# Computational Methods in Astrophysics

Linear Algebra — Matrix Inversion

and

**The Rate Equations** 

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# 1. Introduction

The solution of a set of linear algebraic equations

is the subject of this lab. Here there are M equations for the N unknowns  $x_j$ . The coefficients  $a_{ij}$  and the numbers on the right-hand side are assumed to be known. The set of equations can be written in matrix form,

$$\mathbf{A}\mathbf{x} = \mathbf{b}.\tag{2}$$

Note that we can swap rows without affecting the set of equations at all while swapping the columns means that we need to change the ordering of the variables. In addition we can form linear combinations of the equations without changing the information content.

If the number of equations is larger than the number of unknowns (M > N) then the system is overdetermined and can only be solved in the sense of a least squares fit. In the opposite case (M > N) there is no unique solution. We thus restrict ourselves to the case where M = N, the matrix A is square.

Even with M = N a solution is not guaranteed since the matrix might be singular, i.e., its determinant might be zero. This happens when two or more rows are linear combinations of each other (row degeneracy) or the equations define one or more variables only in a linear combination of each other (column degeneracy). For square matrices column degeneracy implies row degeneracy and vice versa. Since our computer arithmetic is only of limited numerical accuracy the equations we wish to solve can be degenerate numerically even if the "true" equations are not.

Formally, as long as A is not singular, the solution may be written

$$\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b},\tag{3}$$

where  $A^{-1}$  is the inverse of A. However, in most cases it is not necessary to obtain  $A^{-1}$  explicitly since we can obtain a solution without it. There are several ways of doing this, the first being Gaussian elimination which we discuss next.

# 2. Gaussian Elimination

The easiest way to learn about Gaussian elimination is to see it in action. We solve the set of equations

$$2x + 3y - 4z = 12x + 5y - z = 123x + 7y - 3z = 20.$$
(4)

First we subtract half of row one from row 2 and obtain

$$2x + 3y - 4z = 120x + (7/2)y + z = 63x + 7y - 3z = 20.$$
 (5)

Note that there is now a zero in the first column. We can do the same with rows 1 and 3, this time with 3/2 as the factor, to find

$$2x + 3y - 4z = 120x + (7/2)y + z = 60x + (5/2)y + 3z = 2.$$
(6)

The important thing here is that x no longer appears in the last two rows which we must now solve for y and z. Subtracting 5/7 of row 2 from row 3 then gives

$$2x + 3y - 4z = 120x + (7/2)y + z = 60x + 0y + (16/7)z = -16/7.$$
(7)

The last equation now only contains z and can be solved trivially to give z = -1. Knowing z in row two allows us to solve for y, (7/2)y = 7, or y = 2, and finally the first row implies that x = 1. Using the matrix form the reductions look like this:

$$\begin{pmatrix} 2 & 3 & -4 & | & 12 \\ 1 & 5 & -1 & | & 12 \\ 3 & 7 & -3 & | & 20 \end{pmatrix} \xrightarrow{\operatorname{row2-\frac{1}{2} \cdot row1, \ row3-\frac{3}{2} \cdot row1}} \begin{pmatrix} 2 & 3 & -4 & | & 12 \\ 0 & 7/2 & 1 & | & 6 \\ 0 & 5/2 & 3 & | & 2 \end{pmatrix}$$

$$\xrightarrow{\operatorname{row3-\frac{5}{7} \cdot row2}} \begin{pmatrix} 2 & 3 & -4 & | & 12 \\ 0 & 7/2 & 1 & | & 6 \\ 0 & 0 & 16/7 & | & -16/7 \end{pmatrix}$$

and we have saved a little space by writing the right hand side (RHS) as a fourth column.

Thus we have

- reduced the initial matrix to *triangular* form.
- solved the system by *back substitution*.

The algorithm in the general case is then:

```
for all row i do
for all row j > i do
for all column k > i do
subtract l_{ji} = a_{ji}/a_{ii} times a_{ik} from a_{jk} and b_j
and store the result in a_{jk}, b_j
end for
end for
end for
```

for the reduction to U (for "upper") form, followed by:

```
for all row i in descending order do
for all column j > i do
subtract a_{ij} times b_j from b_i
and store the result in b_i
end for
b_i = b_i/a_{ii}
end for
```

There are a few points to note:

- the solution is performed in place so no additional storage is needed.
- in consequence both A and b are destroyed, occasionally a copy may be required.
- the necessary computation time is proportional to  $N^3$ .
- since *U* is triangular the determinant is simply the product of the diagonal elements.
- as written, the algorithm is only applied to a single RHS but this is only for didactic purposes. Any number of RHSs may be treated. In particular, setting **b** equal to the unit matrix will give the inverse of **A** since the solution of

$$Ax = I$$

is

$$x=A^{-1}.$$

In fact, elements of A below the diagonal remain unchanged so that all the information needed to reduce any given RHS is available. We can perform the U reduction for A alone and later reduce and solve for b. This scheme is implemented in the pair of routines lured/reslv (to be found in lured.f90 and reslv.f90).

There is one additional very important point about the algorithm as written:

#### It can fail!

To see why, we change our example slightly:

If we try to divide by the diagonal element  $a_{11}$  we have a problem. The same could happen if any of the  $a_{ii}$  are zero or very small compared to the non-diagonal elements. The solution to this problem is *pivoting*.

# 3. Pivoting

Pivoting is the re-ordering of the equations to avoid divisions by small or zero elements during the reduction process. This is done by searching for the largest element in the present column and bringing it onto the diagonal. Rows and columns that have already been treated are not considered. Looking at the example again,

$$\begin{pmatrix} 0 & 3 & -4 & | & 10 \\ 1 & 5 & -1 & | & 12 \\ 3 & 7 & -3 & | & 20 \end{pmatrix}$$
 (8)

we see that the largest element in the first column is 3 and it appears in the third row. So we swap rows 1 and 3 to obtain

$$\begin{pmatrix}
3 & 7 & -3 & | & 20 \\
1 & 5 & -1 & | & 12 \\
0 & 3 & -4 & | & 10
\end{pmatrix}$$
(9)

and then proceed as before.

