Math 307: Problems for section 2.2

October 16, 2012

Problem: The following formula matrix occurs in a chemical system given by a rock sample [3]. The elements are Si, Al, Fe, Mg, K, H **and** O. **The species are**
qu = quartz (SiO_2)
si = sillimanite (Al_2SiO_5)
Kf = K feldspar ($KAlSi_3O_8$)
st = steam (H_2O)
al = almandine ($Fe_3Al_2Si_3O_{12}$)
py = pyrope ($Mg_3Al_2Si_3O_{12}$)
an = annite ($KFe_3Si_3AlO_{10}(OH)_2$)
ph = phlogopite ($KMg_3Si_3AlO_{10}(OH)_2$)
Fec = Fe-cordierite ($Fe_2Al_4Si_5O_{18}$)
Mgc = Mg-cordierite ($Mg_2Al_4Si_5O_{18}$).
Thus, the formula matrix is

$$A = \begin{array}{c} \\ \mathrm{Si} \\ \mathrm{Al} \\ \mathrm{Fe} \\ \mathrm{Mg} \\ \mathrm{K} \\ \mathrm{H} \\ \mathrm{O} \end{array} \begin{array}{c} \begin{array}{cccccccccc} \mathrm{qu} & \mathrm{si} & \mathrm{Kf} & \mathrm{st} & \mathrm{al} & \mathrm{py} & \mathrm{an} & \mathrm{ph} & \mathrm{Fec} & \mathrm{Mgc} \end{array} \\ \begin{pmatrix} 1 & 1 & 3 & 0 & 3 & 3 & 3 & 3 & 5 & 5 \\ 0 & 2 & 1 & 0 & 2 & 2 & 1 & 1 & 4 & 4 \\ 0 & 0 & 0 & 0 & 3 & 0 & 3 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & 0 & 3 & 0 & 2 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 2 & 2 & 0 & 0 \\ 2 & 5 & 8 & 1 & 12 & 12 & 12 & 12 & 18 & 18 \end{pmatrix} \end{array}$$

(i) Determine possible reactions for this system.
(ii) Is there a fixed ratio of molar amounts of the elements in every possible sample composed of species from this system?

Solution: (i) We must find the null space of A. Using MATLAB/Octave we compute

```
>A=[
1 1 3 0 3 3 3 3 5 5;
0 2 1 0 2 2 1 1 4 4;
0 0 0 0 3 0 3 0 2 0;
0 0 0 0 0 3 0 3 0 2;
0 0 1 0 0 0 1 1 0 0;
0 0 0 2 0 0 2 2 0 0;
2 5 8 1 12 12 12 12 18 18];

>rref(A)
ans =
```

```
  1.00  0.00  0.00  0.00  0.00  0.00  -2.00  -2.00  1.67  1.67
  0.00  1.00  0.00  0.00  0.00  0.00  -1.00  -1.00  1.33  1.33
  0.00  0.00  1.00  0.00  0.00  0.00   1.00   1.00  0.00  0.00
  0.00  0.00  0.00  1.00  0.00  0.00   1.00   1.00  0.00  0.00
  0.00  0.00  0.00  0.00  1.00  0.00   1.00   0.00  0.67  0.00
  0.00  0.00  0.00  0.00  0.00  1.00   0.00   1.00  0.00  0.67
  0.00  0.00  0.00  0.00  0.00  0.00   0.00   0.00  0.00  0.00
```

This shows that the nullspace is 4 dimensionsal and is spanned by

$$
\begin{gathered}
[2,1,-1,-1,-1,0,1,0,0,0]^T \\
[2,1,-1,-1,0,-1,0,1,0,0]^T \\
[-5,-4,0,0,-2,0,0,0,3,0]^T \\
[-5,-4,0,0,0,-2,0,0,0,3]^T
\end{gathered}
$$

Thus the possible reactions are

$$
\begin{aligned}
2\mathrm{qu} + \mathrm{si} + \mathrm{an} &= \mathrm{Kf} + \mathrm{st} + \mathrm{al} \\
2\mathrm{qu} + \mathrm{si} + \mathrm{ph} &= \mathrm{Kf} + \mathrm{st} + \mathrm{py} \\
3\mathrm{Fec} &= 5\mathrm{qu} + 4\mathrm{si} + 2\mathrm{al} \\
3\mathrm{Mgc} &= 5\mathrm{qu} + 4\mathrm{si} + 2\mathrm{py}
\end{aligned}
$$

(ii) We must determine if $N(A^T)$ contains any non-zero vectors. The calculation

```
>rref(A')
ans =

  1.00  0.00  0.00  0.00  0.00  0.00  2.00
  0.00  1.00  0.00  0.00  0.00  0.00  1.50
  0.00  0.00  1.00  0.00  0.00  0.00  1.00
  0.00  0.00  0.00  1.00  0.00  0.00  1.00
  0.00  0.00  0.00  0.00  1.00  0.00  0.50
  0.00  0.00  0.00  0.00  0.00  1.00  0.50
  0.00  0.00  0.00  0.00  0.00  0.00  0.00
  0.00  0.00  0.00  0.00  0.00  0.00  0.00
  0.00  0.00  0.00  0.00  0.00  0.00  0.00
  0.00  0.00  0.00  0.00  0.00  0.00  0.00
```

shows that $N(A^T)$ is one dimensional, spanned by $[-4,-3,-2,-2,-1,-1,2]^T$. Therefore if $\mathbf{b} = [b_1, b_2, b_3, b_4, b_5, b_6, b_7]^T$ are the molar amounts of the species in any sample (listed in the same order as in the formula matrix) then

$$\frac{4b_1 + 3b_2 + 2b_3 + 2b_4 + b_5 + b_6}{2b_7} = 1$$