Kagawa University Economic Review
Vol. 77, No. 3, December 2004, 19−27

The Schur Complements and the Le Chatelier-Braun Principle

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Abstract. By considering the Le Chatelier-Braun principle in thermodynamics for a system of linear equations, we derive a formula which describes how to calculate the inverse of principal submatrices of a real square matrix, based upon the inverse of the given matrix. This formula is related to the Schur complement, and is due to Duncan. Thus, the second term of Schur complement à la Duncan may be interpreted as the matrix of exact Le Chatelier-Braun effects. All proofs are simple and elementary.

Keywords: Duncan identity, Le Chatelier-Braun principle, Reverse bordering method, Schur complements

1 Introduction

Let us consider a system of simultaneous linear equations, $Ax = d$, where A is in $\mathbb{R}^{n\times n}$, the set of n by n $(n \geq 2)$ real matrices, x an n-column variable vector, and d is a given n-column vector. We assume A is regular. Now suppose that the first element of d is increased by unity, then we know the solution x changes by the amount of the first column of the inverse of A. If the last element of the original solution x is to be kept unchanged, thus giving up the last equality in the system of simultaneous equations, the changes in x are represented by the first column of the inverse of the principal submatrix consisting of the first $(n-1)$ columns and $(n-1)$ rows of A. The differences between these two cases show how the solution vector shifts when the last equality is removed from the simultaneous system while keeping the last variable fixed. This situation is where the Le Chatelier-Braun principle may work. In Fujimoto and Ranade[10], a proposition was presented concerning this problem when a given matrix is inverse-positive. (See also Fujimoto[8] and Fujimoto, Herrero and Villar[9].) The point is that the differences between the two inverses of the original matrix and of the principal submatrix are expressed by use of the *inverse* of the original matrix. That is, knowing the signs of A^{-1}, we want to predict whether each element of the solution or equilibrium vector x changes by a greater or a smaller amount than in the original system, when a variable should be fixed, and thus destroying one equation.

When we allow more than one variables to be fixed, and thus removing as many equations, we obtain the inverse of a principal submatrix of a smaller size. When we accomplished this generalization, we found that the resulting formula was already known to Duncan[6], and was used by Brezinski, Morandi, and Redivo-Zaglia[3, p.926] in discussing the reverse bordering method or the bordered inversion method. The formula is also presented in Galántai[12, p.122]. To prove the formula, these authors utilize the Banachiewicz identity in [1], which involves the Schur complement. (For Schur complements, see Ouellette[13]: the reader is referred also to Brezinski[2], Carlson[4], and Cottle[5].)

Following the notation in Ouellette[13] and Galántai[12], let

$$A \equiv \begin{bmatrix} E & F \\ G & H \end{bmatrix} \text{ and } A^{-1} \equiv \begin{bmatrix} \widehat{E} & \widehat{F} \\ \widehat{G} & \widehat{H} \end{bmatrix},$$

where E is in $\mathbb{R}^{p\times p}$, $1 \leq p < n$, and $H \in \mathbb{R}^{q\times q}$, $q = n - p$. Then the Banachiewicz identity in [1] is

$$A^{-1} \equiv \begin{bmatrix} E^{-1} + E^{-1}FS^{-1}GE^{-1} & -E^{-1}FS^{-1} \\ -S^{-1}GE^{-1} & S^{-1} \end{bmatrix},$$

where S is the Schur complement defined by

$$S \equiv (A/E) \equiv H - GE^{-1}F.$$

(This identity was discovered independently by Frazer, Duncan and Collar[7].) From the Banachiewicz identity, it is easy to derive the Duncan identity

$$\widehat{E} = E^{-1} + \widehat{F}(\widehat{H})^{-1}\widehat{G}\ , \text{ or } E^{-1} = (A^{-1}/\widehat{H}) = \widehat{E} - \widehat{F}(\widehat{H})^{-1}\widehat{G}\,.$$

(For derivation, see Brezinski, Morandi, and Redivo-Zaglia[3, p.925], or Galántai[12, p.122].)

It is a matter of simple multiplication of two matrices to prove the Banachiewicz identity. In this paper, however, we derive the Duncan identity first by considering the Le Chatelier-Braun principle for removal of some equations, and then prove the Banachiewicz identity. Therefore, we present one more manifestation of the Schur complement through equilibrium shift in physical systems. The term $(-\widehat{F}(\widehat{H})^{-1}\widehat{G})$ may be interpreted as the matrix of exact Le Chatelier-Braun effects. The exact statement thus made based on the Schur complement à la Duncan makes it easier to understand why the Le Chatelier-Braun principle is not so useful when more than one constraints are removed. One exception is the case in which a given matrix is an M-matrix, thus every principal submatrix is inverse-positive.