Here we have only looked for the largest element in the present column, the procedure is called *partial* pivoting. Of course it is possible to look for the largest element in the remaining sub-matrix, *full* pivoting. In this case, the 7 to be found in row 3 and column 2 would be the chosen pivot. The two columns 1 and 2 and rows 1 and 3 would then be swapped. The advantage in doing this, numerical stability in all cases, is far outweighed by the disadvantages that the increase in bookkeeping brings with it. This is particularly so since, in practice, partial pivoting is equally stable (artificial examples can be constructed for which partial pivoting also fails).

It is instructive to look at a very simple example to see just how badly things can go wrong. We imagine that we are computing to three significant figures and want to solve the following system:

$$\begin{pmatrix} 0.1 & 100 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 100 \\ 3 \end{pmatrix}.$$
 (10)

The usual procedure leads to the new system

$$\begin{pmatrix} 0.1 & 100 \\ 0 & -1000 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 100 \\ -1000 \end{pmatrix}$$
(11)

since the computation of 2 - 1000 and 3 - 1000 in three significant figures will yield -1000 in both cases. Solving for  $x_2$  gives  $x_2 = 1$ , which is correct, but for  $x_1$  we have

$$0.1x_1 + 100 = 100\tag{12}$$

or  $x_1 = 0$ , which is incorrect.

Now we use pivoting which in this case simply implies that we swap the two rows:

$$\begin{pmatrix} 1 & 2 \\ 0.1 & 100 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 100 \end{pmatrix}.$$
 (13)

Now the reduction leads to

$$\begin{pmatrix} 1 & 2 \\ 0 & 100 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 100 \end{pmatrix},$$
 (14)

and the solution for  $x_2$  is 1, while  $x_1$  is given by

$$x_1 + 2 = 3 \tag{15}$$

resulting in  $x_1 = 1$ , which is also correct. It is the ratio of  $a_{11}$  to  $a_{12}$  which is important here. The same situation can, in principle, occur in real applications but is somewhat more unlikely since single precision delivers roughly 6.5 significant figures and double precision something like 15. At some point, however, if the matrix is large enough, rounding errors are capable of producing such a situation so partial pivoting at least is a must.

Finally, we note that the numerical value of the pivot depends on the scaling of the equations. We can multiply row 2 in our example (8) throughout by 1000, say, without changing the actual solution vector. But in this case we would choose row 2 as the pivot instead of 3. To deal with this, *implicit* pivoting can used. The pivot candidates are chosen as if they were normalized so that the sum of the absolute values of the row elements is 1. We look at

$$\frac{|a_{ij}|}{\sum_k |a_{ik}|}.$$
(16)

Turning again to our example, the sum of the elements in row 2 is 7 and the first factor is 1/7. For row 3 the sum is 13, the factor is 3/13 so we would once again choose row 3 as our pivot.

The row interchanges may be represented succinctly by the use of a *permutation* matrix P. For N = 2 the matrix

$$\boldsymbol{P} = \left(\begin{array}{cc} 0 & 1\\ 1 & 0 \end{array}\right) \tag{17}$$

swaps two rows as a simple test will show:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} a_{21} & a_{22} \\ a_{11} & a_{12} \end{pmatrix}.$$
 (18)

In the general case we notice that PI = P by definition so that P for any permutation can be found simply by performing the same operations in the same order on the unit

matrix I. For instance, the P corresponding to the exchange of row 1 with row 3 and then row 2 with row 3 is given by

$$\boldsymbol{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \xrightarrow{\text{swap 1 and 3}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \xrightarrow{\text{swap 2 and 3}} \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = \boldsymbol{P}$$
(19)

Thus, having begun with the system

$$A\mathbf{x} = \mathbf{b},\tag{20}$$

the row interchanges correspond to multiplication of both sides by P,

$$PAx = Pb, (21)$$

and it is this system of equations which is solved. As a final comment, it may be noted that swapping two rows multiplies the determinant by -1, so that counting the number of swaps allows the determinant to be determined.

# 4. LU decomposition

The elements below the diagonal are zero by definition after the reduction. By leaving them unchanged we were able to deal with any number of RHSs. There is however another alternative: we can store the multiplicative factors  $l_{ij}$  in the appropriate elements. Our example was

$$\begin{pmatrix}
2 & 3 & -4 \\
1 & 5 & -1 \\
3 & 7 & -3
\end{pmatrix},$$
(22)

and we reduced the first column to 0 by subtracting 1/2 and 3/2 times the first row from the second and third rows, respectively. We store these factors  $l_{21}$  and  $l_{31}$  in place of  $a_{21}$  and  $a_{31}$ :

$$\begin{pmatrix} 2 & 3 & -4 \\ 1/2 & 7/2 & 1 \\ 3/2 & 5/2 & 3 \end{pmatrix}.$$
 (23)

The final step (for this  $3 \times 3$  matrix) was to subtract 5/7 of the second row from the third. Our final matrix is

$$\begin{pmatrix} 2 & 3 & -4 \\ 1/2 & 7/2 & 1 \\ 3/2 & 5/7 & 16/7 \end{pmatrix}.$$
 (24)

But what is the advantage in doing this? We complete the matrix below the diagonal (L) with 1s on the diagonal and calculate LU (hence the name):

$$\begin{pmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/2 & 5/7 & 1 \end{pmatrix} \begin{pmatrix} 2 & 3 & -4 \\ 0 & 7/2 & 1 \\ 0 & 0 & 16/7 \end{pmatrix} = \begin{pmatrix} 2 & 3 & -4 \\ 1 & 5 & -1 \\ 3 & 7 & -3 \end{pmatrix},$$
(25)

i.e., we have A = LU. Now we can solve

$$Ax = LUx = b \tag{26}$$

in two stages: first we find y from Ly = b followed by x from Ux = y.

