W07-04

Slide 01: In this unit, we will discuss how to find a least squares solution to a linear system.

Slide 02: Let us first recall the definition of a least squares solution of a linear system. Suppose $\boldsymbol{Ax} = \boldsymbol{b}$ is a linear system where the coefficient matrix $\boldsymbol{A}$ is a $m \times n$ matrix.

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A vector $\boldsymbol{u}$ in $\mathbb{R}^n$ is called a least squares solution to the system if the length of the vector $\boldsymbol{b} - \boldsymbol{Au}$ is less than or equal to the length of $\boldsymbol{b} - \boldsymbol{Av}$ for any choice of $\boldsymbol{v}$ in $\mathbb{R}^n$.

Slide 03: What does the least squares solution to the system actually mean if $\boldsymbol{Ax} = \boldsymbol{b}$ is a consistent system? Remember that $\boldsymbol{Ax} = \boldsymbol{b}$ is consistent if and only if $\boldsymbol{b}$ belongs to the column space of $\boldsymbol{A}$.

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In the figure, the green vector $\boldsymbol{b}$ belongs to the column space of $\boldsymbol{A}$

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which means that $\boldsymbol{Ax} = \boldsymbol{b}$ is consistent. Thus in this case, the least squares solution is in fact the exact solution that we know exists. Such a solution would be the best possible since it solves the linear system exactly and the sum of the error squares would be zero.

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In this next figure, the green vector $\boldsymbol{b}$ does not belong to the column space of $\boldsymbol{A}$.

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This means that the linear system is inconsistent. What is a least squares solution in this case?

Slide 04: Let us examine the case of an inconsistent linear system a little further.

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Recall that the column space of $\boldsymbol{A}$ contains all the possible linear combinations of the columns of $\boldsymbol{A}$, which is the set of all $\boldsymbol{Av}$ for all vectors $\boldsymbol{v}$ in $\mathbb{R}^n$. So for example, we have $\boldsymbol{Ax_1}$

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$\boldsymbol{Ax_2}$

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$\boldsymbol{Ax_3}$

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and $\boldsymbol{Ax_4}$ as examples of vectors belonging to the column space of $\boldsymbol{A}$.

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Which vector in the column space of $\boldsymbol{A}$ will be closest to $\boldsymbol{b}$? In particular, which $\boldsymbol{u}$ will be such that $\boldsymbol{Au}$ will be closest to $\boldsymbol{b}$ among all the vectors in the column space of $\boldsymbol{A}$?

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This is where the understanding of orthogonal projection comes in. We know that the vector $\boldsymbol{p}$, which is the projection of $\boldsymbol{b}$ onto the column space of $\boldsymbol{A}$ will be the one closest to $\boldsymbol{b}$. So the vector $\boldsymbol{u}$ that we are looking for is the one such that $\boldsymbol{Au}$ is equal to $\boldsymbol{p}$.

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It is now clear that to find a least squares solution $\boldsymbol{u}$ to the linear system, we will solve the alternative system $\boldsymbol{Ax} = \boldsymbol{p}$.

Slide 05: Let us present our discussion as a theorem. Let $\boldsymbol{Ax} = \boldsymbol{b}$ be a linear system where $\boldsymbol{A}$ is a $m \times n$ matrix. Suppose $\boldsymbol{p}$ is the projection of $\boldsymbol{b}$ onto the column space of $\boldsymbol{A}$. Then the length of the vector $\boldsymbol{b} - \boldsymbol{p}$ is less than or equal to the length of $\boldsymbol{b} - \boldsymbol{Av}$ for any choice of vector $\boldsymbol{v}$ in $\mathbb{R}^n$.

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The distance between $\boldsymbol{b}$ and $\boldsymbol{p}$ is shown here. This distance is the length of the vector $\boldsymbol{b} - \boldsymbol{p}$.

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The theorem states that this distance is the smallest among all the vectors $\boldsymbol{Av}$ in the column space of $\boldsymbol{A}$, when measured from $\boldsymbol{b}$.

Slide 06: Consider the following example with the 3×2 matrix $\boldsymbol{A}$ and V is the column space of $\boldsymbol{A}$.

