CHAPTER II

SUBSPACES, BASES AND DIMENSION

II.1. Subspaces, basis and dimension

Prerequisites and Learning Goals

From your work in previous courses, you should be able to

- Write down a vector as a linear combination of a set of vectors, and express the linear combination in matrix form.
- Define linear independence for a collection of vectors.
- Define a basis for a vector subspace.

After completing this section, you should be able to

- Explain what a vector space is, give examples of vector spaces.
- Define vector addition and scalar multiplication for vector spaces of functions.
- Give a definition of subspace and decide whether a given collection of vectors forms a subspace.
- Recast the dependence or independence of a collection of vectors in \mathbb{R}^n or \mathbb{C}^n as a statement about existence of solutions to a system of linear equations, and use it to decide if a collection of vectors are dependent or independent.
- Define the span of a collection of vectors; show that given a set of vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ the span $\mathrm{span}(\mathbf{v}_1, \dots, \mathbf{v}_k)$ is a subspace; determine when a given vector is in the span.
- Describe the significance of the two parts (independence and span) of the definition of a basis.
- Check if a collection of vectors is a basis.
- Show that any basis for a subspace has the same number of elements.
- Show that any set of k linearly independent vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ in a k dimensional subspace S is a basis of S.
- Define the dimension of a subspace.
- Determine possible reactions from the formula matrix for a chemical system.
- Given the formula matrix for a chemical system, determine if there is a fixed ratio of molar amounts of the elements in every possible sample composed of species in the system.

II.1.1. Vector spaces and subspaces

In your previous linear algebra course, and for most of this course, vectors are *n*-tuples $\begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$ of

numbers, either real or complex. The sets of all *n*-tuples, denoted \mathbb{R}^n or \mathbb{C}^n , are examples of vector spaces.

In more advanced applications vector spaces of functions often occur. For example, an electrical signal can be thought of as a real valued function x(t) of time t. If two signals x(t) and y(t) are superimposed, the resulting signal is the sum that has the value x(t)+y(t) at time t. This motivates the definition of vector addition for functions: the vector sum of the functions x and y is the new function x + y defined by (x + y)(t) = x(t) + y(t). Similarly, if s is a scalar, the scalar multiple sx is defined by (sx)(t) = sx(t). If you think of t as being a continuous index, these definitions mirror the componentwise definitions of vector addition and scalar multiplication for vectors in \mathbb{R}^n or \mathbb{C}^n .

It is possible to give an abstract definition of a vector space as any collection of objects (the vectors) that can be added and multiplied by scalars, provided the addition and scalar multiplication rules obey a set of rules. We won't follow this abstract approach in this course.

A collection of vectors V contained in a given vector space is called a *subspace* if vector addition and scalar multiplication of vectors in V stay in V. In other words, for any vectors $\mathbf{v}_1, \mathbf{v}_2 \in V$ and any scalars c_1 and c_2 , the vector $c_1\mathbf{v}_1 + c_2\mathbf{v}_2$ lies in V too.

In three dimensional space \mathbb{R}^3 , examples of subspaces are lines and planes through the origin. If we add or scalar multiply two vectors lying on the same line (or plane) the resulting vector remains on the same line (or plane). Additional examples of subspaces are the trivial subspace, containing the single vector $\mathbf{0}$, as well as the whole space itself.

Here is another example of a subspace. The set of $n \times n$ matrices can be thought of as an n^2 dimensional vector space. Within this vector space, the set of symmetric matrices (satisfying $A^T = A$) is a subspace. To see this, suppose A_1 and A_2 are symmetric. Then, using the linearity property of the transpose, we see that

$$(c_1 A_1 + c_2 A_2)^T = c_1 A_1^T + c_2 A_2^T = c_1 A_1 + c_2 A_2$$

which shows that $c_1A_1 + c_2A_2$ is symmetric too.

We have encountered subspaces of functions in the section on interpolation. In Lagrange interpolation we considered the set of all polynomials of degree at most m. This is a subspace of the space of functions, since adding two polynomials of degree at most m results in another polynomial, again of degree at most m, and scalar multiplication of a polynomial of degree at most m yields another polynomial of degree at most m.

Another example of a subspace of functions is the set of all functions y(t) that satisfy the differential equation y''(t) + y(t) = 0. To check that this is a subspace, we must verify that if $y_1(t)$ and $y_2(t)$ both solve the differential equation, then so does $c_1y_1(t) + c_2y_2(t)$ for any choice of scalars c_1 and c_2 .

II.1.2. Linear dependence and independence

To begin we review the definition of linear dependence and independence. A linear combination of vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ is a vector of the form

$$\sum_{i=1}^{k} c_i \mathbf{v}_i = c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2 + \dots + c_k \mathbf{v}_k$$

for some choice of numbers c_1, c_2, \ldots, c_k .

The vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ are called *linearly dependent* if there exist numbers c_1, c_2, \dots, c_k that are not all zero, such that the linear combination $\sum_{i=1}^k c_i \mathbf{v}_i = \mathbf{0}$

On the other hand, the vectors are called *linearly independent* if the only linear combination of the vectors equaling zero has every $c_i = 0$. In other words

$$\sum_{i=1}^{k} c_i \mathbf{v}_i = \mathbf{0} \quad \text{implies} \quad c_1 = c_2 = \dots = c_k = 0$$

For example, the vectors $\begin{bmatrix} 1\\1\\1 \end{bmatrix}$, $\begin{bmatrix} 1\\0\\1 \end{bmatrix}$ and $\begin{bmatrix} 7\\1\\7 \end{bmatrix}$ are linearly dependent because

$$1 \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + 6 \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} - 1 \begin{bmatrix} 7 \\ 1 \\ 7 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

If $\mathbf{v}_1, \dots, \mathbf{v}_k$ are linearly dependent, then at least one of the \mathbf{v}_i 's can be written as a linear combination of the others. To see this suppose that

$$c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \dots + c_k\mathbf{v}_k = \mathbf{0}$$

with not all of the c_i 's zero. Then we can solve for any of the \mathbf{v}_i 's whose coefficient c_i is not zero. For instance, if c_1 is not zero we can write

$$\mathbf{v}_1 = -(c_2/c_1)\mathbf{v}_2 - (c_3/c_1)\mathbf{v}_3 - \dots - (c_k/c_1)\mathbf{v}_k$$

This means any linear combination we can make with the vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ can be achieved without using \mathbf{v}_1 , since we can simply replace the occurrence of \mathbf{v}_1 with the expression on the right.

Sometimes it helps to have a geometrical picture. In three dimensional space \mathbb{R}^3 , three vectors are linearly dependent if they lie in the same plane.

The columns of a matrix in echelon form are linearly independent if and only if every column is a pivot column. We illustrate this with two examples.

The matrix $\begin{bmatrix} 1 & * & * \\ 0 & 2 & * \\ 0 & 0 & 3 \end{bmatrix}$ is an example of a matrix in echelon form where each column is a pivot column. Here * denotes an arbitrary entry.

To see that the columns are linearly independent suppose that

$$c_1 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} * \\ 2 \\ 0 \end{bmatrix} + c_3 \begin{bmatrix} * \\ * \\ 3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Then, equating the bottom entries we find $3c_3 = 0$ so $c_3 = 0$. But once we know $c_3 = 0$ then the equation reads

$$c_1 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} * \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

which implies that $c_2 = 0$ too, and similarly $c_1 = 0$

Similarly, for a matrix in echelon form (even if, as in the example below, it is not completely reduced), the pivot columns are linearly independent. For example the first, second and fifth columns in the matrix

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 5 & 5 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

are independent. However, the non-pivot columns can be written as linear combination of the pivot columns. For example

$$\begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix} = - \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

so if there are non-pivot columns, then the set of all columns is linearly dependent. This is particularly easy to see for a matrix in reduced row echelon form, like

$$\begin{bmatrix} 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 2 & 5 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

In this case the pivot columns are standard basis vectors (see below), which are obviously independent. It is easy to express the other columns as linear combinations of these.

Recall that for a matrix U in echelon form, the presence or absence of non-pivot columns determines whether the homogeneous equation $U\mathbf{x} = \mathbf{0}$ has any non-zero solutions. By the discussion above, we can say that the columns of a matrix U in echelon form are linearly dependent exactly when the homogeneous equation $U\mathbf{x} = \mathbf{0}$ has a non-zero solution.

In fact, this is true for any matrix. Suppose that the vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ are the columns of a matrix A so that

$$A = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_k \end{bmatrix}.$$

If we put the coefficients c_1, c_2, \ldots, c_k into a vector

$$\mathbf{c} = \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_k \end{bmatrix}$$

then

$$A\mathbf{c} = c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \dots + c_k\mathbf{v}_k$$

is the linear combination of the columns $\mathbf{v}_1, \dots, \mathbf{v}_k$ with coefficients c_i .

Now it follows directly from the definition of linear dependence that the columns of A are linearly dependent if there is a non-zero solution \mathbf{c} to the homogeneous equation

$$A\mathbf{c} = \mathbf{0}$$

On the other hand, if the only solution to the homogeneous equation is $\mathbf{c} = \mathbf{0}$ then the columns $\mathbf{v}_1, \dots, \mathbf{v}_k$ are linearly independent.

To compute whether a given collection of vectors is dependent or independent we can place them in the columns of a matrix A and reduce to echelon form. If the echelon form has only pivot columns, then the vectors are independent. On the other hand, if the echelon form has some non-pivot columns, then the equation $A\mathbf{c} = \mathbf{0}$ has some non-zero solutions and so the vectors are dependent.

Let's try this with the vectors in the example above in MATLAB/Octave.

```
>V2=[1 0 1]';
>V3=[7 1 7]';
>A=[V1 V2 V3]
A =
1 1 7
1 0 1
```

>V1=[1 1 1]';

>rref(A)

ans =

1 0 1 0 1 6 0 0 0

Since the third column is a non-pivot column, the vectors are linearly dependent.