The second equation is solved by the same algorithm as before:

```
for all row i in descending order do
for all column j > i do
subtract a_{ij} times b_j from b_i
and store the result in b_i
end for
b_i = b_i/a_{ii}
end for
```

Since *L* is also triangular, the algorithm to solve Ly = b is similar:

```
for all row i in ascending order do
for all column j < i do
subtract a_{ij} times b_j from b_i
and store the result in b_i
end for
end for
```

and we have explicitly set the diagonal elements to 1.

In general L has only elements on and below the diagonal, we call them  $l_{ij}$  with the understanding that  $l_{ij} = 0$  for j > i. Similarly the elements of U are  $u_{ij}$  with  $u_{ij} = 0$  for j < i. This gives us  $N^2$  equations for  $N^2 + N$  unknowns. They read

$$i < j: \quad l_{i1}u_{1j} + l_{i2}u_{2j} + \dots + l_{ii}u_{ij} = a_{ij}$$
  

$$i = j: \quad l_{i1}u_{1j} + l_{i2}u_{2j} + \dots + l_{ii}u_{jj} = a_{jj}$$
  

$$i > j: \quad l_{i1}u_{1j} + l_{i2}u_{2j} + \dots + l_{ij}u_{jj} = a_{ij}.$$
(27)

We are free to choose N of these unknowns and we set  $l_{ii} = 1$ . The solution is then found using Crout's algorithm:

for all column j in ascending order do
 for all row i, i < j do
 calculate</pre>

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$
(28)

end for for all row i, i > j do calculate

$$l_{ij} = \frac{1}{u_{jj}} \left( a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj} \right)$$
(29)

#### end for end for

Then  $u_{ij}$  is the reduced upper matrix and the  $l_{ij}$  are the corresponding multiplicative factors as described above. For i = j the two equations are identical apart from the division by the pivot element  $u_{jj}$  so pivoting can be introduced by performing the U reduction completely and then for i = j make the choice for the pivot and continue with the L reduction. Subroutines implementing this scheme with implicit pivoting are to be found in ludcmp.f90 and lubksb.f90 (from *Numerical Recipes*).

### 5. Special cases

If you have information about the structure of the matrix you should use it, as the speed and accuracy can be increased dramatically. In the solution of differential equations using differencing, band matrices occur frequently. These are such that the matrix has non-zero elements only in bands on and close to the diagonal. A diagonal matrix is the simplest, the next simplest being a tridiagonal matrix and we look at this example in more detail. The equations are

$$a_i x_{i-1} + b_i x_i + c_i x_{i+1} = d_i \tag{30}$$

with  $a_1 = c_n = 0$ . In matrix form this reads

$$\begin{pmatrix} b_{1} & c_{1} & & & & 0 \\ a_{2} & b_{2} & c_{2} & & & & \\ & a_{3} & b_{3} & c_{3} & & & & \\ & & & \ddots & & & \\ & & & & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & & & & & a_{n} & b_{n} \end{pmatrix} \begin{pmatrix} x_{1} \\ x_{2} \\ x_{3} \\ \vdots \\ x_{n-1} \\ x_{n} \end{pmatrix} = \begin{pmatrix} d_{1} \\ d_{2} \\ d_{3} \\ \vdots \\ d_{n-1} \\ d_{n} \end{pmatrix}$$
(31)

The solution is a simple application of the Gaussian elimination we saw earlier.

The first equation has solution

$$\boldsymbol{x}_{1} = -\boldsymbol{b}_{1}^{-1}\boldsymbol{c}_{1}\boldsymbol{x}_{2} + \boldsymbol{b}_{1}^{-1}\boldsymbol{d}_{1} \equiv \boldsymbol{e}_{1}\boldsymbol{x}_{2} + \boldsymbol{v}_{1}.$$
(32)

The equation is written in this way because the system could be *block* tridiagonal with  $a_i, b_i, c_i$  matrices and  $x_i, d_i$  vectors. Substituting this result into the second equation we obtain (22)

$$\boldsymbol{x}_2 = \boldsymbol{e}_2 \boldsymbol{x}_3 + \boldsymbol{v}_2 \tag{33}$$

$$\boldsymbol{e}_2 = -(\boldsymbol{b}_2 + \boldsymbol{a}_2 \boldsymbol{e}_1)^{-1} \boldsymbol{c}_2 \tag{34}$$

$$\boldsymbol{v}_2 = (\boldsymbol{b}_2 + \boldsymbol{a}_2 \boldsymbol{e}_1)^{-1} (\boldsymbol{d}_2 - \boldsymbol{a}_2 \boldsymbol{v}_1)$$
(35)

and in the general case

$$\boldsymbol{x}_i = \boldsymbol{e}_i \boldsymbol{x}_{i+1} + \boldsymbol{v}_i \tag{36}$$

$$\boldsymbol{e}_i = -(\boldsymbol{b}_i + \boldsymbol{a}_i \boldsymbol{e}_{i-1})^{-1} \boldsymbol{c}_i \tag{37}$$

$$\boldsymbol{v}_{i} = (\boldsymbol{b}_{i} + \boldsymbol{a}_{i}\boldsymbol{e}_{i-1})^{-1}(\boldsymbol{d}_{i} - \boldsymbol{a}_{i}\boldsymbol{v}_{i-1})$$
(38)

For i = n we have  $c_n = 0$  and thus  $e_n = 0$  and  $x_n = v_n$ . Having found  $v_n$ , the equations (36) can then be used to derive all the  $x_i$ , the back-substitutions. There are several points to note here:

- *a*, *b*, *c* can be stored as vectors.
- The algorithm is now *O*(*n*).
- The algorithm can be extended to more bands in an obvious way.

