Linear Algebra is Your Friend: Least Squares Solutions to Overdetermined Linear Systems

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Most engineering students are quite familiar with least squares regression analysis of experimental data on Y versus X plots using EXCEL or other similar spreadsheet software programs. They use the reported coefficient of determination, R^2, as a measure of the "closeness of fit". Most chemical engineering students, however, are not well versed enough with the concepts of modern day computational techniques for finding the least squares solution or with the application of linear algebra for determining the best solution to overdetermined linear systems of equations.

For chemical engineers these systems commonly result from material balance analysis of multicomponent flow through processing equipment. Take the very simple example of a Prism membrane system used in the senior lab course at the Ralph E. Martin Department of Chemical Engineering at the University of Arkansas shown in Figure 1[1]. It is used for separating a pressurized air stream into an oxygen rich stream and a nitrogen rich stream.

Figure 1 Prism Membrane Separation System

Traditional material balance analysis would involve obtaining a unique solution by writing an overall balance and an oxygen component balance over the membrane system:

$$(1)*F = (1)*N_p + (1)* N_{np} \qquad \text{(eq. 1)}$$

$$(0.21)*F = (Y_{O2})_p* N_p + (Y_{O2})_{np}* N_{np} \qquad \text{(eq. 2)}$$

or, alternatively, an overall balance and a nitrogen component balance,

$$(0.79)*F = (Y_{N2})_p* N_p + (Y_{N2})_{np}* N_{np} \qquad \text{(eq. 3)}$$

but not all three because the component balances sum to give the overall balance and therefore all three equations are not strictly independent. Furthermore, traditionally the mole fractions, y, of each stream are forced to sum to 1.0. However, when each flow rate is individually determined by flow meters and when each mole fraction is determined individually by sensors (except for the inlet air), the student is faced with obtaining the "best" solution to the overdetermined system of equations that has uncertainty introduced due to the inaccuracy of instrumentation.

Consider the following example data taken during an experiment using the equipment above:

F- Total molar flow rate of air through the system as measured by the dry gas meter,1.98 mole/min

Inlet air composition certified by the air supplier as 21 mole% O_2 and 79 mole% N_2

N_p - Molar flow rate of permeate exit stream as measured by the rotameter, 0.150 mole/min

N_{np} -Molar flow rate of the non-permeate exit stream as measured by the rotameter,1.86 mole/min

$(Y_{xx})_p$ –Component mole fraction of the permeate stream measured by sensors as 42 mole% O_2 and 60 mole% N_2 where $_{xx}$ represents either O_2 or N_2

$(Y_{xx})_{np}$ - Component mole fraction of the non-permeate stream measured by sensors as 19 mole% O_2 and 84 mole % N_2 where $_{xx}$ represents either O_2 or N_2

Thus, an overdetermined system of linear equations is formed, having matrix format represented by the classical A**x**=**b** system of linear equations (eq. 4). The symbol A is an m by n matrix consisting of the coefficients of the N_p and N_{np} flow streams in each equation; **x** is an n-vector representing the molar flow rates variables themselves (F, N_p, N_{np}). The m-vector **b** represents the total and individual component molar flow rates of material flowing through the system.

$$\begin{pmatrix} 1 & 1 \\ 0.42 & 0.19 \\ 0.60 & 0.84 \end{pmatrix} \cdot (\mathbf{x}) = \begin{pmatrix} 1.980 & 1.980 \\ 0.417 & 0.416 \\ 1.652 & 1.564 \end{pmatrix} \qquad \text{eq. 4}$$

$$A \cdot (\mathbf{x}) = b$$

Several items need to be noted with respect to the system of equations represented by equation 4. First, one notes that matrix A, the mole fractions of the permeate and the non-permeate streams do not sum to one due to inaccuracy of the compositional sensors. Secondly, **b** presents two different column vectors representing two different modeling approaches for determining the total amount of each component, oxygen and nitrogen, flowing through the system. The first column vector in b denotes the total flow of each component by assuming that both permeate and non-permeate stream flow meters are accurate as well as each compositional sensor. The second column vector in **b** represents the total component flows by assuming the feed dry gas flow meter is accurate and assuming the composition of atmospheric air to be 79% nitrogen and 21% oxygen. Further, note that in this case the only significant difference between these two modeling approaches shows up in the total nitrogen flow.

The least squares type problem may be formally defined mathematically by Datta[2] as finding the n-vector **x** such that the norm of the residual vector, $\| A\mathbf{x}-\mathbf{b} \|_2$, is a minimum. This is synonymous to saying the sum of the squares of the individual residuals is a minimum. This technique was first published by A. M. Legendre in 1806 although Carl Friedrich Gauss actually used it in astronomical calculations as early as 1797[3].

Solving equations 1 and 2 simultaneously, then equations 1 and 3 simultaneously, followed by simultaneously solving equations 2 and 3, results in differ values of N_n and N_{np} . Table 1 presents the resulting flow rates and each respective residual using the first column vector of **b**.