II.1.3. Span

Given a collection of vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ we may form a subspace of all possible linear combinations. This subspace is called $\operatorname{span}(\mathbf{v}_1, \dots, \mathbf{v}_k)$ or the space spanned by the \mathbf{v}_i 's. It is a subspace because if we start with any two elements of $\operatorname{span}(\mathbf{v}_1, \dots, \mathbf{v}_k)$, $\operatorname{say} c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \dots + c_k\mathbf{v}_k$ and $d_1\mathbf{v}_1 + d_2\mathbf{v}_2 + \dots + d_k\mathbf{v}_k$ then a linear combination of these linear combinations is again a linear combination since

$$s_1(c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \dots + c_k\mathbf{v}_k) + s_2(d_1\mathbf{v}_1 + d_2\mathbf{v}_2 + \dots + d_k\mathbf{v}_k) = (s_1c_1 + s_2d_1)\mathbf{v}_1 + (s_1c_2 + s_2d_2)\mathbf{v}_2 + \dots + (s_1c_k + s_2d_k)\mathbf{v}_k$$

For example the span of the three vectors $\begin{bmatrix} 1\\0\\0 \end{bmatrix}$, $\begin{bmatrix} 0\\1\\0 \end{bmatrix}$ and $\begin{bmatrix} 0\\0\\1 \end{bmatrix}$ is the whole three dimensional

space, because every vector is a linear combination of these. The span of the four vectors $\begin{bmatrix} 1\\0\\0 \end{bmatrix}$,

$$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \text{ and } \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \text{ is the same.}$$

II.1.4. Basis

A collection of vectors $\mathbf{v}_1, \dots, \mathbf{v}_k$ contained in a subspace V is called a basis for that subspace if

- 1. $\operatorname{span}(\mathbf{v}_1,\ldots,\mathbf{v}_k)=V$, and
- 2. $\mathbf{v}_1, \dots, \mathbf{v}_k$ are linearly independent.

Condition (1) says that any vector in V can be written as a linear combination of $\mathbf{v}_1, \dots, \mathbf{v}_k$. Condition (2) says that there is exactly one way of doing this. Here is the argument. Suppose there are two ways of writing the same vector $\mathbf{v} \in V$ as a linear combination:

$$\mathbf{v} = c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2 + \dots + c_k \mathbf{v}_k$$
$$\mathbf{v} = d_1 \mathbf{v}_1 + d_2 \mathbf{v}_2 + \dots + d_k \mathbf{v}_k$$

Then by subtracting these equations, we obtain

$$\mathbf{0} = (c_1 - d_1)\mathbf{v}_1 + (c_2 - d_2)\mathbf{v}_2 + \dots + (c_k - d_k)\mathbf{v}_k$$

Linear independence now says that every coefficient in this sum must be zero. This implies $c_1 = d_1$, $c_2 = d_2 \dots c_k = d_k$.

Example: \mathbb{R}^n has the standard basis $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n$ where

$$\mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \end{bmatrix} \quad \mathbf{e}_2 = \begin{bmatrix} 0 \\ 1 \\ \vdots \end{bmatrix} \quad \cdots$$

Another basis for \mathbb{R}^2 is $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$. To see this, notice that saying that any vector \mathbf{y} can be written in a unique way as $c_1 \begin{bmatrix} 1 \\ 1 \end{bmatrix} + c_2 \begin{bmatrix} 1 \\ -1 \end{bmatrix}$ is the same as saying that the equation

$$\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \mathbf{x}$$

always has a unique solution. This is true.

A basis for the vector space \mathcal{P}_2 of polynomials of degree at most two is given by $\{1, x, x^2\}$. These polynomials clearly span \mathcal{P}_2 since every polynomial $p \in \mathcal{P}_2$ can be written as a linear combination $p(x) = c_0 \cdot 1 + c_1 x + c_2 x^2$. To show independence, suppose that $c_0 \cdot 1 + c_1 x + c_2 x^2$ is the zero polynomial. This means that $c_0 \cdot 1 + c_1 x + c_2 x^2 = 0$ for every value of x. Taking the first and second derivatives of this equation yields that $c_1 + 2c_2 x = 0$ and $2c_2 = 0$ for every value of x. Substituting x = 0 into each of these equations we find $c_0 = c_1 = c_2 = 0$.

Notice that if we represent the polynomial $p(x) = c_0 \cdot 1 + c_1 x + c_2 x^2 \in \mathcal{P}_2$ by the vector of coefficients $\begin{bmatrix} c_0 \\ c_1 \\ c_2 \end{bmatrix} \in \mathbb{R}^3$, then the vector space operations in \mathcal{P}_2 are mirrored perfectly in \mathbb{R}^3 . In other words, adding or scalar multiplying polynomials in \mathcal{P}_2 is the same as adding or scalar multiplying the corresponding vectors of coefficients in \mathbb{R}^3 .

This sort of correspondence can be set up whenever we have a basis $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_k$ for a vector space V. In this case every vector \mathbf{v} has a unique representation $c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \dots + c_k\mathbf{v}_k$ and we

can represent the vector $\mathbf{v} \in V$ by the vector $\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_k \end{bmatrix} \in \mathbb{R}^k$ (or \mathbb{C}^k). In some sense this says that we

can always think of finite dimensional vector spaces as being copies of \mathbb{R}^n or \mathbb{C}^n . The only catch is that the the correspondence that gets set up between vectors in V and vectors in \mathbb{R}^n or \mathbb{C}^n depends on the choice of basis.

