The Generalised Inverse
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The generalised inverse

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Introduction

If we have a system of m linear equations to solve, it is a great simplification to write them in matrix form

$$\mathbf{Ax} = \mathbf{b},$$

where $\mathbf{A}$ is an $m \times n$ matrix of coefficients, $\mathbf{b}$ is an m-dimensional vector of constants and $\mathbf{x}$ is an n-dimensional vector of unknowns. It is one of the benefits of this representation that, providing

(i) $m = n$, and
(ii) $\mathbf{A}$ is non-singular (i.e. $\mathbf{A}^{-1}$ exists),

then $$\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

is the solution, where $\mathbf{A}^{-1}$ is the $n \times n$ matrix that satisfies $\mathbf{A}^{-1}\mathbf{A} = \mathbf{AA}^{-1} = \mathbf{I}$.

Something of the power of the matrix method, displayed by this result, is lost however when either $m \neq n$ or $\mathbf{A}$ is singular. For in this case, almost by definition, $\mathbf{A}^{-1}$ does not exist and we have to be content with statements such as "the solution does/does not exist", "there is one/are many solutions", etc. In fact, it seems that the best we can do is to describe the entire set of solutions as $\mathbf{z} = \mathbf{a} + \mathbf{k}$, where $\mathbf{a}$ is some particular solution to $\mathbf{Ax} = \mathbf{b}$ and $\mathbf{k}$ is any vector from $K(\mathbf{A})$, the kernel of $\mathbf{A}$. (Recall that the kernel, or null space, of $\mathbf{A}$ is the subspace of all solutions to $\mathbf{Ax} = \mathbf{0}$.)

Things are not as bad as they seem; for, as we shall see, there exists a matrix $\mathbf{A}^g$ (of dimensions $n \times m$), known as the "generalised inverse" of $\mathbf{A}$ (whether $\mathbf{A}$ is square or rectangular, singular or non-singular!), such that

$$\mathbf{z} = \mathbf{A}^g\mathbf{b}$$

is a particular solution to $\mathbf{Ax} = \mathbf{b}$. And, a somewhat more unexpected result,

$$\mathbf{z} = \mathbf{A}^g\mathbf{b} + (\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{w}$$

represents the entire set of solutions as $\mathbf{w}$, an arbitrary n-dimensional vector, varies over all possible values. This is a remarkable result in that it is subject to only one mild condition—that a solution exists at all—and $\mathbf{A}^g$ even provides a simple test for this condition!

A numerical example

Consider the four equations in three unknowns specified by the matrix equation

$$\begin{bmatrix} 2 & 0 & -2 \\ 1 & -1 & 0 \\ 3 & -1 & -2 \\ 1 & 1 & -2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 3 \\ 5 \\ -1 \end{bmatrix}.$$

$$\mathbf{A} \qquad \mathbf{x} = \mathbf{b}.$$

These can be solved by the usual elimination method (see [1]), which gives

$$\begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \\ 0 \\ 0 \end{bmatrix}$$

and hence

$$x_1 - x_3 = 1, \; x_2 - x_3 = -2.$$

Thus (writing $x_3 = \lambda$)

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1+\lambda \\ \lambda - 2 \\ \lambda \end{bmatrix}$$

gives all the solutions as λ varies over all possible values. We will use this example throughout to illustrate the techniques introduced.

It should be pointed out that elimination is usually to be preferred to the calculation of $\mathbf{A}^g$, or $\mathbf{A}^{-1}$ for that matter, when solving any *particular* set of equations. The power of $\mathbf{A}^g$ lies in being able to supply the solution to *all* equations involving the coefficient matrix $\mathbf{A}$.

What makes a solution?

If $\mathbf{z} = \mathbf{Gb}$ is a solution to $\mathbf{Ax} = \mathbf{b}$, what properties must $\mathbf{G}$ have?