# 6. Astrophysical application

A star with mass not too different from that of our Sun will, at the end of its life, throw off its outer envelope, leaving the remnant star to contract and heat up, then cool down to ultimately become a white dwarf. The envelope will be illuminated by the hot star and is observed as a planetary nebula. Planetary nebulae come in all shapes and sizes as the pictures below show. They are of considerable interest since the elemental abundances are representative of the outer layers of the star as the nebula was thrown off, giving clues about stellar evolution. Also, since they have large diameters, they are very bright and with their distinctive forbidden-line spectra (see below) they are easy to spot in galaxies even well outside the local group. Their optical properties make them good standard candles with well known physics allowing the Hubble constant to be determined independently of Cepheids.



**Figure 1:** A selection of images of planetary nebulae from the HST. They are: a) Hb 5 "Hubble's Double Bubble"; b) MyCn 18 "Hourglass Nebula"; c) IC 418 "Spirograph Nebula"; d) M 57 "Ring Nebula"; e) NGC 6543 "Cat's Eye Nebula"; f) NGC 2392 "Eskimo Nebula".

The physics of such a nebula is particularly simple. Photoionization by stellar photons is negligible to a first approximation due to geometrical effects (the nebula is large, the star small) and densities are small so that photons escape immediately. Thus radiative transfer need not be considered. Under such circumstances the strengths of wellchosen line pairs can be used to give a direct measure of the temperature and the electron density.

The strength of a spectral emission line is given by the particle number density  $n_i$  of the upper level multiplied by the transition probability  $A_i$ ,

$$j_i = n_i A_i. \tag{39}$$

The latter is an atomic physical quantity and can be taken as given. Normally ratios of two lines belonging to the same ion are used, as in this case abundances and other complicating factors do not play a rôle. Thus we have

$$\frac{j_i}{j_j} = \frac{n_i A_i}{n_j A_j} \tag{40}$$

and since the As are known, the line strength ratio depends on the population ratio  $n_i/n_j$ . In thermodynamic equilibrium this ratio is given by the Boltzmann formula

$$\frac{n_i}{n_j} = \frac{g_i}{g_j} \exp\left(-\frac{E_i - E_j}{kT}\right),\tag{41}$$

 $g_i$  and  $g_j$  being the statistical weights and  $E_i$  and  $E_j$  the excitation energies of levels *i* and *j*, respectively. The Boltzmann constant is *k* and the temperature is *T*. Of course, thermodynamic equilibrium is not possible in a nebula but if the densities are high enough so that collisional processes are more efficient than radiative ones, then *Local Thermodynamic Equilibrium* can apply and the Boltzmann formula can be used with local values of the temperature, the line ratio does not depend on the density.

In the opposite extreme, at very low densities, every excitation of the atom by a collision will lead directly to a line photon. Only collisions involving the ground state (population  $n_1$ ) need be considered since none of the other levels will be significantly populated. Thus we have

$$n_i A_i = n_1 n_e q_{1i}(T)$$
 (42)

$$n_j A_j = n_1 n_e q_{1j}(T)$$
 (43)

and the line ratio is given by

$$\frac{j_i}{j_j} = \frac{q_{1i}(T)}{q_{1j}(T)}.$$
(44)

There is again no dependence on the density  $n_e$ . The collision rates  $q_{1i}(T)$  and  $q_{1j}(T)$  are calculated or measured by atomic physicists and are given. Normally, the downward

rate

$$q_{i1}(T) = \frac{8.629 \times 10^{-6}}{q_i T^{1/2}} \Omega(T)$$
(45)

is to be preferred since  $\Omega(T)$  is a slowly varying function of temperature. The upward rate is then given by detailed balance to be

$$q_{1i}(T) = \frac{g_i}{g_1} \exp\left(-\frac{E_i - E_1}{kT}\right) q_{i1}(T).$$
 (46)

At intermediate densities the picture is more complicated and the populations must be derived from the equations of *statistical equilibrium*. They simply balance the number of transitions into a level and those leaving it. So for a level *i* the equation reads

$$n_i \sum_j P_{ij} = \sum_j n_j P_{ji}.$$
(47)

The sum extends, in principle, over all possible levels *j* but in practice only a few terms are necessary. The transition rate  $P_{ij}$  includes contributions from collisional  $C_{ij} = n_e q_{ij}$  and radiative processes but the latter are only to be included in the downward rates. For three levels the three equations will read ( $n_1$  is the ground level):

$$n_1(C_{12} + C_{13}) = n_2(C_{21} + A_{21}) + n_3(C_{31} + A_{31})$$
(48)

$$n_2(C_{21} + A_{21} + C_{23}) = n_1C_{12} + n_3(C_{32} + A_{32})$$
(49)

$$n_3(C_{31} + A_{31} + C_{32} + A_{32}) = n_1C_{13} + n_2C_{23}.$$
(50)

Note that these are linearly dependent as, for example, the third is equal to the sum of the other two. So we need a further equation to close the system, e.g., for the total number density N,

$$n_1 + n_2 + n_3 = N. (51)$$

If we only deal with line ratios the actual value of N is not important. Having derived T and  $n_e$  from suitable line ratios, the element abundance N is determined separately from the individual line strengths. This is a much more complicated question, however (for instance, several ionization stages will need to be considered), and we shall not investigate it here.

Instead we will look at line ratios in doubly (O II) and singly (O II) ionized oxygen, the line ratios of which are temperature and density sensitive, respectively.