It is intuitively clear that, say, a plane in three dimensions will always have a basis of two vectors. Here is an argument that shows that any two bases for a subspace S of \mathbb{R}^k or \mathbb{C}^k will always have the same number of elements. Let $\mathbf{v}_1, \ldots, \mathbf{v}_n$ and $\mathbf{w}_1, \ldots, \mathbf{w}_m$ be two bases for a subspace S. Let's

try to show that n must be the same as m. Since the \mathbf{v}_i 's span V we can write each \mathbf{w}_i as a linear combination of \mathbf{v}_i 's. We write

$$\mathbf{w}_j = \sum_{i=1}^n a_{i,j} \mathbf{v}_i$$

for each $j=1,\ldots,m$. Let's put all the coefficients into an $n\times m$ matrix $A=[a_{i,j}]$. If we form the matrix $k\times m$ matrix $W=[\mathbf{w}_1|\mathbf{w}_2|\cdots|\mathbf{w}_m]$ and the $k\times n$ matrix $V=[\mathbf{v}_1|\mathbf{v}_2|\cdots|\mathbf{v}_m]$ then the equation above can be rewritten

$$W = VA$$

To understand this construction consider the two bases $\left\{ \begin{bmatrix} 1\\0\\-1 \end{bmatrix}, \begin{bmatrix} 1\\-1\\0 \end{bmatrix} \right\}$ and $\left\{ \begin{bmatrix} 4\\2\\-6 \end{bmatrix}, \begin{bmatrix} 1\\-2\\1\\1 \end{bmatrix} \right\}$

for a subspace in \mathbb{R}^3 (in fact this subspace is the plane through the origin with normal vector $\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$).

Then we may write

$$\begin{bmatrix} 4\\2\\-6 \end{bmatrix} = 6 \begin{bmatrix} 1\\0\\-1 \end{bmatrix} - 2 \begin{bmatrix} 1\\-1\\0 \end{bmatrix}$$
$$\begin{bmatrix} 1\\-2\\1 \end{bmatrix} = -\begin{bmatrix} 1\\0\\-1 \end{bmatrix} + 2\begin{bmatrix} 1\\-1\\0 \end{bmatrix}$$

and the equation W = VA for this example reads

$$\begin{bmatrix} 4 & 1 \\ 2 & -2 \\ -6 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & -1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 6 & -1 \\ -2 & 2 \end{bmatrix}$$

Returning now to the general case, suppose that m > n. Then A has more columns than rows. So its echelon form must have some non-pivot columns which implies that there must be some non-zero solution to $A\mathbf{c} = \mathbf{0}$. Let $\mathbf{c} \neq \mathbf{0}$ be such a solution. Then

$$W\mathbf{c} = VA\mathbf{c} = \mathbf{0}$$

But this is impossible because the columns of W are linearly dependent. So it can't be true that m > n. Reversing the roles of V and W we find that n > m is impossible too. So it must be that m = n.

We have shown that any basis for a subspace S has the same number of elements. Thus it makes sense to define the *dimension* of a subspace S to be the number of elements in any basis for S.

Here is one last fact about bases: any set of k linearly independent vectors $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ in a k dimensional subspace S automatically spans S and is therefore a basis. To see this (in the case that S is a subspace of \mathbb{R}^n or \mathbb{C}^n) we let $\{\mathbf{w}_1, \dots, \mathbf{w}_k\}$ be a basis for S, which also will have k elements. Form $V = [\mathbf{v}_1| \dots | \mathbf{v}_k]$ and $W = [\mathbf{w}_1| \dots | \mathbf{w}_k]$. Then the construction above gives V = WA for a $k \times k$ matrix A. The matrix A must be invertible. Otherwise there would be a non-zero solution \mathbf{c} to $A\mathbf{c} = \mathbf{0}$. This would imply $V\mathbf{c} = WA\mathbf{c} = \mathbf{0}$ contradicting the independence of the rows of V. Thus we can write $W = VA^{-1}$ which shows that every \mathbf{w}_k is a linear combination of \mathbf{v}_i 's.

This shows that the \mathbf{v}_i 's must span S because every vector in S is a linear combination of the basis vectors \mathbf{w}_k 's which in turn are linear combinations of the \mathbf{v}_i 's.

As an example of this, consider again the space \mathcal{P}_2 of polynomials of degree at most 2. We claim that the polynomials $\{1, (x-a), (x-a)^2\}$ (for any constant a) form a basis. We already know that the dimension of this space is 3, so we only need to show that these three polynomials are independent. The argument for that is almost the same as before.

II.2. The four fundamental subspaces for a matrix

From your work in previous courses, you should be able to

- Recognize and use the property of transposes for which $(AB)^T = B^T A^T$ for any matrices A and B.
- Define the inner (dot) product of two vectors, and its properties (symmetry, linearity), and explain its geometrical meaning.
- Use the inner product to decide if two vectors are orthogonal, and to compute the angle between two vectors.
- State the Cauchy-Schwarz inequality and know for which vectors the inequality is an equality.
- For a linear system classify variables as basic and free.