In section 2 our notation is explained, and section 3 presents our propositions. In section 4, an interpretation of the matrix $(-\widehat{F}(\widehat{H})^{-1}\widehat{G})$ is given in terms of equilibrium displacements after removal of some equations. The following section 5 includes a natural generalization of Schur complement à la Duncan to function spaces. The final section 6 gives numerical examples and two remarks.

2 Notation

The (i, j) element of a matrix $A \in \mathbb{R}^{n\times n}$, $n \geq 2$, is written as a_{ij}, and the i-th element of a vector x as x_i. The identity matrix in $\mathbb{R}^{n\times n}$ is denoted by I_n.The inequality signs for comparison of two matrices A and $B \in \mathbb{R}^{n\times n}$ are as follows:

$A \geq B$ iff $a_{ij} \geq b_{ij}$;
$A > B$ iff $a_{ij} \geq b_{ij}$ and $A \neq B$;
$A \gg B$ iff $a_{ij} > b_{ij}$.

In section 5, the symbol $L(\mathfrak{X})$ means a Banach space of functions on a measurable set $\mathfrak{X}$, and T is a linear operator from $L(\mathfrak{X})$ to itself.

3 Propositions

We first present a theorem which derives the Duncan identity directly, and is a generalization of Theorem 3.3 in Fujimoto and Ranade [10].

Theorem 1 (Duncan[6]) *Let us suppose a given matrix A and $\widehat{H}$ are regular. Then, E is also regular, and the difference between two corresponding elements in the inverses of E and A is given as*

$$\widehat{E} - E^{-1} = \widehat{F}(\widehat{H})^{-1}\widehat{G}\ , \text{ or } \ E^{-1} = (A^{-1}/\widehat{H}) = \widehat{E} - \widehat{F}(\widehat{H})^{-1}\widehat{G}\,.$$

Proof. We adapt the proof for Theorem 3.3 in Fujimoto and Ranade [10], and consider two matrix equations:

$$A\begin{bmatrix} X & U \\ V & W \end{bmatrix} = I_n, \text{ and} \tag{1}$$

$$EY = I_p\,, \tag{2}$$

where $X \in \mathbb{R}^{p\times p}$, $U \in \mathbb{R}^{p\times q}$, $V \in \mathbb{R}^{q\times p}$, and $W \in \mathbb{R}^{q\times q}$, while Y is in $\mathbb{R}^{p\times p}$. We know

$$X = \widehat{E},\ U = \widehat{F}, V = \widehat{G}, \text{ and } W = \widehat{H}.$$

Subtracting the second equation (2) from the top p equations of (1), we get

$$A\begin{bmatrix} X - Y & U \\ V & W \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ -GY & I_q \end{bmatrix}, \text{ or} \tag{3}$$

$$\begin{bmatrix} X - Y & U \\ V & W \end{bmatrix} = A^{-1}\begin{bmatrix} 0 & 0 \\ -GY & I_q \end{bmatrix} = \begin{bmatrix} \widehat{E} & \widehat{F} \\ \widehat{G} & \widehat{H} \end{bmatrix}\begin{bmatrix} 0 & 0 \\ -GY & I_q \end{bmatrix}. \tag{4}$$

From these, follow

$$X - Y = -\widehat{F}GY\,,\ \text{and}\ \ V = -\widehat{H}GY.$$

From the latter, we have $GY = -(\widehat{H})^{-1}V = -(\widehat{H})^{-1}\widehat{G}$, which is substituted to the former, yielding $\widehat{E} - Y = \widehat{F}(\widehat{H})^{-1}\widehat{G}$, i.e., $Y = \widehat{E} - \widehat{F}(\widehat{H})^{-1}\widehat{G}$. Proceeding backward in this proof, we know from eq.(2) that Y is the inverse of E. ■

Theorem 2 (Banachiewicz[1]) *Let us suppose a given matrix A and its principal submatrix E are regular. Then*

$$A^{-1} = \begin{bmatrix} E^{-1} + E^{-1}FS^{-1}GE^{-1} & -E^{-1}FS^{-1} \\ -S^{-1}GE^{-1} & S^{-1} \end{bmatrix}.$$

Proof. Since

$$(A^{-1})^{-1} = \begin{bmatrix} E & F \\ G & H \end{bmatrix},$$

and E is assumed to be regular, we can apply the Duncan identity to A^{-1} and $\widehat{H}$, obtaining $(\widehat{H})^{-1} = H - GE^{-1}F = S$, from which comes out $\widehat{H} = S^{-1}$. Now we can write

$$A^{-1} = \begin{bmatrix} E^{-1} + \widehat{F}S\widehat{G} & \widehat{F} \\ \widehat{G} & S^{-1} \end{bmatrix}. \tag{5}$$

