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CS-575

Homework 5

1) Work is shown below:

1) Let A be a 2×2 Lower triangular matrix and solve $Ax = b$ by forward sub. Show that barring overflow or underflow, the computed solution \hat{x} satisfies $(A+F)\hat{x} = b$ where $f_{ij} \leq 2\epsilon |a_{ij}|$.

$$\Rightarrow Ax = b$$

$$f1(Ax = b) \leftarrow \text{solution is } \hat{x}$$

There exists F matrix such that

$$(A+F)\hat{x} = b$$

$2 \times 1 \rightarrow$

$$\Rightarrow \begin{bmatrix} x \\ \end{bmatrix} f1(a_{11}x = b) + f1(a_{12}x = b) \\ + f1(a_{21}x = b) + f1(a_{22}x = b) \\ \text{where } \hat{x} = \frac{b}{(1+\delta)} \quad a_{ij}$$

$$\Rightarrow \frac{a_{11}\hat{x}}{1+\delta} + \frac{a_{12}\hat{x}}{1+\delta} + \frac{a_{21}\hat{x}}{1+\delta} + \frac{a_{22}\hat{x}}{1+\delta} = b$$

$$\text{Let } \frac{1}{1+\delta} = 1+\hat{\delta}$$

$$\text{where } |\hat{\delta}| \leq \epsilon_m + O(\epsilon_m^2)$$

$$\Rightarrow (a_{11}(1+\hat{\delta}) + a_{12}(1+\hat{\delta}) + a_{21}(1+\hat{\delta}))\hat{x} = b$$

$$\Rightarrow (a_{11} + a_{11}\hat{\delta} + a_{12} + a_{12}\hat{\delta} + a_{21} + a_{21}\hat{\delta} + a_{22} + a_{22}\hat{\delta})\hat{x} = b$$

$$\Rightarrow \underbrace{(a_{11} + a_{12} + a_{21} + a_{22})}_A + \underbrace{(a_{11}\hat{\delta} + a_{12}\hat{\delta} + a_{21}\hat{\delta} + a_{22}\hat{\delta})}_F \hat{x} = b$$

$$\Rightarrow (A+F)\hat{x} = b \quad \checkmark \text{ DONE}$$

therefore Forward substitution
is backward stable.

2) For the next problem we were given a table of molecular weights for six nitric oxides. We were to use these weights and derive various equations and solutions using our equations.

- a) The first part of the question asks us to derive a simple equation for the nitric oxides that we observe. I found the equation $W_{a,b} = W_N * a + W_O * b$ to satisfy as an equation for the observed weights listed in the table. This simple equation is derived from the fact that the weights of both of the elements in the compound are weighted differently based on the molecular weight measurement. The a and b variables are corresponding to the number of atoms that appear in the current nitric oxide state.
- b) For this part of the question, we must now derive the normal equations from the equation we found in the first part of this question. The normal equation formula is $A^T A x = A^T b$ and I found for this equation that it is specifically where:

$$1W_N + 1W_O + c = 30.006$$

$$2W_N + 1W_O + c = 44.013$$

$$1W_N + 2W_O + c = 46.006$$

$$2W_N + 3W_O + c = 76.012$$

$$2W_N + 4W_O + c = 92.011$$

$$2W_N + 5W_O + c = 108.010$$

or in matrix/vector form

$$A = [1 \ 1 \ 1, 2 \ 1 \ 1, 1 \ 2 \ 1, 2 \ 3 \ 1, 2 \ 4 \ 1, 2 \ 5 \ 1]$$

$$b = [30.006, 44.013, 46.006, 76.012, 92.011, 108.010]$$

$$x = [W_N \ W_O \ c]$$

Our goal is to find the values of W_N , W_O , and c that minimize S . We can do this by taking the partial derivatives of S with respect to W_N , W_O , and c and setting them equal to zero. Our function is structured as $ax + by + c$, where our job is to find the values of W_N , W_O , and c that best fit the data

which the normal equations above directly solves for each coefficient. There is an extra column of 1's added in **A** to our system here to accommodate for the **c** coefficient.