After completing this section, you should be able to

- Define the four fundamental subspaces N(A), R(A), $N(A^T)$, and $R(A^T)$, associated to a matrix A and its transpose A^T , and show that they are subspaces.
- Express the Gaussian elimination process performed to reduce a matrix A to its row reduced echelon form matrix U as a matrix factorization, A = EU, using elementary matrices, and perform the steps using MATLAB/Octave.
- Compute bases for each of the four fundamental subspaces N(A), R(A), $N(A^T)$ and $R(A^T)$ of a matrix A; infer information on a matrix given the bases of its fundamental subspaces.
- Define and compute the rank of a matrix.
- State the formulas for the dimension of each of the four subspaces and explain why they are true; when possible, use such formulas to find the dimension of the subspaces.
- Explain what it means for two subspaces to be orthogonal $(V \perp W)$ and for one subspace to be the orthogonal complement of another $(V = W^{\perp})$.
- State which of the fundamental subspaces are orthogonal to each other and explain why, verify the orthogonality relations in examples, and use the orthogonality relation for R(A) to test whether the equation $A\mathbf{x} = \mathbf{b}$ has a solution.

II.2.1. Nullspace N(A) and Range R(A)

There are two important subspaces associated to any matrix. Let A be an $n \times m$ matrix. If \mathbf{x} is m dimensional, then $A\mathbf{x}$ makes sense and is a vector in n dimensional space.

The first subspace associated to A is the *nullspace* (or *kernel*) of A denoted N(A) (or Ker(A)). It is defined as all vectors \mathbf{x} solving the homogeneous equation for A, that is

$$N(A) = \{\mathbf{x} : A\mathbf{x} = \mathbf{0}\}$$

This is a subspace because if $A\mathbf{x}_1 = \mathbf{0}$ and $A\mathbf{x}_2 = \mathbf{0}$ then

$$A(c_1\mathbf{x}_1 + c_2\mathbf{x}_2) = c_1A\mathbf{x}_1 + c_2A\mathbf{x}_2 = \mathbf{0} + \mathbf{0} = \mathbf{0}.$$

The nullspace is a subspace of m dimensional space \mathbb{R}^m .

The second subspace is the range (or column space) of A denoted R(A) (or C(A)). It is defined as all vectors of the form $A\mathbf{x}$ for some \mathbf{x} . From our discussion above, we see that R(A) is the the span (or set of all possible linear combinations) of its columns. This explains the name "column space". The range is a subspace of n dimensional space \mathbb{R}^n .

The four fundamental subspaces for a matrix are the nullspace N(A) and range R(A) for A together with the nullspace $N(A^T)$ and range $R(A^T)$ for the transpose A^T .

II.2.2. Finding basis and dimension of N(A)

Example: Let

$$A = \begin{bmatrix} 1 & 3 & 3 & 10 \\ 2 & 6 & -1 & -1 \\ 1 & 3 & 1 & 4 \end{bmatrix}.$$

To calculate a basis for the nullspace N(A) and determine its dimension we need to find the solutions to $A\mathbf{x} = \mathbf{0}$. To do this we first reduce A to reduced row echelon form U and solve $U\mathbf{x} = \mathbf{0}$ instead, since this has the same solutions as the original equation.

ans =

This means that
$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$
 is in $N(A)$ if

$$\begin{bmatrix} 1 & 3 & 0 & 1 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

We now divide the variables into basic variables, corresponding to pivot columns, and free variables, corresponding to non-pivot columns. In this example the basic variables are x_1 and x_3 while the free variables are x_2 and x_4 . The free variables are the parameters in the solution. We can solve for the basic variables in terms of the free ones, giving $x_3 = -3x_4$ and $x_1 = -3x_2 - x_4$. This leads to

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -3x_2 - x_4 \\ x_2 \\ -3x_4 \\ x_4 \end{bmatrix} = x_2 \begin{bmatrix} -3 \\ 1 \\ 0 \\ 0 \end{bmatrix} + x_4 \begin{bmatrix} -1 \\ 0 \\ -3 \\ 1 \end{bmatrix}$$

The vectors $\begin{bmatrix} -3\\1\\0\\0 \end{bmatrix}$ and $\begin{bmatrix} -1\\0\\-3\\1 \end{bmatrix}$ span the nullspace since every element of N(A) is a linear combination

of them. They are also linearly independent because if the linear combination on the right of the equation above is zero, then by looking at the second entry of the vector (corresponding to the first free variable) we find $x_2 = 0$ and looking at the last entry (corresponding to the second free variable) we find $x_4 = 0$. So both coefficients must be zero.

To find a basis for N(A) in general we first compute U = rref(A) and determine which variables are basic and which are free. For each free variable we form a vector as follows. First put a 1 in the position corresponding to that free variable and a zero in every other free variable position. Then fill in the rest of the vector in such a way that $U\mathbf{x} = \mathbf{0}$. (This is easy to do!) The set all such vectors - one for each free variable - is a basis for N(A).

II.2.3. The matrix version of Gaussian elimination

How are a matrix A and its reduced row echelon form U = rref(A) related? If A and U are $n \times m$ matrices, then there exists an invertible $n \times n$ matrix such that

$$A = EU$$
 $E^{-1}A = U$

This immediately explains why the N(A) = N(U), because if $A\mathbf{x} = \mathbf{0}$ then $U\mathbf{x} = E^{-1}A\mathbf{x} = \mathbf{0}$ and conversely if $A\mathbf{x} = \mathbf{0}$ then $U\mathbf{x} = EA\mathbf{x} = \mathbf{0}$.

What is this matrix E? It can be thought of as a matrix record of the Gaussian elimination steps taken to reduce A to U. It turns out performing an elementary row operation is the same as multiplying on the left by an invertible square matrix. This invertible square matrix, called an elementary matrix, is obtained by doing the row operation in question to the identity matrix.