From the identity $AA^{-1} = I_n$, we have $E\widehat{F} + FS^{-1} = 0$. Thus, $\widehat{F} = -E^{-1}FS^{-1}$. Similarly, from $A^{-1}A = I_n$, we get $\widehat{G} = -S^{-1}GE^{-1}$. Substituting these into the RHS of eq.(5), completes the proof. ■

When H is a nonzero scalar, i.e., $q = 1$, it is easy to have the following corollary, which is Theorem 3.3 in Fujimoto and Ranade [10, p.62].

Corollary 3 *Suppose that H is a scalar, a_{nn}, the inverse of A has its last column and the bottom row non-negative, and that $|A| > 0$ and $|E| > 0$. Then each element of the inverse of E^{-1} is less than or equal to the corresponding element of the inverse of A, i.e., $\widehat{E}$.*

Proof. Since $\widehat{H} = |E|\,/\,|A| > 0$, $\widehat{F} \geq 0$, and $\widehat{G} \geq 0$, the desired result follows from Theorem 1. ■

This result can be interpreted as expressing a sort of Le Chatelier-Braun principle as is explained in Fujimoto and Ranade[10, p.65]. However, when q becomes larger than one, say $q = 2$, that is, two equations are removed at the same time, we cannot predict the directions of changes even when the inverse of A has the last two columns and the bottom two rows positive. (See a numerical example in section 6.) One exception is the case in which a given matrix A is an M-matrix.

Corollary 4 *If A is an M-matrix, then each principal submatrix is inverse-positive, and the smaller is the size of a principal submatrix, the smaller are the elements of its inverse or they remain unchanged. That is,* $\widehat{F}(\widehat{H})^{-1}\widehat{G} > 0$.

Proof. Since each principal submatrix of an M-matrix is again an M-matrix, it is inverse-positive. Thus, we can apply Corollary 3 successively. ■

This corollary is proved in Fujimoto, Herrero and Villar [9] using an iterative method, and the inequality $\widehat{F}(\widehat{H})^{-1}\widehat{G} > 0$ does not seem trivial unless we know the LHS is the difference between $\widehat{E}$ and E^{-1}. (The essence of this result was generalized to an indecomposable system of nonlinear M-functions in Fujimoto [8].)

4 An Interpretation

In thermodynamics, the Le Chatelier principle means a prediction of direction in which an equilibrium shifts when a *direct* parametrical change takes place in the system, while the Le Chatelier-Braun principle is concerned with the situation where a disturbance is introduced *indirectly.* Recently this distinction has become almost lost, and both dictate that the equilibrium changes in order to reduce the effects caused by external disturbances directly or indirectly, thus implying possible stability of the new equilibrium. The Le Chatelier principle is normally proved using the positive definiteness of the Hessian matrix at the equilibrium: the definiteness is guaranteed through minimization of a certain energy. In our framework, an equilibrium described by a system of simultaneous linear equations, $Ax = d$, is perturbed by changes in d while fixing some variables at the previous equilibrium levels and removing as many equations, and so the Le Chatelier-Braun principle may work.

Our proof of Theorem 3.1 can give a natural interpretation of the matrix

$$(-\widehat{F}(\widehat{H})^{-1}\widehat{G}).$$

First, we imagine that a series of n disturbances have taken place separately, in each of which d_i, for $i = 1$ to n, is increased by one. These disturbances are represented by I_n in eq.(1), and all the resulting displacements are given as $\begin{bmatrix} X & U \\ V & W \end{bmatrix}$ in eq.(1). The displacements, Y, when the bottom q variables remain unchanged and destroying as many bottom equations, are described by eq.(2). Direct and indirect effects are all contained in the elements of the inverse A^{-1} and $Y(= E^{-1})$. The matrix $(-GY)$ in eq.(3) shows the discrepancy created in the bottom q equations by the shift from X to Y in the first p variables. Thus, once $\widehat{G}$ and $\widehat{H}$, inclusive of all direct and indirect effects, are known, we can calculate $(-GY)$ as

$$-GY = (\widehat{H})^{-1}V = (\widehat{H})^{-1}\widehat{G},$$

using the bottom q equations of eq.(4). If, in addition, $\widehat{E}$ and $\widehat{F}$ are known, it follows from the top p equations, i.e., $X - Y = -\widehat{F}GY$, that

$$\widehat{E} - E^{-1} = -\widehat{F}GY = \widehat{F}(\widehat{H})^{-1}\widehat{G}.$$

Thus, the displacement matrix $(-\widehat{F}(\widehat{H})^{-1}\widehat{G})$ between two equilibria X and Y may be called the matrix of *exact* Le Chatelier-Braun effects.