By definition, $\mathbf{Az} = \mathbf{b}$ if and only if $\mathbf{z}$ is a solution; hence $\mathbf{AGb} = \mathbf{b}$ is the simple condition that $\mathbf{G}$ has to satisfy. Now at this point it is tempting to rush on and claim that, as $\mathbf{AGb} = \mathbf{b}$, $\mathbf{AG}$ must be the identity $\mathbf{I}$; but in this case $\mathbf{AGy} = \mathbf{y}$ for *all* $\mathbf{y}$, and this is far more than we require. If $\mathbf{AGy} = \mathbf{y}$ for *only* $\mathbf{y} = \mathbf{b}$ we still have a solution to $\mathbf{Ax} = \mathbf{b}$.

However, for $\mathbf{G}$ to be of any use, we would like $\mathbf{AGb} = \mathbf{b}$ for as many different $\mathbf{b}$s as possible. As a solution to $\mathbf{Ax} = \mathbf{b}$ only exists if $\mathbf{b}$ is in the image space $\mathrm{Im}(\mathbf{A})$ of $\mathbf{A}$, the best we could possibly ask is for $\mathbf{G}$ to satisfy $\mathbf{AGb} = \mathbf{b}$ for all $\mathbf{b}$ in $\mathrm{Im}(\mathbf{A})$. Such a matrix $\mathbf{G}$ is known as a *generalised inverse* of $\mathbf{A}$, and is written $\mathbf{A}^g$.

A matrix definition of $\mathbf{A}^g$

Our current definition of $\mathbf{A}^g$ is difficult to work with, as it involves $\mathrm{Im}(\mathbf{A})$. We can, however, obtain a simple matrix definition of $\mathbf{A}^g$ free of any reference to $\mathrm{Im}(\mathbf{A})$ as follows. If $\mathbf{x}$ is an arbitrary n-dimensional vector, $\mathbf{y} = \mathbf{Ax}$ is a vector in $\mathrm{Im}(\mathbf{A})$. Thus the condition

$$\mathbf{AA}^g\mathbf{y} = \mathbf{y} \quad \text{for all } \mathbf{y} \text{ in } \mathrm{Im}(\mathbf{A})$$

becomes

$$\mathbf{AA}^g\mathbf{Ax} = \mathbf{Ax} \quad \text{for all vectors } \mathbf{x};$$

that is, if $\mathbf{A}^g$ is a generalised inverse according to our first definition, then $\mathbf{AA}^g\mathbf{A} = \mathbf{A}$. It is not difficult to show that the converse is also true. This property is the basis of the more usual definition of a generalised inverse; viz., a matrix $\mathbf{G}$ such that $\mathbf{AGA} = \mathbf{A}$.

A generalised inverse of $\mathbf{A}$, the matrix of coefficients in our example, is

$$\mathbf{A}^g = \frac{1}{18}\begin{bmatrix} 1 & 2 & 3 & -1 \\ 1 & -4 & -3 & 5 \\ -2 & 2 & 0 & -4 \end{bmatrix},$$

as may be verified by showing that $\mathbf{AA}^g\mathbf{A} = \mathbf{A}$. (Details of the calculation of $\mathbf{A}^g$ are given later.)

Existence and everything

Let us now examine what $\mathbf{A}^g$ can do for us.

THEOREM 1. *A solution to* $\mathbf{Ax} = \mathbf{b}$ *exists if and only if* $\mathbf{AA}^g\mathbf{b} = \mathbf{b}$.

PROOF. If $\mathbf{AA}^g\mathbf{b} = \mathbf{b}$ then $\mathbf{A}^g\mathbf{b}$ is clearly a solution.

Conversely if a solution exists, $\mathbf{z}$ say, then $\mathbf{Az} = \mathbf{b}$. Therefore

$$\mathbf{AA}^g\mathbf{Az} = \mathbf{b} \quad (\text{using } \mathbf{AA}^g\mathbf{A} = \mathbf{A}),$$

and so

$$\mathbf{AA}^g\mathbf{b} = \mathbf{b} \quad (\text{using } \mathbf{Az} = \mathbf{b}).$$

THEOREM 2. *The complete set of solutions to* $\mathbf{Ax} = \mathbf{b}$ *is given by*

$$\mathbf{z} = \mathbf{A}^g\mathbf{b} + (\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{w}$$

as $\mathbf{w}$, *an arbitrary n-dimensional vector, varies over all possible values.*

PROOF. We already have, by Theorem 1, that $\mathbf{A}^g\mathbf{b}$ is a particular solution. If we can show that $(\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{w}$ gives every vector in $K(\mathbf{A})$ and no other, then, by our earlier remark, we have all the solutions.