Suppose we start with the matrix

The first elementary row operation that we want to do is to subtract twice the first row from the second row. Let's do this to the 3×3 identity matrix I (obtained with eye(3) in MATLAB/Octave) and call the result E1

```
>E1 = eye(3)
E1 =
   1
       0
            0
   0
       1
            0
       0
            1
>E1(2,:) = E1(2,:)-2*E1(1,:)
E1 =
   1
            0
  -2
            0
        1
   0
       0
            1
```

Now if we multiply E1 and A we obtain

which is the result of doing that elementary row operation to A. Let's do one more step. The second row operation we want to do is to subtract the first row from the third. Thus we define

$$>E2 = eye(3)$$

E2 =

1 0 0 0 1 0 0 0 1

$$>E2(3,:) = E2(3,:)-E2(1,:)$$

E2 =

1 0 0 0 1 0 -1 0 1

and we find

ans =

which is one step further along in the Gaussian elimination process. Continuing in this way until we eventually arrive at U so that

$$E_k E_{k-1} \cdots E_2 E_1 A = U$$

Thus A=EU with $E=E_1^{-1}E_2^{-1}\cdots E_{k-1}^{-1}E_k^{-1}$. For the example above it turns out that

$$E = \begin{bmatrix} 1 & 3 & -6 \\ 2 & -1 & -18 \\ 1 & 1 & -9 \end{bmatrix}$$

which we can check:

```
>A=[1 3 3 10;2 6 -1 -1;1 3 1 4]
A =
    1
          3
               3
                    10
    2
          6
               -1
                    -1
    1
>U=rref(A)
U =
   1
       3
            0
                 1
   0
            1
                 3
                 0
>E=[1 3 -6; 2 -1 -18; 1 1 -9];
>E*U
ans =
    1
                    10
    2
              -1
                    -1
    1
               1
```

If we do a partial elimination then at each step we can write A = E'U' where U' is the resulting matrix at the point we stopped, and E' is obtained from the Gaussian elimination step up to that point. A common place to stop is when U' is in echelon form, but the entries above the pivots have not been set to zero. If we can achieve this without doing any row swaps along the way then E' turns out to be lower triangular matrix. Since U' is upper triangular, this is called the LU decomposition of A.

II.2.4. A basis for R(A)

The ranges or column spaces R(A) and R(U) are not the same in general, but they are related. In fact, the vectors in R(A) are exactly all the vectors in R(U) multiplied by E, where E is the invertible matrix in the equation A = EU. We can write this relationship as

$$R(A) = ER(U)$$

To see this notice that if $\mathbf{x} \in R(U)$, that is, $\mathbf{x} = U\mathbf{y}$ for some \mathbf{y} then $E\mathbf{x} = EU\mathbf{y} = A\mathbf{y}$ is in R(A). Conversely if $\mathbf{x} \in R(A)$, that is, $\mathbf{x} = A\mathbf{y}$ for some \mathbf{y} then $\mathbf{x} = EE^{-1}A\mathbf{y} = EU\mathbf{y}$ so \mathbf{x} is E times a vector in R(U).

Now if we can find a basis $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_k$ for R(U), the vectors $E\mathbf{u}_1, E\mathbf{u}_2, \dots, E\mathbf{u}_k$ form a basis for R(A). (Homework exercise)

But a basis for the column space R(U) is easy to find. They are exactly the pivot columns of U. If we multiply these by E we get a basis for R(A). But if

$$A = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \cdots & \mathbf{a}_m \end{bmatrix}, \quad U = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \cdots & \mathbf{u}_m \end{bmatrix}$$

then the equation A = EU can be written

$$\begin{bmatrix} \mathbf{a}_1 \middle| \mathbf{a}_2 \middle| \cdots \middle| \mathbf{a}_m \end{bmatrix} = \begin{bmatrix} E\mathbf{u}_1 \middle| E\mathbf{u}_2 \middle| \cdots \middle| E\mathbf{u}_m \end{bmatrix}$$

From this we see that the columns of A that correspond to pivot columns of U form a basis for R(A). This implies that the dimension of R(A) is the number of pivot columns in U.

II.2.5. The rank of a matrix

We define the rank of the matrix A, denoted r(A) to be the number of pivot columns of U. Then we have shown that for an $n \times m$ matrix A

$$\dim(R(A)) = r(A)$$
$$\dim(N(A)) = m - r(A)$$

II.2.6. Bases for $R(A^T)$ and $N(A^T)$

Of course we could find $R(A^T)$ and $N(A^T)$ by computing the reduced row echelon form for A^T and following the steps above. But then we would miss an important relation between the dimensions of these spaces.

Let's start with the column space $R(A^T)$. The columns of A^T are the rows of A (written as column vectors instead of row vectors). So $R(A^T)$ is the row space of A.