### 6.1. Temperature-dependent O III

Two lines will be sensitive to temperature if the respective upper levels have a large energy difference. In O III the lines at  $\lambda\lambda4959$ , 5007 and  $\lambda4363$  (see Fig. 2) have upper levels <sup>1</sup>D and <sup>1</sup>S that are more than 20000 cm<sup>-1</sup> apart. The ratio of the populations of the two levels is proportional to the Boltzmann factor exp(-20000/kT) which will be sensitive up to temperatures where  $kT \approx 20000$  (with kT in cm<sup>-1</sup>). Since the electron density only appears linearly in the equations, the exponential factor dominates.

The relevant atomic data are shown in Table 1. They have been taken from the book on Gaseous Nebulae by Osterbrock. Of particular interest is the fact that all the levels belong to the  $2p^2$  configuration, the two valence electrons can both be labelled with 2p. Transitions among the 5 levels are *forbidden* since no change in the electron configuration takes place. As a consequence, the radiative transition probabilities are very small, the largest is only  $1.82 \text{ sec}^{-1}$ . For comparison, the transition probabilities allow collisions to produce relatively large populations in the excited states even though the electron densities are low (perhaps  $10^3 \text{ cm}^{-3}$ ). The collisional rates are so small that the atoms are far from thermodynamic equilibrium so forbidden lines in emission are among the strongest to be seen in Planetary nebulae as illustrated in Fig. 4.

```
! Number of levels
5
3P0
                       ! For each level:
     1
             0.0
3P1
     3
           113.178
                          - a label,
                       Į.
3P2
     5
           306.174
                       ļ
                          - the statistical weight,
     5
1D2
        20273.27
                       !
                          - the energy.
150
     1
        43185.74
1
   2
      0.54
            2.6e-5
                       ! For each pair of levels:
1
   3
      0.27
             3.0e-11
                         - two indices,
                       !
1
   4
      0.24
            2.7e-6
                       1
                         - the effective collision strength,
1
   5
      0.03
            0.0
                       ! - the radiative transition probability.
2
   3
      1.29
            9.8e-5
2
   4
      0.72
             6.7e-3
2
   5
      0.09
            0.22
3
   4
      1.21
            2.0e-2
3
   5
      0.16
             7.8e-4
   5
4
      0.62
            1.8
```

 Table 1: Input data for O III.



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**Figure 2:** Energy level (Grotrian) diagram for O III. Solid arrows indicate line transitions in the ultraviolet part of the spectrum, dashed arrows in the visual range, and dotted in the infrared. The separation of the  ${}^{3}P$  levels has been exaggerated for clarity.

#### 6.2. Density-dependent O II

The levels of O II all belong to the  $2p^3$  configuration so that the lines are forbidden, as was the case for the O III. On the other hand, the energy level structure is completely different (see Fig. 3). The energy levels appear in pairs, doublets. The ratio of the strengths of the two lines from the  $^2D$  levels to the ground state is primarily sensitive to the electron density. This is simply because the energy difference is only 20 cm<sup>-1</sup>, as can be seen from Table 2, so that the Boltzmann factor,  $\exp(-20/kT)$ , is approximately 1 even at very low temperatures. Thus there is almost no sensitivity to temperature.

As we shall see later, the ratio of the two lines and their wavelength separation is small so that the observations are difficult, making O  $\pi$  a far from ideal case.

As a final comment, the collision rates are in fact dependent on temperature and for accurate work a table should be read in and interpolated upon. However, the principle is the same, only the numerical values appearing in the rate equations are slightly different, and we omit this detail here.

```
! Number of levels
5
4S3_2
                     ! For each level:
      4
              0.0
         26810.55
2D5_2 6
                     ! - a label.
2D3_2 4
         26830.57
                     ! - the statistical weight,
2P3_2 4
                     ! - the energy.
         40468.01
2P1 2 2
         40470.00
1
  2 0.80
           3.6e-5
                     ! For each pair of levels:
                     ! - two indices,
1
  3
     0.54
           1.8e-4
1
  4
     0.27
           5.8e-2
                     ! - the effective collision strength,
                     ! - the radiative transition probability.
1
  5
     0.13 2.4e-2
2
  3
     1.17
            1.3e-7
2
  4
     0.73
           0.11
2
  5
     0.30
           5.6e-2
3
  4 0.41
           5.8e-2
3
  5
     0.28 9.4e-2
4
  5 0.29 1.4e-10
```

 Table 2: Input data for O II.



**Figure 3:** Energy level (Grotrian) diagram for O II. Only the relevant transitions are shown. Level separations have been exaggerated for clarity.



**Figure 4:** An amateur spectrum of the Saturn nebula. Note the strength of the O III  $(= O^{+2})$  lines. (Credit: Mais Observatory.)

### 7. Exercises

#### **Exercise 1**

Solve the equations

| 2w         | + | 2x | + | 3у         | + | 1z         | = | 0  |      |
|------------|---|----|---|------------|---|------------|---|----|------|
| 3 <i>w</i> | + | 4x | _ | 2y         | + | 5 <i>z</i> | = | 4  | (52) |
| -5w        | + | 5x | _ | 1 <i>y</i> | _ | 2z         | = | 3  | (32) |
| -w         | _ | x  | _ | 3 <i>y</i> | + | 3z         | = | -2 |      |

using Gaussian elimination.

#### **Exercise 2**

Solve the same system of equations as before

| 2w         | + | 2x | + | 3у         | + | 1z         | = | 0  |      |
|------------|---|----|---|------------|---|------------|---|----|------|
| 3 <i>w</i> | + | 4x | _ | 2y         | + | 5z         | = | 4  | (52) |
| -5w        | + | 5x | _ | 1 <i>y</i> | _ | 2z         | = | 3  | (55) |
| -w         | — | x  | _ | 3 <i>y</i> | + | 3 <i>z</i> | = | -2 |      |

this time using LU decomposition.