Consider $\mathbf{k} = (\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{w}$. Then

$$\mathbf{Ak} = \mathbf{A}(\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{w} = (\mathbf{A} - \mathbf{AA}^g\mathbf{A})\mathbf{w} = (\mathbf{A} - \mathbf{A})\mathbf{w} = \mathbf{0},$$

and every vector of the form $(\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{w}$ is a member of $K(\mathbf{A})$.

Now suppose $\mathbf{k}$ is a vector in the kernel of $\mathbf{A}$, so that $\mathbf{Ak} = \mathbf{0}$. Then, as $(\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{k} = (\mathbf{k} - \mathbf{A}^g\mathbf{Ak}) = (\mathbf{k} - \mathbf{A}^g\mathbf{0}) = \mathbf{k}$, every vector in $K(\mathbf{A})$ may be written in the form $(\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{w}$.

We can now obtain the complete set of solutions to our example, using Theorem 2 and the value for $\mathbf{A}^g$ given earlier. The reader is invited to show that:

(i) $\mathbf{AA}^g\mathbf{b} = \mathbf{b}$.

(ii) A particular solution is given by

$$\mathbf{z} = \mathbf{A}^g\mathbf{b} = \tfrac{1}{3}\begin{bmatrix} 4 \\ -5 \\ 1 \end{bmatrix}.$$

(iii) $$(\mathbf{I} - \mathbf{A}^g\mathbf{A})\mathbf{w} = \tfrac{1}{3}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}\begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix},$$

and therefore $\begin{bmatrix} \lambda' \\ \lambda' \\ \lambda' \end{bmatrix}$, where $\lambda' = \frac{1}{3}(w_1 + w_2 + w_3)$, is in $K(\mathbf{A})$.

(iv) $$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \tfrac{1}{3}\begin{bmatrix} 4 \\ -5 \\ 1 \end{bmatrix} + \begin{bmatrix} \lambda' \\ \lambda' \\ \lambda' \end{bmatrix}$$

is equivalent to our earlier solution, i.e.

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 + \lambda \\ \lambda - 2 \\ \lambda \end{bmatrix}, \quad \text{where } \lambda = \lambda' + \tfrac{1}{3}.$$

We now have all the results promised in the introduction, but we have by no means exhausted the usefulness of the generalised inverse in the solution of linear equations. The reader is referred to [2] for more details.

Calculating $\mathbf{A}^g$

The calculation of $\mathbf{A}^g$ is mainly of theoretical interest, for as we have already noted the use of $\mathbf{A}^g$ (or $\mathbf{A}^{-1}$ when $\mathbf{A}$ is square and non-singular) is not the best way to obtain numerical solutions to any *particular* linear problem. Nevertheless a simple method for constructing a generalised inverse is given below, which at least serves to demonstrate that $\mathbf{A}^g$ always exists.

Assume that $\mathbf{A}$ (of dimensions $m \times n$) is of rank r, that is has r linearly independent rows. Then

(i) take r independent rows of $\mathbf{A}$ to form the matrix $\mathbf{B}$;

(ii) calculate $\mathbf{C} = \mathbf{AB}^{\mathrm{T}}(\mathbf{BB}^{\mathrm{T}})^{-1}$ (note that $\mathbf{BB}^{\mathrm{T}}$ is always non-singular: why?);

(iii) $\mathbf{A}^g = \mathbf{B}^{\mathrm{T}}(\mathbf{BB}^{\mathrm{T}})^{-1}(\mathbf{C}^{\mathrm{T}}\mathbf{C})^{-1}\mathbf{C}^{\mathrm{T}}$.

There are better ways of calculating $\mathbf{A}^g$, but they all involve more advanced concepts such as eigenvectors (see [2]).

The application of this method to the coefficient matrix $\mathbf{A}$ of our example results in the $\mathbf{A}^g$ given earlier. As the rank of $\mathbf{A}$ is 2, the reader may repeat the calculation by selecting *any* two rows of $\mathbf{A}$ to form the matrix $\mathbf{B}$. (The first two are a good choice, leading to simple arithmetic.)