It turns out that $R(A^T)$ and $R(U^T)$ are the same. This follows from A = EU. To see this take the transpose of this equation. Then $A^T = U^T E^T$. Now suppose that $\mathbf{x} \in R(A^T)$. This means that $\mathbf{x} = A^T \mathbf{y}$ for some \mathbf{y} . But then $\mathbf{x} = U^T E^T \mathbf{y} = U^T \mathbf{y}'$ where $\mathbf{y}' = E^T \mathbf{y}$ so $\mathbf{x} \in R(U^T)$. Similarly, if $\mathbf{x} = U^T \mathbf{y}$ for some \mathbf{y} then $\mathbf{x} = U^T E^T (E^T)^{-1} \mathbf{y} = A^T (E^T)^{-1} \mathbf{y} = A^T \mathbf{y}'$ for $\mathbf{y}' = (E^T)^{-1} \mathbf{y}$. So every vector in $R(U^T)$ is also in $R(A^T)$. Here we used that E and hence E^T is invertible.

Now we know that $R(A^T) = R(U^T)$ is spanned by the columns of U^T . But since U is in reduced row echelon form, its non-zero columns of U^T are independent (homework exercise). Therefore, the

non-zero columns of U^T form a basis for $R(A^T)$. There is one of these for every pivot. This leads to

$$\dim(R(A^T)) = \mathrm{r}(A) = \dim(R(A))$$

The final subspace to consider is $N(A^T)$. From our work above we know that

$$\dim(N(A^T)) = n - \dim(R(A^T)) = n - r(A).$$

Finding a basis is trickier. It might be easiest to find the reduced row echelon form of A^T . But if we insist on using A = EU or $A^T = U^T E^T$ we could proceed by multiplying on the right be the inverse of E^T . This gives

$$A^T (E^T)^{-1} = U^T$$

Now notice that the last n - r(A) columns of U^T are zero, since U is in reduced row echelon form. So the last n - r(A) columns of $(E^T)^{-1}$ are in the nullspace of A^T . They also have to be independent, since $(E^T)^{-1}$ is invertible.

Thus the last n - r(A) of $(E^T)^{-1}$ form a basis for $N(A^T)$.

From a practical point of view, this is not so useful since we have to compute the inverse of a matrix. It might be just as easy to reduce A^T . (Actually, things are slightly better if we use the LU decomposition. The same argument shows that the last n - r(A) columns of $(L^T)^{-1}$ also form a basis for $N(A^T)$. But L^T is an upper triangular matrix, so its inverse is faster to compute.)

II.2.7. Orthogonal vectors and subspaces

In preparation for our discussion of the orthogonality relations for the fundamental subspaces of matrix we review some facts about orthogonal vectors and subspaces.

Recall that the dot product, or inner product of two vectors

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

is denoted by $\mathbf{x} \cdot \mathbf{y}$ or $\langle \mathbf{x}, \mathbf{y} \rangle$ and defined by

$$\mathbf{x}^T \mathbf{y} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^n x_i y_i$$

Some important properties of the inner product are symmetry

$$\mathbf{x}\cdot\mathbf{y}=\mathbf{y}\cdot\mathbf{x}$$

and linearity

$$(c_1\mathbf{x}_1 + c_2\mathbf{x}_2) \cdot \mathbf{y} = c_1\mathbf{x}_1 \cdot \mathbf{y} + c_2\mathbf{x}_2 \cdot \mathbf{y}.$$

The (Euclidean) norm, or length, of a vector is given by

$$\|\mathbf{x}\| = \sqrt{\mathbf{x} \cdot \mathbf{x}} = \sqrt{\sum_{i=1}^{n} x_i^2}$$

An important property of the norm is that $\|\mathbf{x}\| = 0$ implies that $\mathbf{x} = \mathbf{0}$.

The geometrical meaning of the inner product is given by

$$\mathbf{x} \cdot \mathbf{y} = \|\mathbf{x}\| \|\mathbf{y}\| \cos(\theta)$$

where θ is the angle between the vectors. The angle θ can take values from 0 to π .

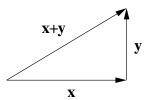
The Cauchy–Schwarz inequality states

$$|\mathbf{x} \cdot \mathbf{y}| \le ||\mathbf{x}|| ||\mathbf{y}||.$$

It follows from the previous formula because $|\cos(\theta)| \le 1$. The only time that equality occurs in the Cauchy–Schwarz inequality, that is $\mathbf{x} \cdot \mathbf{y} = \|\mathbf{x}\| \|\mathbf{y}\|$, is when $\cos(\theta) = \pm 1$ and θ is either 0 or π . This means that the vectors are pointed in the same or in the opposite directions.

The vectors \mathbf{x} and \mathbf{y} are orthogonal if $\mathbf{x} \cdot \mathbf{y} = 0$. Geometrically this means either that one of the vectors is zero or that they are at right angles. This follows from the formula above, since $\cos(\theta) = 0$ implies $\theta = \pi/2$.

Another way to see that $\mathbf{x} \cdot \mathbf{y} = 0$ means that vectors are orthogonal is from Pythagoras' formula. If \mathbf{x} and \mathbf{y} are at right angles then $\|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 = \|\mathbf{x} + \mathbf{y}\|^2$.



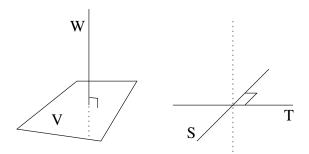
But $\|\mathbf{x} + \mathbf{y}\|^2 = (\mathbf{x} + \mathbf{y}) \cdot (\mathbf{x} + \mathbf{y}) = \|\mathbf{x}\|^2 + \|\mathbf{y}\|^2 + 2\mathbf{x} \cdot \mathbf{y}$ so Pythagoras' formula holds exactly when $\mathbf{x} \cdot \mathbf{y} = 0$.

