Numerics Problem

Mass Spectrometry analysis gives a series of peak height readings for various ion masses. For each peak, the height $h_j$ is contributed to by the various constituents. These make different contributions $c_{i,j}$ per unit concentration $p_i$ so that the relation

$$h_j = \sum_{i=1}^{n} c_{i,j}p_i$$

holds, with $n$ being the number of components present. Carahan (1964) gives the values shown in the following table for $c_{i,j}$:

<table>
<thead>
<tr>
<th>Peak number</th>
<th>Component</th>
<th>CH$_4$</th>
<th>C$_2$H$_4$</th>
<th>C$_2$H$_6$</th>
<th>C$_3$H$_4$</th>
<th>C$_3$H$_8$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td>0.165</td>
<td>0.202</td>
<td>0.317</td>
<td>0.234</td>
<td>0.182</td>
</tr>
<tr>
<td>2</td>
<td></td>
<td>27.7</td>
<td>0.862</td>
<td>0.062</td>
<td>0.073</td>
<td>0.131</td>
</tr>
<tr>
<td>3</td>
<td></td>
<td>0</td>
<td>22.35</td>
<td>13.05</td>
<td>4.420</td>
<td>6.001</td>
</tr>
<tr>
<td>4</td>
<td></td>
<td>0</td>
<td>0</td>
<td>11.28</td>
<td>0</td>
<td>1.110</td>
</tr>
<tr>
<td>5</td>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>9.850</td>
<td>1.684</td>
</tr>
<tr>
<td>6</td>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>15.94</td>
</tr>
</tbody>
</table>

Answer the following questions.

a. How many equations are there? How many unknowns? How is this problem like the matrix problems solved in the statistics portion of the class? There are 6 equations and 5 unknowns. This makes this problem over determined, much like the problems that were solved when considering the least squares problem, such as when fitting curves to data. As such, there (generally) does not exist a solution that satisfies all equations, one just that finds the solution which is best in an average sense.

b. Write a function to solve for the vector $p$, given a vector $h$.

This question is to test your understanding of the method, as well as the syntax of writing an equation.
function [p]=testQ5(h)

\[ c = \begin{bmatrix} 0.165 & 0.202 & 0.317 & 0.234 & 0.182 \\ 27.7 & 0.862 & 0.062 & 0.073 & 0.131 \\ 0 & 22.35 & 13.05 & 4.420 & 6.001 \\ 0 & 0 & 11.28 & 0 & 1.110 \\ 0 & 0 & 0 & 9.850 & 1.684 \\ 0 & 0 & 0 & 0 & 15.94 \end{bmatrix}; \]

% Solve the system of equations
p = c\h;

c  Try your function if a sample had measured peak heights of \(h_1 = 5.20, h_2 = 61.7, h_3 = 149.2, h_4 = 79.4, h_5 = 89.3, h_6 = 69.3\). Report the values of \(p_i\) for each component.

Using your function you should get:

\[ p = \begin{bmatrix} 2.1701 & 0.0021 & 6.6112 & 8.3227 & 4.3476 \end{bmatrix}; \]  \(2\)

d  Give your answer to the previous question if the total of all \(p_i\) values is 21.53.

We can now add a seventh equation to the system:

\[ p_1 + p_2 + p_3 + p_4 + p_5 = 21.53 \]  \(3\)

This information is entered by adding a new row to the matrix, and a 21.53 to the right hand side vector.

Notice that before the additional information, the sum of \(p\) is 21.4537. After adding the additional equation, we get sum of \(p\) equals 21.4546. Still not 21.53. It is a least squares solution, no equation is satisfied. You might weight this equation higher, and I’d be excited to see such a solution.

The vector of \(p\) is \[2.1702 0.0020 6.6114 8.3233 4.3477\]