The proof that $\mathbf{A}^g$ so constructed satisfies $\mathbf{AA}^g\mathbf{A} = \mathbf{A}$ depends on noting that, as $\mathbf{B}$ consists of any r independent rows of $\mathbf{A}$, the remaining rows can be written as linear combinations of the rows of $\mathbf{B}$. (If this were not the case $\mathbf{A}$ would be of rank greater than r.) Putting this another way, $\mathbf{A}$ may be written as $\mathbf{XB}$, where $\mathbf{X}$ is the $r \times m$ matrix used to form the linear combinations of the rows of $\mathbf{B}$. It is not difficult to show that $\mathbf{X}$ is of rank r and that $\mathbf{X} = \mathbf{C}$. Thus $\mathbf{A} = \mathbf{CB}$ and, as

$$\begin{aligned}\mathbf{AA}^g\mathbf{A} &= \mathbf{C}(\mathbf{BB}^{\mathrm{T}})(\mathbf{BB}^{\mathrm{T}})^{-1}(\mathbf{C}^{\mathrm{T}}\mathbf{C})^{-1}(\mathbf{C}^{\mathrm{T}}\mathbf{C})\mathbf{B} \\ &= \mathbf{CB} = \mathbf{A},\end{aligned}$$

we have proved that our method for constructing $\mathbf{A}^g$ always works.

How many $\mathbf{A}^g$*s?*

Now that we have shown that $\mathbf{A}^g$ exists, the next question is: is $\mathbf{A}^g$ unique? Having gone to so much trouble to find a particular $\mathbf{A}^g$, it is surprising to find that there may be many matrices that could serve as a generalised inverse. When $\mathbf{A}$ is non-singular then $\mathbf{A}^g = \mathbf{A}^{-1}$ and is unique, but in all other cases there is an infinite number of matrices that satisfy $\mathbf{AA}^g\mathbf{A} = \mathbf{A}$.

However, the particular $\mathbf{A}^g$ constructed according to our previous algorithm is unique (that is, it does not depend on the initial selection of the r independent rows) and is usually referred to as *the* generalised inverse or the Moore/Penrose (M/P) inverse.

The M/P inverse satisfies three extra conditions:

(1) $\mathbf{A}^g\mathbf{A}\mathbf{A}^g = \mathbf{A}^g$,

(2) $(\mathbf{A}\mathbf{A}^g)^{\mathrm{T}} = \mathbf{A}\mathbf{A}^g$,

(3) $(\mathbf{A}^g\mathbf{A})^{\mathrm{T}} = \mathbf{A}^g\mathbf{A}$,

and it is an interesting (but difficult) exercise in matrix algebra to show that any matrix $\mathbf{G}$ that satisfies $\mathbf{AGA} = \mathbf{A}$ and (1)–(3) is unique (see [2]).

Conclusion

The generalised inverse provides a closed solution to a problem that crops up in most areas of mathematics, and makes theoretical calculations with singular matrices almost as easy as with non-singular matrices. We can go on to classify all the possible types of solution to $\mathbf{Ax} = \mathbf{b}$ according to the rank of $\mathbf{A}$ and solve problems of the "least squares" type without exhausting all of the possibilities. Finally, to offer a glimpse of wider (but less practical) horizons, the inverses in other mathematical objects can be "generalised"; e.g. the generalised inverse of a in a ring R is an element a^g in R such that $aa^ga = a$.

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Georg Wolff (1886–1977)

At the International Congress of Mathematicians in Rome in 1908 the decision was taken to found the International Commission for Mathematical Instruction. The various national sub-commissions arranged to produce a series of reports, describing the state of mathematical education in their different countries for presentation at the next congress at Cambridge in 1912. The British contribution comprised 43 papers, covering over 900 pages, in two volumes published by the Board of Education (*Special reports on educational subjects*, XXVI and XXVII: Teaching of Mathematics in the United Kingdom, HMSO, 1912). These papers were written by the leading mathematicians and educators of the day, and they are still compelling reading.