Download the programs (la\_progs.tar) from the web page. When you have unpacked the archive (tar xvf la\_progs.tar) you will have two directories, TEST and PN, and we will begin with TEST. Enter the following

```
cd TEST
ifort -c precision.f90
ifort -o test *.f90
```

or

```
cd TEST
gfortran -c precision.f90
gfortran -o test *.f90
```

to compile the package. You should inspect the various subroutines to find out what they do and how they do it. With the help of these notes this should be straightforward. Note that ludcmp and lubksb have been taken from *Numerical Recipes*. You can change from single to double precision by changing the value of the variable 1.e0 to 1.d0 in precision.f90. Read the comments carefully for more information. Pay particular attention to the warning about compiling the module first before the rest of the routines.

You can start the program with

./test

and you will be offered 4 options:

- 1) fill the matrix with random values (default)
- 2) the hilbert matrix
- 3) a user-defined matrix: edit user.f90 first
- 4) read a matrix and a RHS from mat.dat

for each of the first 3 you will then need to give the size of the required matrix and which pair ludcmp/lubksb or lured/reslv you wish to use.

#### An intermezzo: the Hilbert matrix

The Hilbert matrix is a very strange beast. Its elements are easy to define,

$$H_{ij} = 1/(i+j-1), (54)$$

and its inverse has elements

$$(H^{-1})_{ij} = (-1)^{i+j}(i+j+1)\binom{n+i-1}{n-j}\binom{n+j-1}{n-i}\binom{n-i}{i-1}^2,$$
(55)

where the notation  $\binom{n}{j}$  is the binomial coefficient defined by

$$\binom{n}{j} = \frac{n!}{j!(n-j)!}.$$
(56)

The interesting property of the matrix is that its determinant is one divided by 1, 12, 2160, 6048000, 266716800000, and so on, making it an extremely stringent test for any numerical linear algebra solution routine.

Table 3: Determinant of the first few Hilbert matrices.

n det(H)  
1 1  
2 
$$8.33333 \times 10^{-2}$$
  
3  $4.62963 \times 10^{-4}$   
4  $1.65344 \times 10^{-7}$   
5  $3.74930 \times 10^{-12}$   
6  $5.36730 \times 10^{-18}$ 

#### **Exercise 3**

Perform the following in single precision:

- a. Choose option 1 and compare the error for a number of matrix sizes (100s to 1000s) and for both algorithm pairs. How fast does it grow? Does the algorithm become unusable? For these runs start the program with time ./test, take the user entry as an indication of the computer time used. Plot this logarithmically and compare the slope with the predicted value of 3. (Note that large matrices may not fit into the available memory in which case the system will write data to disk as needed, making the execution times much longer. This is called *paging*. You can use the top command in another window to see if this is happening. CPU usage below 90% for any period is a good sign that this is the case.)
- **b.** Choose option 2 and compare the error for a number of matrix sizes and for both algorithm pairs. Here the matrix size should be small (< 20).
- **c.** Choose option 3 and for 3 different choices of matrix perform similar tests. You will need to edit and change user. f90 appropriately and then recompile the program (see above).
- **d.** Option 4 is included chiefly for pedagogical purposes but with an appropriate input data set you can check your answers from Exercises 1 and 2 (see mat1.dat).

#### **Exercise 4**

Perform the same tests as in Exercise 3 but in double precision and compare your results. You will need to edit precision.f90 and recompile the program.

#### **Exercise 5**

Solve the following tridiagonal matrix.

$$\begin{pmatrix} 2 & 1 & 0 & 0 & 0 \\ 1 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 1 & 2 & 1 \\ 0 & 0 & 0 & 1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{pmatrix}$$
(57)

#### **Exercise 6**

Write a subroutine to solve a tridiagonal matrix. Use this routine to check your solution to Exercise 5.

#### **Exercise 7**

For this exercise

```
cd ../PN
ifort -c precision.f90
ifort -o line *.f90
./line | tee output
```

The input is simple. You will be asked to calculate data for oii or oiii. Then for oiii, which is temperature dependent, you should enter a density, while a temperature is needed for oii. For each ion you should perform 2 or 3 runs with a different output file for each run. Then plot your results for each ion, line intensity ratio versus temperature for oiii and versus density for oii. Comment on your results.

#### Advanced task 1

The subject of this lab has been to solve the set of linear equations

$$Ax = b. (58)$$

In fact, we have only found an approximate solution that satisfies the perturbed equation

$$A(\mathbf{x} + \delta \mathbf{x}) = \mathbf{b} + \delta \mathbf{b}.$$
 (59)

The difference between the two gives an equation for  $\delta x$  in terms of  $\delta b$ ,

$$A\delta \boldsymbol{x} = \delta \boldsymbol{b},\tag{60}$$

while  $\delta \boldsymbol{b}$  is known from Eqn. 59,

$$A\delta \boldsymbol{x} = \boldsymbol{A}(\boldsymbol{x} + \delta \boldsymbol{x}) - \boldsymbol{b}. \tag{61}$$

This last equation can be used to improve the current solution and may be applied iteratively. The A and b on the RHS are the original matrix and vector, so a copy is needed. Since the RHS is the current error vector it must be calculated as accurately as possible, double precision should be used.

Your mission, should you choose to accept it, is to write a subroutine to implement this algorithm (no peeking in *Numerical Recipes*). You should use ludcmp/lubksb and write a test program.

#### Advanced task 2

S II and S III are very similar to O II and O III in their atomic physical properties and so can be used in a similar way to derive temperatures and densities. Construct input data sets suitable for use with line. The necessary data are to be found in the appendix.

#### Advanced task 3

**lured/reslv** as written do not use pivoting. Modify them to use partial or implicit pivoting. You may use **ludcmp/lubksb** as an example. Once more you should test your routines to ensure that they are correct.