- c) Lastly, we were asked to perform the least squares fit to estimate the atomic weights for nitrogen and oxygen. I am going to make a pre-estimate using no calculations that this will return values near or exactly $W_N = 14.007$, $W_O = 15.999$. I plugged in my data into python and used NumPy's least squares solver to approximate the two values of my atomic weight of nitrogen and oxygen. I found that they were very close to my pre-estimations and it is very interesting to note the values down to the 16th digit. On the next page, you can see my code and the output. Below you can see my approximation of the entire equation.

$$f(a,b) = 14.006729729729736*a + 115.9992972972973*b + 0.00032432432427764724$$

Initialization and set up:

```
# W_a,b = W_N*a + W_O*b
# W_a,b = a*(14.007) + b*(15.999)
# W_N = 14.007
# W_O = 15.999
W_N = np.array([1, 2, 1, 2, 2, 2])
W_O = np.array([1, 1, 2, 3, 4, 5])
W_AB_ALL = np.array([30.006, 44.013, 46.006, 76.012, 92.011, 108.010])

# Create coefficient matrix
A = np.vstack([W_N, W_O, np.ones(len(W_N))]).T
print(A)
```

```
[[1.  1.  1.]
 [2.  1.  1.]
 [1.  2.  1.]
 [2.  3.  1.]
 [2.  4.  1.]
 [2.  5.  1.]
```

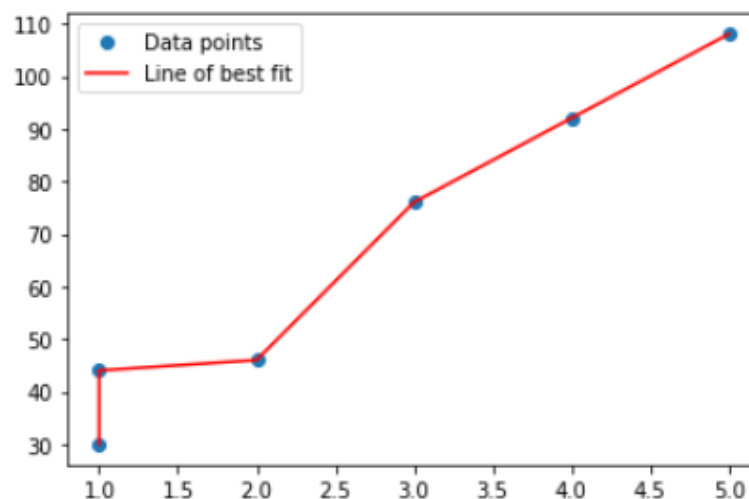
Solving the system and the estimate:

```
# Fit the system using least squares
m1, m2, c = np.linalg.lstsq(A, W_AB_ALL, rcond=None)[0]

print('W_N Estimate:', m1)
print('W_O Estimate:', m2)
print('c Estimate:', c)
```

```
W_N Estimate: 14.006729729729736
W_O Estimate: 15.9992972972973
c Estimate: 0.00032432432427764724
```

Plot of fitted estimation:



3) Work is shown below:

3) If $Ax=b$ has a solution, then the set of solutions must equal to the set of solutions of $A^T Ax = A^T b$

Solution: \hat{x} of $A^T Ax = A^T b$

Solution: \hat{y} of $Ax=b$

$Ax=b$ has a solution \hat{x}
 $A\hat{x}=b$ where \hat{x} is the solution

$A^T Ax = A^T b$ has a solution \hat{y}
 $A^T A\hat{y} = A^T b$

So...

$$A^T A\hat{y} = A^T b$$

$$A^T (A\hat{y}) = A^T b$$

$$A^T (b) = A^T b$$

$$A^T b = A^T b \quad \checkmark \text{ DONE}$$

Therefore $\hat{x} = \hat{y}$ in the sense that they are both a solution to their respective systems. This indicates a solution for both $Ax=b$ with \hat{x} and $A^T Ax = A^T b$ with \hat{y} . We can now say that the solution set are equal for both $A^T Ax = A^T b$ and $Ax=b$.

4) Work is shown below:

4) Given a $m \times m$ matrix A , let $A = QR$ where Q is an $m \times m$ orthogonal matrix and R is an $m \times m$ upper triangular matrix.

a) Show $|\det(Q)| = 1$

$$\Rightarrow |\det(Q)|$$

$$\Rightarrow |\det(Q Q^T)|$$

$$\Rightarrow |\det(I)|$$

$$\Rightarrow |1|$$

$$\Rightarrow 1 \quad \text{therefore } |\det(Q)| = 1$$

✓ DONE

b) Let a_j and r_j refer to the j^{th} cols of A and R respectively.