More concretely, let us consider the case dealt with jointly by both Corollaries 3 and 4. Suppose for simplicity of discussion that $\widehat{H}$ is a positive scalar, and $\widehat{F}$ and $\widehat{G}$ are strictly positive vectors and $\widehat{E}$ is a strictly positive matrix. When d_1 is increased by unity, x_1 and x_n are also increased to the new equilibrium values x_1^* and x_n^* because $\widehat{E}_{11} > 0$ and $\widehat{G}_1 > 0$. Then, keeping x_n fixed at the level before the disturbance, implies decreasing x_n^*, which in turn would be equivalent to an decrease in d_n as a parametrical change because $\widehat{H}$ is a positive scalar. In the end, this will cause x_1^* to decrease since $\widehat{F}_1 > 0$. Therefore, the effect on x_1 of the increase in d_1 is smaller when the last element x_n is fixed and the last equation is removed. In sum, removal of the last equation attenuates the effect of the disturbance produced by increasing d_1.

5 A Generalization to Function Spaces

It is now not difficult to extend the results in section 3 to function spaces. Suppose a measure space, $\mathfrak{X}$ with its measure μ, is divided into two measurable sets P and Q such that $P \cup Q = \mathfrak{X}$, $P \cap Q = \emptyset$, $\mu(P) \neq 0$, and $\mu(Q) \neq 0$. We assume that a given linear operator T from $L(\mathfrak{X})$ to itself has its inverse T^{-1}. By considering the restrictions of domains of functions to P or Q, we can conceive the decompositions of T and T^{-1} as

$$T = \begin{bmatrix} E & F \\ G & H \end{bmatrix} \text{ and } T^{-1} = \begin{bmatrix} \widehat{E} & \widehat{F} \\ \widehat{G} & \widehat{H} \end{bmatrix},$$

exactly as in the case of a finite dimension. When two operators E and $\widehat{H}$ are invertible, the same proof that is employed for Theorem 1 applies, interpreting I_n, I_p and I_q as the identity maps on the respective subspaces, and we have $\widehat{E} - E^{-1} = \widehat{F}(\widehat{H})^{-1}\widehat{G}$ or $E^{-1} = (T^{-1}/\widehat{H}) = \widehat{E} - \widehat{F}(\widehat{H})^{-1}\widehat{G}$. Concerning a special case of M-operator we have published a paper in this journal([11]).

6 A Numerical Example and Remarks

Consider the following 4 by 4 matrix and its inverse:

$$A \equiv \begin{bmatrix} -6.0 & 5.5 & 6.0 & -5.0 \\ 5.0 & -4.5 & -6.0 & 5.0 \\ 10.0 & -10.0 & -10.0 & 10.0 \\ -9.0 & 9.0 & 11.0 & -10.0 \end{bmatrix} \text{ and } A^{-1} = \begin{bmatrix} 1.0 & 3.0 & 1.0 & 2.0 \\ 2.0 & 4.0 & 1.0 & 2.0 \\ 1.0 & 1.0 & 1.0 & 1.0 \\ 2.0 & 2.0 & 1.1 & 1.0 \end{bmatrix}.$$

When

$$E = \begin{bmatrix} -6.0 & 5.5 & 6.0 \\ 5.0 & -4.5 & -6.0 \\ 10.0 & -10.0 & -10.0 \end{bmatrix},$$

we can confirm Corollary 3 because

$$\begin{aligned} E^{-1} &= \begin{bmatrix} -6.0 & 5.5 & 6.0 \\ 5.0 & -4.5 & -6.0 \\ 10.0 & -10.0 & -10.0 \end{bmatrix}^{-1} \\ &= \begin{bmatrix} -3.0 & -1.0 & -1.2 \\ -2.0 & 0 & -1.2 \\ -1.0 & -1.0 & -0.1 \end{bmatrix} \ll \begin{bmatrix} 1.0 & 3.0 & 1.0 \\ 2.0 & 4.0 & 1.0 \\ 1.0 & 1.0 & 1.0 \end{bmatrix} = \widehat{E}. \end{aligned}$$

When we set

$$E = \begin{bmatrix} -6.0 & 5.5 \\ 5.0 & -4.5 \end{bmatrix},$$

$$\begin{aligned} E^{-1} &= \begin{bmatrix} -6.0 & 5.5 \\ 5.0 & -4.5 \end{bmatrix}^{-1} \\ &= \begin{bmatrix} 9.0 & 11.0 \\ 10.0 & 12.0 \end{bmatrix} \gg \begin{bmatrix} 1.0 & 3.0 \\ 2.0 & 4.0 \end{bmatrix} = \widehat{E}. \end{aligned}$$

Note that though the matrix A has the bottom two rows and the last two columns positive, removal of bottom two equations while fixing the last two variables gives rise to a very different picture, compared with the case of removal of a single equation separately.