# 8. Appendix

The energy level notation is  ${}^{2S+1}L_J$ , *S* being the total spin and *L* the total orbital angular momentum (this is expressed as a letter whereby "*S*" means L = 0, "*P*" means L = 1, and "*D*" means L = 2). The total angular momentum is J = L+S. The statistical weight of any level is simply 2J + 1 while the statistical weight of a term is (2S + 1)(2L + 1). These weights are such that  $\sum (2J + 1) = (2S + 1)(2L + 1)$ . The electron configurations (of O II and S II) are denoted by  $2s^22p^3$  and  $3s^23p^3$ . They are not important here but the fact that they are very similar means that the energy level structure is very similar and that the two elements are chemically related.

Osterbrock has saved space in his tabulations by making use of some elementary properties of the collision strengths. For instance the  ${}^{3}P \leftrightarrow {}^{1}D$  collision strength between the two terms  ${}^{3}P$  and  ${}^{1}D$  in O III and S III splits into three collision strengths between the levels  ${}^{3}P_{0,1,2} \leftrightarrow {}^{1}D_{2}$  according to the statistical weights:

$$\Omega({}^{3}P_{0} \leftrightarrow {}^{1}D_{2}) = \frac{(2J+1)}{(2S+1)(2L+1)} \Omega\left({}^{2S+1}L \leftrightarrow {}^{2S'+1}L'\right)$$
(62)

$$=\frac{(2\cdot 0+1)}{3\cdot (2\cdot 1+1)}\Omega({}^{3}P\leftrightarrow {}^{1}D)$$
(63)

$$=\frac{1}{9}\Omega({}^{3}P\leftrightarrow{}^{1}D) \tag{64}$$

and so on. We have used this to write out the tables in full. You can check your values by comparing with the O  $\pi$  and O  $\pi$  numbers given in the text and the input data files.

### 8.1. Atomic data for O II and S II

|               | Оп              |          | Sп            |                 |          |  |  |
|---------------|-----------------|----------|---------------|-----------------|----------|--|--|
| Configuration | Level           | Energy   | Configuration | Level           | Energy   |  |  |
| $2s^22p^3$    | ${}^{4}S_{3/2}$ | 0.0      | $3s^23p^3$    | ${}^{4}S_{3/2}$ | 0.0      |  |  |
| $2s^2 2p^3$   | $^{2}D_{5/2}$   | 26810.55 | $3s^23p^3$    | $^{2}D_{3/2}$   | 14852.94 |  |  |
| $2s^22p^3$    | $^{2}D_{3/2}$   | 26830.57 | $3s^23p^3$    | $^{2}D_{5/2}$   | 14884.73 |  |  |
| $2s^2 2p^3$   | ${}^{2}P_{3/2}$ | 40468.01 | $3s^23p^3$    | ${}^{2}P_{1/2}$ | 24524.83 |  |  |
| $2s^22p^3$    | ${}^{2}P_{1/2}$ | 40470.00 | $3s^23p^3$    | ${}^{2}P_{3/2}$ | 24571.54 |  |  |

**Table 4:** O II and S II energy levels in  $cm^{-1}$  from the NIST website. Note the ordering.

**Table 5:** O II and S II radiative data (Einstein A coefficients in units of  $\sec^{-1}$ ) from the book *Astrophysics of Gaseous Nebulae* by Osterbrock.

| Transition                                    | Оп                    | S II                 |  |  |
|---|-----------------------|----------------------|--|--|
| ${}^{4}S_{3/2} \leftrightarrow {}^{2}D_{5/2}$ | $3.6 \times 10^{-5}$  | $2.6 \times 10^{-4}$ |  |  |
| ${}^{4}S_{3/2} \leftrightarrow {}^{2}D_{3/2}$ | $1.8 \times 10^{-4}$  | $8.8 	imes 10^{-4}$  |  |  |
| ${}^{4}S_{3/2} \leftrightarrow {}^{2}P_{3/2}$ | $5.8 \times 10^{-2}$  | $2.2 \times 10^{-1}$ |  |  |
| ${}^{4}S_{3/2} \leftrightarrow {}^{2}P_{1/2}$ | $2.4 \times 10^{-2}$  | $9.1 \times 10^{-2}$ |  |  |
| ${}^{2}D_{5/2} \leftrightarrow {}^{2}D_{3/2}$ | $1.3 \times 10^{-7}$  | $3.3 \times 10^{-7}$ |  |  |
| $^{2}D_{5/2} \leftrightarrow ^{2}P_{3/2}$     | $1.1 \times 10^{-1}$  | $1.8 \times 10^{-1}$ |  |  |
| ${}^{2}D_{5/2} \leftrightarrow {}^{2}P_{1/2}$ | $5.6 \times 10^{-2}$  | $7.8 \times 10^{-2}$ |  |  |
| $^{2}D_{3/2} \leftrightarrow ^{2}P_{3/2}$     | $5.8 \times 10^{-2}$  | $1.3 \times 10^{-1}$ |  |  |
| ${}^{2}D_{3/2} \leftrightarrow {}^{2}P_{1/2}$ | $9.4 \times 10^{-2}$  | $1.6 \times 10^{-1}$ |  |  |
| ${}^{2}P_{3/2} \leftrightarrow {}^{2}P_{1/2}$ | $1.4 \times 10^{-10}$ | $1.0 \times 10^{-6}$ |  |  |

**Table 6:** O II and S II collision strengths ( $\Omega$ ) from the book *Astrophysics of Gaseous Nebulae* by Osterbrock. The collision strength is dimensionless.