Show $\|a_j\|_2 = \|r_j\|_2$

$$\Rightarrow \|a_j\|_2$$

$$\Rightarrow \|Q^T r_j\|_2$$

$$\Rightarrow \|Q^T Q r_j\|_2$$

$$\Rightarrow \|I r_j\|_2$$

$$\Rightarrow \|r_j\|_2$$

$$\Rightarrow \|r_j\|_2 \quad \text{therefore } \|a_j\|_2 = \|r_j\|_2$$

✓ DONE

c) Use the last results to prove:

$$|\det(A)| \leq \prod_{j=1}^m \|a_j\|_2$$

$$= |\det(A)|$$

$$= |\det(QR)|$$

$$= |\det(Q) \cdot \det(R)|$$

$$= |1 \cdot \det(R)|$$

$$= |\det(R)|$$

$$\leq \prod_{j=1}^m \|r_j\|$$

$$\leq \prod_{j=1}^m \|a_j\|$$

therefore

$$|\det(A)| \leq \prod_{j=1}^m \|a_j\|_2$$

✓ DONE

5) Work is shown below:

5) Show that if $Q \in \mathbb{R}^{m \times m}$ is orthogonal, then
 $\|AQ\|_2 = \|QA\|_2 = \|A\|_2$
for any $A \in \mathbb{R}^{m \times m}$

Show:

$$\|AQ\|_2 = \|QA\|_2$$

$$\begin{aligned} \text{LHS} \Rightarrow & \|AQ\|_2 = (AQ)^T (AQ) \\ & = Q^T A^T A Q \\ & = Q^T Q^T A^T A Q Q^T \\ & = A^T A Q Q^T \\ & = A^T A I \\ & = A^T A \leftarrow \end{aligned}$$

$$\begin{aligned} \text{RHS} \Rightarrow & \|QA\|_2 \\ & = (QA)^T (QA) \\ & = Q^T A^T Q A \\ & = Q^T Q A^T A \\ & = I A^T A \\ & = A^T A \leftarrow \end{aligned}$$

$A^T A = A^T A$
LHS = RHS
therefore

$$\|AQ\|_2 = \|QA\|_2$$

✓ DONE

Show:

$$\|QA\|_2 = \|A\|_2$$

$$\Rightarrow \|QA\|_2$$

$$= \max_{x \in \mathbb{R}^n} \frac{\|QAx\|_2}{\|x\|_2}$$

$$= \max_{x \in \mathbb{R}^n} \frac{\|Q\|_2 \|Ax\|_2}{\|x\|_2}$$

$$= \max_{x \in \mathbb{R}^n} \frac{\|Ax\|_2}{\|x\|_2}$$

$$= \|A\|_2 \quad \text{therefore} \quad \|QA\|_2 = \|A\|_2 \quad \checkmark \text{ DONE}$$

6) Work is shown below:

6) Find a $u \in \mathbb{R}^2$ with $\|u\|_2 = 1$ such that,

$$Q_u \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

Here Q_u is the Householder reflector associated with u .

$$Q_u = I - 2uu^T \quad x = \begin{bmatrix} 2 \\ 1 \end{bmatrix} \quad y = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$u = \pm \frac{x - y}{\|x - y\|_2}$$

$$= \pm \frac{\begin{bmatrix} 2 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \end{bmatrix}}{\|\begin{bmatrix} 2 \\ 1 \end{bmatrix} - \begin{bmatrix} 1 \\ 2 \end{bmatrix}\|_2}$$

$$= \pm \frac{\begin{bmatrix} 1 \\ -1 \end{bmatrix}}{\|\begin{bmatrix} 1 \\ -1 \end{bmatrix}\|_2}$$

$$= \pm \frac{\begin{bmatrix} 1 \\ -1 \end{bmatrix}}{\sqrt{1^2 + (-1)^2}}$$

$$= \pm \frac{\begin{bmatrix} 1 \\ -1 \end{bmatrix}}{\sqrt{2}}$$

$$= \pm \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix} \quad \checkmark \text{ DONE}$$

$$u = \pm \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}$$