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The column space of $\boldsymbol{A}$ has already been discussed in a previous unit, where we had found an orthogonal basis for V using Gram-Schmidt Process and then subsequently computed the projection of $\boldsymbol{b}$ onto V. The projection $\boldsymbol{p}$ was found to be $(2, 2, 2)$.

Slide 07: What is a least squares solution to $\boldsymbol{Ax} = \boldsymbol{b}$ and how can we use the vector $\boldsymbol{p}$ to find the answer?

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We have already seen that $\begin{pmatrix} x \\ y \end{pmatrix}$ is a least squares solution if and only if

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$\begin{pmatrix} x \\ y \end{pmatrix}$ is a solution to the linear system $\boldsymbol{Ax} = \boldsymbol{p}$. Upon solving, we find that we have a unique least squares solution in the form of $x = 0$, $y = 2$.

Slide 08: The method of finding a least squares solution to $\boldsymbol{Ax} = \boldsymbol{b}$ that we have seen previously requires the computation of the orthogonal projection of $\boldsymbol{b}$ onto the column space of $\boldsymbol{A}$. This may be cumbersome, especially when we do not have an orthogonal basis for the column space of $\boldsymbol{A}$ that we can readily use. The theorem that we are going to see now allows us to find a least squares solution to $\boldsymbol{Ax} = \boldsymbol{b}$ without needing to find the projection of $\boldsymbol{b}$ onto the column space of $\boldsymbol{A}$. The statement of the theorem is that $\boldsymbol{x}$ is a least squares solution to $\boldsymbol{Ax} = \boldsymbol{b}$ if and only if $\boldsymbol{x}$ is a solution to another matrix equation $\boldsymbol{A}^T\boldsymbol{Ax} = \boldsymbol{A}^T\boldsymbol{b}$, called the normal equation, as highlighted in blue.

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We will now prove this theorem. First, let $\boldsymbol{u_1}, \boldsymbol{u_2}$ to $\boldsymbol{u_n}$ be the columns of $\boldsymbol{A}$.

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So the column space of $\boldsymbol{A}$ is the linear span of $\boldsymbol{u_1}$ to $\boldsymbol{u_n}$. Let us call this subspace V.

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Theoretically, without computing the projection $\boldsymbol{p}$ explicitly, we know that $\boldsymbol{x}$ is a least squares solution to the linear system $\boldsymbol{Ax} = \boldsymbol{b}$ if and only if $\boldsymbol{x}$ is a solution to $\boldsymbol{Ax} = \boldsymbol{p}$.

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This means that $\boldsymbol{Ax}$ is the projection of $\boldsymbol{b}$ onto V.

Slide 09: What can we say about the vector $\boldsymbol{Ax}$? We know that it is a vector in the column space of $\boldsymbol{A}$ but more importantly, the difference between $\boldsymbol{b}$

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and $\boldsymbol{Ax}$ will give us a vector that is orthogonal to the space V.

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For $\boldsymbol{b} - \boldsymbol{Ax}$ to be orthogonal to V, this is equivalent to saying that it is orthogonal to the set of vectors that spans V, namely the $\boldsymbol{u_i}$'s. Thus the dot product between $\boldsymbol{u_i}$ and $(\boldsymbol{b} - \boldsymbol{Ax})$ will be zero for all $i = 1$ to n.

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Let us consider the dot product between $\boldsymbol{u_1}$ and $(\boldsymbol{b} - \boldsymbol{Ax})$. This can be written as a matrix product where $\boldsymbol{u_i}$ is a row matrix and $(\boldsymbol{b} - \boldsymbol{Ax})$ is a column matrix. The result of this matrix product is zero, since they dot product is zero.

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Likewise, the dot product between $\boldsymbol{u_2}$ and $(\boldsymbol{b} - \boldsymbol{Ax})$ can be written as a matrix product as shown, which results in zero as well.

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We continue to write the dot product as matrix product, until the last term $\boldsymbol{u_n}$.

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It is now easy to see that the row matrices $\boldsymbol{u_1}$ to $\boldsymbol{u_n}$, collectively is in fact the matrix $\boldsymbol{A}^T$, since they were the columns of $\boldsymbol{A}$. Thus, we now have the matrix equation $\boldsymbol{A}^T$ premultiplied to $(\boldsymbol{b} - \boldsymbol{Ax})$ equals to $\boldsymbol{0}$.