One more example is concerned with the case of M-matrix treated in Corollary 4. Let

$$A \equiv \begin{bmatrix} 1 & -0.1 & -0.2 & -0.3 \\ -0.2 & 2 & -0.2 & -0.3 \\ -0.1 & -0.2 & 3 & -0.1 \\ -0.2 & -0.1 & -0.1 & 4 \end{bmatrix} \quad \text{and}$$

$$A^{-1} \approx \begin{bmatrix} 1.0373 & 0.06371 & 0.07621 & 0.08448 \\ 0.1165 & 0.5126 & 0.04355 & 0.04827 \\ 0.04421 & 0.03686 & 0.3392 & 0.01456 \\ 0.05588 & 0.01692 & 0.01338 & 0.2558 \end{bmatrix}.$$

When

$$\widehat{H} \approx \begin{bmatrix} 0.3392 & 0.01456 \\ 0.01338 & 0.2558 \end{bmatrix} \text{ and } (\widehat{H})^{-1} \approx \begin{bmatrix} 2.9546 & -0.1682 \\ -0.1546 & 3.9183 \end{bmatrix},$$

we have

$$\widehat{F}(\widehat{H})^{-1}\widehat{G} \approx \begin{bmatrix} 0.07621 & 0.08448 \\ 0.04355 & 0.04827 \end{bmatrix} \begin{bmatrix} 2.9546 & -0.1682 \\ -0.1546 & 3.9183 \end{bmatrix} \begin{bmatrix} 0.04421 & 0.03686 \\ 0.05588 & 0.01692 \end{bmatrix}$$

$$\approx \begin{bmatrix} 0.02716 & 0.01320 \\ 0.01552 & 0.007545 \end{bmatrix} > 0.$$

If

$$\widehat{H} \approx \begin{bmatrix} 0.5126 & 0.04355 & 0.04827 \\ 0.03686 & 0.3392 & 0.01456 \\ 0.01692 & 0.01338 & 0.2558 \end{bmatrix} \text{ and } (\widehat{H})^{-1} \approx \begin{bmatrix} 1.9800 & -0.2400 & -0.3600 \\ -0.2100 & 2.9802 & -0.1300 \\ -0.1200 & -0.1400 & 3.9399 \end{bmatrix},$$

then

$$\widehat{F}(\widehat{H})^{-1}\widehat{G} \approx \begin{bmatrix} 0.06371 & 0.07621 & 0.08448 \end{bmatrix} \begin{bmatrix} 1.9800 & -0.2400 & -0.3600 \\ -0.2100 & 2.9802 & -0.1300 \\ -0.1200 & -0.1400 & 3.9399 \end{bmatrix} \begin{bmatrix} 0.1165 \\ 0.04421 \\ 0.05588 \end{bmatrix}$$

$$\approx 0.03726 > 0.$$

These inequalities verify Corollary 4.

Remark 1 From the Banachiewicz identity or eq.(5), it easily follows that $|A^{-1}| = |E^{-1}| \cdot |S^{-1}|$. Thus we have the original result due to Schur [14], $|A| = |E| \cdot |S|$. We can then deduce $|S^{-1}| \cdot |A| = |E|$, i.e, $\left|\widehat{H}\right| \cdot |A| = |E|$. (See the proof of Theorem 2.) This is the Jacobi determinant identity.

Remark 2 The Le Chatelier-Braun principle may work well when *only one* 'disturbance' takes place. As we can observe from the first example in the above, however, when two or more constraints are removed by fixing as many variables, it may be wrong to add those individual effects that can be well predicted separately by the principle. Our Theorem 1 may be able to give some useful *qualitative* information in special cases such as the one in Corollaries 3 and 4, or more generally when the sign patterns of the inverse of $\widehat{H}$ can be found by those of $\widehat{H}$ only. Indeed, as Carlson[4, p.273] wrote, "They(Schur complement matrices) will continue to be of use to mathematicians and users of mathematics as long as partitioned matrices and restrictions of linear operators to subspaces are studied."

Acknowledgment. Thanks are due to Mr Genta Kido, assistant librarian, who helped the authors to obtain the photocopies of some references.

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