| Transition                                    | Оп   | Ѕп   | Transition                                    | Оп   | Ѕп   |
|---|------|------|---|------|------|
| ${}^{4}S_{3/2} \leftrightarrow {}^{2}D_{5/2}$ | 0.80 | 4.19 | ${}^{2}D_{5/2} \leftrightarrow {}^{2}P_{3/2}$ | 0.73 | 4.79 |
| ${}^{4}S_{3/2} \leftrightarrow {}^{2}D_{3/2}$ | 0.54 | 2.79 | ${}^{2}D_{5/2} \leftrightarrow {}^{2}P_{1/2}$ | 0.30 | 2.56 |
| ${}^{4}S_{3/2} \leftrightarrow {}^{2}P_{3/2}$ | 0.27 | 1.52 | ${}^{2}D_{3/2} \leftrightarrow {}^{2}P_{3/2}$ | 0.41 | 3.38 |
| ${}^{4}S_{3/2} \leftrightarrow {}^{2}P_{1/2}$ | 0.13 | 0.76 | ${}^{2}D_{3/2} \leftrightarrow {}^{2}P_{1/2}$ | 0.28 | 1.52 |
| ${}^{2}D_{5/2} \leftrightarrow {}^{2}D_{3/2}$ | 1.17 | 7.59 | ${}^{2}P_{3/2} \leftrightarrow {}^{2}P_{1/2}$ | 0.29 | 2.38 |

### 8.2. Atomic data for O m and S m

**Table 7:** O III and S III energy levels in  $cm^{-1}$  from the NIST website. Here the ordering is the same.

|               | Ош            |          | S III         |               |         |  |  |
|---------------|---------------|----------|---------------|---------------|---------|--|--|
| Configuration | Level         | Energy   | Configuration | Level         | Energy  |  |  |
| $2s^22p^2$    | ${}^{3}P_{0}$ | 0.0      | $3s^23p^2$    | ${}^{3}P_{0}$ | 0.0     |  |  |
| $2s^2 2p^2$   | ${}^{3}P_{1}$ | 113.178  | $3s^23p^2$    | ${}^{3}P_{1}$ | 298.69  |  |  |
| $2s^2 2p^2$   | ${}^{3}P_{2}$ | 306.174  | $3s^23p^2$    | ${}^{3}P_{2}$ | 833.08  |  |  |
| $2s^2 2p^2$   | ${}^{1}D_{2}$ | 20273.27 | $3s^23p^2$    | ${}^{1}D_{2}$ | 11322.7 |  |  |
| $2s^22p^2$    | ${}^{1}S_{0}$ | 43185.74 | $3s^23p^2$    | ${}^{1}S_{0}$ | 27161.0 |  |  |

**Table 8:** O III and S III radiative data (Einstein A coefficients in units of  $\sec^{-1}$ ) from the book *Astrophysics of Gaseous Nebulae* by Osterbrock.

| Transition                                | Ош                    | Sш                   |
|---|-----------------------|----------------------|
| ${}^{3}P_{0} \leftrightarrow {}^{3}P_{1}$ | $2.6 \times 10^{-5}$  | $4.7 \times 10^{-4}$ |
| ${}^{3}P_{0} \leftrightarrow {}^{3}P_{2}$ | $3.0 \times 10^{-11}$ | $4.6 \times 10^{-8}$ |
| ${}^{3}P_{0} \leftrightarrow {}^{1}D_{2}$ | $2.7 \times 10^{-6}$  | $5.8 \times 10^{-6}$ |
| ${}^{3}P_{1} \leftrightarrow {}^{3}P_{2}$ | $9.8 \times 10^{-5}$  | $2.1 \times 10^{-3}$ |
| ${}^{3}P_{1} \leftrightarrow {}^{1}D_{2}$ | $6.7 \times 10^{-3}$  | $2.2 \times 10^{-2}$ |
| ${}^{3}P_{1} \leftrightarrow {}^{1}S_{0}$ | $2.2 \times 10^{-1}$  | $8.0 	imes 10^{-1}$  |
| ${}^{3}P_{2} \leftrightarrow {}^{1}D_{2}$ | $2.0 \times 10^{-2}$  | $5.8 \times 10^{-2}$ |
| ${}^{3}P_{2} \leftrightarrow {}^{1}S_{0}$ | $7.8 \times 10^{-4}$  | $1.0 \times 10^{-2}$ |
| ${}^{1}D_{2} \leftrightarrow {}^{1}S_{0}$ | $1.8 \times 10^0$     | $2.2 \times 10^{0}$  |

**Table 9:** O III and S III collision strengths ( $\Omega$ ) from the book *Astrophysics of Gaseous Nebulae* by Osterbrock. The collision strength is dimensionless.

| Transition                                | Ош   | Sш   | Transition                                | Ош   | Sш   |
|---|------|------|---|------|------|
| ${}^{3}P_{0} \leftrightarrow {}^{3}P_{1}$ | 0.54 | 2.64 | ${}^{3}P_{1} \leftrightarrow {}^{1}D_{2}$ | 0.72 | 2.80 |
| ${}^{3}P_{0} \leftrightarrow {}^{3}P_{2}$ | 0.27 | 1.11 | ${}^{3}P_{1} \leftrightarrow {}^{1}S_{0}$ | 0.09 | 0.40 |
| ${}^{3}P_{0} \leftrightarrow {}^{1}D_{2}$ | 0.24 | 0.93 | ${}^{3}P_{2} \leftrightarrow {}^{1}D_{2}$ | 1.21 | 4.66 |
| ${}^{3}P_{0} \leftrightarrow {}^{1}S_{0}$ | 0.03 | 0.13 | ${}^{3}P_{2} \leftrightarrow {}^{1}S_{0}$ | 0.16 | 0.66 |
| ${}^{3}P_{1} \leftrightarrow {}^{3}P_{2}$ | 1.29 | 5.79 | ${}^{1}D_{2} \leftrightarrow {}^{1}S_{0}$ | 0.62 | 1.88 |