\mathbf{X}\mathbf{W}_k = \mathbf{T}_k^\star$ we obtain an approximation of $\mathbf{X}$ by multiplying both sides of the equation from the right with $\mathbf{W}_k^t$:

$$\mathbf{X} \approx \mathbf{X}\mathbf{W}_k\mathbf{W}_k^t = \mathbf{T}_k\mathbf{B}_k\mathbf{W}_k^t \overset{\text{def}}{=} \mathbf{X}_k.$$

Here $\mathbf{W}_k\mathbf{W}_k^t$ projects the $\mathbf{X}$-rows onto $\mathcal{K}_k(\mathbf{X}^t\mathbf{X}, \mathbf{X}^t\mathbf{y})$.

Exercise 8:
Recall from Lecture-notes4 the (truncated) pseudo-inverse for the rank k approximation of $\mathbf{X}$ obtained by the SVD.

Suggest a similar definition $\widetilde{\mathbf{X}}_k^\dagger$ based on the bi-diagonal factorization $\widetilde{\mathbf{X}}_k = \mathbf{T}_k\mathbf{B}_k\mathbf{W}_k^t$ that is consistent with calculation of the PLSR regression coeffs $\boldsymbol{\beta}_k$.

The PLS regression problem

Recall:

The ordinary least squares (OLS) problem for any linear system $\mathbf{X}\boldsymbol{\beta} = \mathbf{y}$ corresponds to solving

$$\min_{\boldsymbol{\beta}} \|\mathbf{X}\boldsymbol{\beta} - \mathbf{y}\|_2 \quad \text{subject to} \quad \min \|\boldsymbol{\beta}\|_2$$

always has a unique solution $\widehat{\boldsymbol{\beta}}$ called the *pseudoinverse solution*. This solution characterized by satisfying the two conditions

$$\mathbf{X}^t\mathbf{X}\boldsymbol{\beta} = \mathbf{X}^t\mathbf{y}, \qquad \boldsymbol{\beta} \in Span(\mathbf{X}^t) \subseteq \mathbb{R}^n,$$

lin comb of the x-rows

i.e., $\widehat{\boldsymbol{\beta}}$ is the solution of the associated normal equations that is also contained in the row subspace of $\mathbf{X}$.

The **PLS approximations** $\boldsymbol{\beta}_k$, $k = 1, 2, \ldots$ to the least squares problem can be defined as the estimates generated by k steps of the NIPALS PLS algorithm.

However, a definition of the approximate k-component PLS solutions should be independent of a particular algorithm.

We therefore define the *PLS approximation* $\boldsymbol{\beta}_k$ as *the solution of the restricted problem*

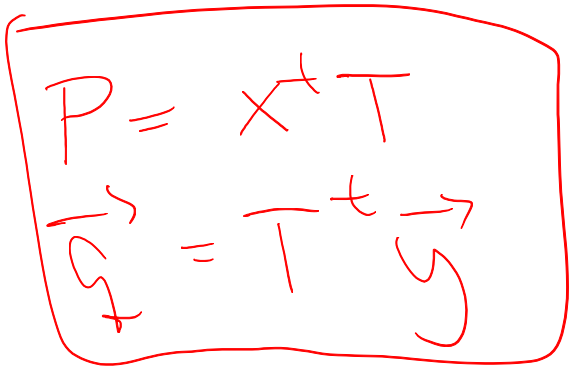
$$\min_{\boldsymbol{\beta}} \|\mathbf{X}\boldsymbol{\beta} - \mathbf{y}\|_2, \quad \text{subject to} \quad \boldsymbol{\beta} \in \mathcal{K}_k(\mathbf{X}^t\mathbf{X}, \mathbf{X}^t\mathbf{y}).$$

From latter definition, alternative algorithms for finding the PLS approximations can be studied (see Björck & Indahl, 2017)).

$\hat{\beta}_k$ means that $\hat{\beta}_k$ is a lin comb of W_k - columns.

Julia-code for the NIPALS PLS

```
1  using LinearAlgebra, Statistics
2  function PLS_nip(X, y; mc = 2)
3  # b0, B, T, W, P, q = PLS_nip(X,y; mc = 6)
4  m,n = size(X)
5  mc  = min(mc, min(n,m)-1)
6  # Scores (T), weights (W) and X-loadings (P):
7  T   = zeros(m,mc); W = zeros(n,mc); P = zeros(n,mc)
8  q   = zeros(1,mc); # the y-loadings
9  mx  = mean(X, dims=1) # - X-column mean values.
10 my  = mean(y, dims=1)[1] # - mean of responses y.
11 y  = y.- my;           # - centered response vector.
12 X  = X.- mx;           # - centered X-data
13 for a = 1:mc
14     w = X'y;  w = w/norm(w);  W[:,a] = w;
15     t = X*w;  t = t/norm(t);  T[:,a] = t;
16     P[:,a] = X't;          X = X - t*P[:,a]';
17     q[a]   = (y't)[1];     y = y - q[a].*t;
18 end
19 # The regression-coeffs (B) and constant terms (b0):
20 B  = cumsum((W/triu(P'W)).*q, dims = 2);
21 b0 = my .- mx*B;
22 return b0, B, T, W, P, q;
23 end
```



Exercise 9:
Extend last weeks programming exercise with the Julia-script RR_PCR_Exercise.jl to include PLS-modelling with the same number of components as for PCR.

Some useful "local" contributions to PLS-modelling:

- **Much faster cross-validation in PLSR-modelling by avoiding redundant calculations, see Liland et al. (2020)**. About fast selection/validation of PLS models.

- **ROSA - a fast extension of partial least squares regression for multiblock data analysis, Liland et al. (2016)**. Multiblock data analysis (a.k.a. *data fusion*) is about combining different measurements (data matrices) obtained from the same set of samples.

- **Canonical partial least squares - a unified PLS approach to classification and regression problems, see Indahl et al. (2009)**. About estimating latent variables in multivariate classification and regression problems where more than one response variable is available.