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This can be easily simplified to give the normal equation $\boldsymbol{A}^T\boldsymbol{Ax} = \boldsymbol{A}^T\boldsymbol{b}$ as desired. The proof is thus complete.

Slide 10: Let us return to the example on fitting a set of 6 data points into a non linear equation involving three physical quantities r, s and t. This was discussed in a previous unit and we saw how it can be modeled as an inconsistent linear system where exact solutions for c, d and e do not exist. How can we find a least squares solution using the normal equation? We first identify the coefficient matrix $\boldsymbol{A}$ and constant matrix $\boldsymbol{b}$ as shown.

Slide 11: By the theorem we have just established, $\boldsymbol{x}$ is a least squares solution to $\boldsymbol{Ax} = \boldsymbol{b}$ if and only if it is a solution to the normal equation. Thus we need to compute the matrices $\boldsymbol{A}^T\boldsymbol{A}$ and $\boldsymbol{A}^T\boldsymbol{b}$, which we have shown here.

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We now solve the normal equation $\boldsymbol{A}^T\boldsymbol{Ax} = \boldsymbol{A}^T\boldsymbol{b}$, which can be done via the usual Gaussian elimination method.

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Upon doing so, we obtain $c = 0.9275$, $d = 0.9225$ and $e = 0.315$ as the least squares solution to the linear system $\boldsymbol{Ax} = \boldsymbol{b}$.

Slide 12: Consider the next example where V is the linear span of 3 vectors from $\mathbb{R}^4$. We would like to compute the projection of $(1, 1, 1, 1)$ onto V.

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You should appreciate the fact that if we did not have the normal equation method, we can still proceed to solve this problem by first finding an orthogonal basis for V and then use the orthogonal projection theorem to compute the projection of $(1, 1, 1, 1)$ onto V. However, this would be quite tedious. Now with the normal equation method, we can first construct a matrix $\boldsymbol{A}$ with the 3 vectors forming the colmuns of $\boldsymbol{A}$. In this case, the column space of $\boldsymbol{A}$ will be the space V. We also let $\boldsymbol{b} = (1, 1, 1, 1)$, the vector which we would like to project onto V.

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To use the normal equation method, we first obtain a least squares solution $\boldsymbol{Ax} = \boldsymbol{b}$.

Slide 13: Solving the normal equation $\boldsymbol{A}^T\boldsymbol{Ax} = \boldsymbol{A}^T\boldsymbol{b}$,

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we obtain a general solution as shown here.

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Notice that it is perfectly possible for the normal equation to have infinitely many solutions as the square matrix $\boldsymbol{A}^T\boldsymbol{A}$ may not necessarily be invertible. In this example we see that there are infinitely many least squares solution, as the general solution involves one arbitrary parameter.

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Any one of the inifinitely many solutions can now be chosen, say we choose $(\frac{2}{5}, \frac{4}{5}, 0)$ as our least squares solution

Slide 14: then from our understanding of least squares solutions, we know that they solve the linear system $\boldsymbol{Ax} = \boldsymbol{p}$, where $\boldsymbol{p}$ is the orthogonal projection of $\boldsymbol{b}$ onto the column space of $\boldsymbol{A}$. Thus with our choice of $(\frac{2}{5}, \frac{4}{5}, 0)$, we premultiply $\boldsymbol{A}$ to it in order to obtain $\boldsymbol{p}$, the orthogonal projection of $\boldsymbol{b}$ onto V. We have thus solved this problem in a indirect way by the normal equation method, rather than to compute the projection using the orthogonal projection theorem, which requires an orthogonal basis for V.

Slide 15: To summarise this unit,

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We see that a least squares solution $\boldsymbol{u}$ to the linear system $\boldsymbol{Ax} = \boldsymbol{b}$ is one that solves $\boldsymbol{Ax} = \boldsymbol{p}$ where $\boldsymbol{p}$ is the projection of $\boldsymbol{b}$ onto the column space of $\boldsymbol{A}$.

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We then proved a very useful theorem that allows us to find a least squares solution to $\boldsymbol{Ax} = \boldsymbol{b}$ by solving a normal equation.