Table 1 Simultaneous Pair-Wise Solutions to Equations 1-3

	Equations 1 & 2	**Equations 1 & 3**	**Equations 2 & 3**	**Measured Values**
$\mathbf{N_n}$	0.177	0.124	0.152	0.150
$\mathbf{N_{np}}$	1.802	1.866	1.858	1.860
∑ **Residuals***	0.031	0.018	0.030	0.030

*$\| A\mathbf{x}-\mathbf{b} \|_2$

The values of the permeate flow rate varies by up to 42%, while the value of the sum of the residuals varies by up to 72%. Therefore, the question arises as to how to determine the "least squares" solution to the above overdetermined system of linear equations, i.e. minimize the sum of the residuals to determine the best value of N_n and N_{np}. Linear algebra offers a variety of methods for doing this, each one having their individual advantages and disadvantages depending on such factors as computer time (cost), precision required, conditioning of the system of equations, etc. The method used for the simple example of this paper is known as the "normal equations" solution resulting in the unique least squares solution to the original system of equations provided the matrix, A , has rank of n, which it does.

This method involves left multiplying through by A^T and then using a fundamental theorem of linear algebra which states that

$$\mathbf{x} = (A^T A)^{-1} A^T b \qquad \text{(eq. 5)}$$

is the unique solution for which we are looking.

MATLAB is a readily available and a convenient computer language for making such matrix algebraic manipulations[4]. The MATLAB output for the example discussed above is shown below:

A = 1.0000e+000 1.0000e+000

4.2000e-001 1.9000e-001

6.0000e-001 8.4000e-001

b = 1.9800e+000

4.1700e-001

1.6520e+000

Answers returned by MATLAB for values of **x** are:

N_n = 1.2395e-001

N_{np} = 1.8663e+000

with the sum of the residuals = 0.01763

While the least squares solution is nearly the same as solving equations 1 and 3, it does a better job of satisfying all three equations than any of the other solutions obtained by simply solving any 2 of the 3 equations. The least squares solution for the second column of **b** is

N_n = 2.7128e-001

N_{np} = 1.6898e+000

with the sum of the residuals = 0.03241. And finally, the least squares solution for the 5 different equations is

N_n = 1.9458e-001

N_{np} = 1.7790e+000

with the sum of the residuals = 0.06288. One might argue the merits of one model over another, for example, the least squares solution for the first column of **b** satisfies all three equations better than solving equations 2 and 3, but the solution to equations 2 and 3 gives a solution which is closer to the measured values. But in the measured values, the overall balance is violated much more than with the least squares solution. Which is "more correct"? Is there an experimental error in the measured values or the measured rotameter solution? Which right hand side model is better? Since one can compute a best approximate solution to an overdetermined system, one can include competing and even inconsistent models as components (sets of equations) of the least squares model.

So, hence the title "linear algebra is your friend". Much more complicated problems exist with much larger matrices which require careful consideration of the method used for the least squares solution. An example of a much larger system of equations would be the modeling of a simple flash vessel calculation that separates a compressed liquid stream comprised of more than 100 components into two lower pressure vapor and liquid streams.

The least squares problem always has a unique solution as long as the columns of A are linearly independent. If the columns are dependent, then there are infinitely many solutions. In the case that the columns of A are close to being linearly dependent, sensor inaccuracies (or the computer's rounding errors) can make it difficult or even impossible to compute an accurate solution. In this case one can turn to alternatives to the normal equations approach which are more robust, but more costly in terms of computer time. The normal equations approach to solving an m by n LS problem requires approximately $mn^2 + n^3/3$ floating point operations (FLOPS). The standard alternative to this approach, the Householder QR factorization, requires about $2mn^2 - 2n^3/3$ FLOPS, but solves a wider class of problems. The Modified Gram-Schmidt QR factorization requires about $2mn^2$ FLOPS and is as robust as the Householder approach. The "Rolls-Royce" of LS methods is based on a singular value decomposition (SVD) of A, which requires about $2mn^2 + 11n^3$ FLOPS. These techniques are standard fair in software packages like Matlab, SAS, Mathematica, Maple, etc, and do not require any special expertise to use. If the problem is quite large, then memory requirements and/or computer time may allow no choice but the normal equations approach, but otherwise the Householder QR is popular as a good balance of speed and robustness.

Every engineer need not be an expert in linear algebra computations but every engineering curriculum should include a fundamental course in linear algebra so that the engineer is aware of its capabilities. This will allow engineers to take advantage of the expertise available when applicable. Again, these calculation techniques are currently in use in software and process simulators readily available for use by the process engineer. However, the engineer needs to have at least a rudimentary knowledge of the principles behind these calculations.

1. CHEG 4332, Lab III Experimentation Manuel, Ralph E. Martin Department of Chemical Engineering, University of Arkansas, Fayetteville, AR 200.1
2. Data, Biswa Nath, *Numerical Linear Algebra and Applications*, Thomson Custom Publishing, 2003.
3. Leon, Steven J, *Linear Algebra with Applications*, Prentice Hall, Upper Saddle River, NJ, 5th Edition, 1998.
4. Moore, Holly, *MATLAB for Engineers*, Prentice Hall, Upper Saddle River, NJ, 2007.

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