Updating $\left(\underline{\underline{A}}^T\underline{\underline{A}}\right)^{-1}$ with the Addition and Removals of Columns in $\underline{\underline{A}}$

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1 Overview

The algorithm aims to solve the following problem:

1. We have a matrix $\underline{\underline{A}}$ and we have calculated the inverse $\left(\underline{\underline{A}}^T\underline{\underline{A}}\right)^{-1}$.
2. We now add or remove a column $\underline{v}$ to the matrix $\underline{\underline{A}}$, forming matrix $\underline{\underline{A}}'$.
3. We want to calculate $\left(\underline{\underline{A}}'^T\underline{\underline{A}}'\right)^{-1}$ given our knowledge of $\left(\underline{\underline{A}}^T\underline{\underline{A}}\right)^{-1}$, instead of from scratch.

2 Background Theory

2.1 Matrix-Inversion Lemma

It is known that for correctly-sized matrices $\underline{\underline{A}}$, $\underline{\underline{U}}$, $\underline{\underline{C}}$ and $\underline{\underline{V}}$,

$$\left(\underline{\underline{A}}+\underline{\underline{U}}\,\underline{\underline{C}}\,\underline{\underline{V}}\right)^{-1}=\underline{\underline{A}}^{-1}-\underline{\underline{A}}^{-1}\underline{\underline{U}}\left(\underline{\underline{C}}^{-1}+\underline{\underline{V}}\,\underline{\underline{A}}^{-1}\underline{\underline{U}}\right)^{-1}\underline{\underline{V}}\,\underline{\underline{A}}^{-1}\,. \tag{1}$$

For the special case of adding the outer product of two column vectors $\underline{u}$ an $\underline{v}$, we obtain

$$\left(\underline{\underline{A}}+\underline{u}\,\underline{v}\right)^{-1}=\underline{\underline{A}}^{-1}-c\underline{\underline{A}}^{-1}\underline{u}\,\underline{v}^T\underline{\underline{A}}^{-1}\,, \tag{2}$$

where

$$c=\frac{1}{1+\underline{u}^T\underline{\underline{A}}^{-1}\underline{v}}\,. \tag{3}$$

2.2 Inverting a Partitioned Matrix

The inverse of a partitioned matrix can be expressed as

$$\begin{bmatrix}\underline{\underline{A_{11}}} & \underline{\underline{A_{12}}}\\ \underline{\underline{A_{21}}} & \underline{\underline{A_{22}}}\end{bmatrix}^{-1}=\begin{bmatrix}\underline{\underline{F_{11}^{-1}}} & -\underline{\underline{F_{11}^{-1}}}\,\underline{\underline{A_{12}}}\,\underline{\underline{A_{22}^{-1}}}\\ -\underline{\underline{A_{22}^{-1}}}\,\underline{\underline{A_{21}}}\,\underline{\underline{F_{11}^{-1}}} & \underline{\underline{F_{22}^{-1}}}\end{bmatrix}^{-1}\,, \tag{4}$$

where

$$\underline{\underline{F_{11}^{-1}}} = \underline{\underline{A_{11}^{-1}}}+\underline{\underline{A_{11}^{-1}}}\,\underline{\underline{A_{12}}}\,\underline{\underline{F_{22}^{-1}}}\,\underline{\underline{A_{21}}}\,\underline{\underline{A_{11}^{-1}}}\,, \tag{5}$$

$$\underline{\underline{F_{22}^{-1}}} = \underline{\underline{A_{22}^{-1}}}+\underline{\underline{A_{22}^{-1}}}\,\underline{\underline{A_{21}}}\,\underline{\underline{F_{11}^{-1}}}\,\underline{\underline{A_{12}}}\,\underline{\underline{A_{22}^{-1}}}\,. \tag{6}$$

3 Algorithms for Adding and Removing Columns

Inputs: original matrix $\underline{\underline{A}}$, inverse $\underline{\underline{B}} = \left(\underline{\underline{A}}^T \underline{\underline{A}}\right)^{-1}$, column vector $\underline{v}$, column index j

Outputs: updated inverse $\underline{\underline{B}}' = \left(\underline{\underline{A}}'^T \underline{\underline{A}}'\right)^{-1}$

Procedure:

1. $\underline{u_1} \leftarrow \underline{\underline{A}}^T \underline{v}$
2. $\underline{u_2} \leftarrow \underline{\underline{B}}\underline{u_1}$
3. $d \leftarrow \left(\underline{v}^T \underline{v} - \underline{u_1}^T \underline{u_2}\right)^{-1}$
4. $\underline{u_3} \leftarrow d\underline{u_2}$
5. $\underline{\underline{Q}} \leftarrow \underline{\underline{B}} + d\underline{u_2}\underline{u_2}^T$
6. $\underline{\underline{B}}' \leftarrow \begin{bmatrix} \underline{\underline{Q}} & -\underline{u_3} \\ -\underline{u_3}^T & d \end{bmatrix}$
7. Permute the last row of $\underline{\underline{B}}'$ to row j, and permute the last column of $\underline{\underline{B}}'$ to column j.

Algorithm 1: Algorithm for updating $\left(\underline{\underline{A}}^T \underline{\underline{A}}\right)^{-1}$ upon adding a column $\underline{v}$ to $\underline{\underline{A}}$ at column index j.

Inputs: original matrix $\underline{\underline{A}}$, inverse $\underline{\underline{B}} = \left(\underline{\underline{A}}^T \underline{\underline{A}}\right)^{-1}$, column index j

Outputs: updated inverse $\underline{\underline{B}}' = \left(\underline{\underline{A}}'^T \underline{\underline{A}}'\right)^{-1}$

Procedure:

1. Permute row j to the last row of $\underline{\underline{B}}'$, and permute column j to the last column of $\underline{\underline{B}}$.
2. $\underline{\underline{Q}} \leftarrow \underline{\underline{B_{1:n-1,1:n-1}}}$ (i.e., remove last row and last column from $\underline{\underline{B}}$)
3. $d \leftarrow B_{nn}$
4. $\underline{u_3} \leftarrow \underline{\underline{B_{1:n-1,n}}}$
5. $\underline{u_2} \leftarrow \frac{1}{d}\underline{u_3}$
6. $\underline{\underline{B}}' \leftarrow \underline{\underline{Q}} - d\underline{u_2}\underline{u_2}^T$

Algorithm 2: Algorithm for updating $\left(\underline{\underline{A}}^T \underline{\underline{A}}\right)^{-1}$ upon removing a column $\underline{v}$ from $\underline{\underline{A}}$ at column index j.