To compute the inner product of (column) vectors X and Y in MATLAB/Octave we use the formula $\mathbf{x} \cdot \mathbf{y} = \mathbf{x}^T \mathbf{y}$. Thus the inner product can be computed using X'*Y. (If X and Y are row vectors, the formula is X*Y'.)

The norm of a vector X is computed by norm(X). In MATLAB/Octave inverse trig functions are computed with asin(), acos() etc. So the angle between column vectors X and Y could be computed as

> acos(X'*Y/(norm(X)*norm(Y)))

Two subspaces V and W are said to be orthogonal if every vector in V is orthogonal to every vector in W. In this case we write $V \perp W$.



In this figure $V \perp W$ and also $S \perp T$.

A related concept is the orthogonal complement. The orthogonal complement of V, denoted V^{\perp} , is the subspace containing all vectors orthogonal to V. In the figure $W = V^{\perp}$ but $T \neq S^{\perp}$ since T contains only some of the vectors orthogonal to S.

If we take the orthogonal complement of V^{\perp} we get back the original space V: This is certainly plausible from the pictures. It is also obvious that $V \subseteq (V^{\perp})^{\perp}$, since any vector in V is perpendicular to vectors in V^{\perp} . If there were a vector in $(V^{\perp})^{\perp}$ not contained in V we could subtract its projection onto V (defined in the next chapter) and end up with a non-zero vector in $(V^{\perp})^{\perp}$ that is also in V^{\perp} . Such a vector would be orthogonal to itself, which is impossible. This shows that

$$(V^{\perp})^{\perp} = V.$$

One consequence of this formula is that $V = W^{\perp}$ implies $V^{\perp} = W$. Just take the orthogonal complement of both sides and use $(W^{\perp})^{\perp} = W$.

II.2.8. Orthogonality relations for the fundamental subspaces of a matrix

Let A be an $n \times m$ matrix. Then N(A) and $R(A^T)$ are subspaces of \mathbb{R}^m while $N(A^T)$ and R(A) are subspaces of \mathbb{R}^n .

These two pairs of subspaces are orthogonal:

$$N(A) = R(A^T)^{\perp}$$
$$N(A^T) = R(A)^{\perp}$$

We will show that the first equality holds for any A. The second equality then follows by applying the first one to A^T .

These relations are based on the formula

$$(A^T \mathbf{x}) \cdot \mathbf{y} = \mathbf{x} \cdot (A\mathbf{y})$$

This formula follows from the product formula $(AB)^T = B^T A^T$ for transposes, since

$$(A^T\mathbf{x})\cdot\mathbf{y}=(A^T\mathbf{x})^T\mathbf{y}=\mathbf{x}^T(A^T)^T\mathbf{y}=\mathbf{x}^TA\mathbf{y}=\mathbf{x}\cdot(A\mathbf{y})$$

First, we show that $N(A) \subseteq R(A^T)^{\perp}$. To do this, start with any vector $\mathbf{x} \in N(A)$. This means that $A\mathbf{x} = \mathbf{0}$. If we compute the inner product of \mathbf{x} with any vector in $R(A^T)$, that is, any vector of the form $A^T\mathbf{y}$, we get $(A^T\mathbf{y}) \cdot \mathbf{x} = \mathbf{y} \cdot A\mathbf{x} = \mathbf{y} \cdot \mathbf{0} = 0$. Thus $\mathbf{x} \in R(A^T)^{\perp}$. This shows $N(A) \subseteq R(A^T)^{\perp}$.

Now we show the opposite inclusion, $R(A^T)^{\perp} \subseteq N(A)$. This time we start with $\mathbf{x} \in R(A^T)^{\perp}$. This means that \mathbf{x} is orthogonal to every vector in $R(A^T)$, that is, to every vector of the form $A^T\mathbf{y}$. So $(A^T\mathbf{y}) \cdot \mathbf{x} = \mathbf{y} \cdot (A\mathbf{x}) = \mathbf{0}$ for every \mathbf{y} . Pick $\mathbf{y} = A\mathbf{x}$. Then $(A\mathbf{x}) \cdot (A\mathbf{x}) = ||A\mathbf{x}||^2 = \mathbf{0}$. This implies $A\mathbf{x} = \mathbf{0}$ so $\mathbf{x} \in N(A)$. We can conclude that $R(A^T)^{\perp} \subseteq N(A)$.

These two inclusions establish that $N(A) = R(A^T)^{\perp}$.

Let's verify these orthogonality relations in an example. Let

$$A = \begin{bmatrix} 1 & 2 & 1 & 1 \\ 1 & 3 & 0 & 1 \\ 2 & 5 & 1 & 2 \end{bmatrix}$$

Then

$$\operatorname{rref}(A) = \begin{bmatrix} 1 & 0 & 3 & 1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \operatorname{rref}(A^T) = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Thus we get

$$N(A) = \operatorname{span} \left\{ \begin{bmatrix} -3\\1\\1\\0 \end{bmatrix}, \begin{bmatrix} -1\\0\\0\\1 \end{bmatrix} \right\}$$

$$R(A) = \operatorname{span} \left\{ \begin{bmatrix} 1\\1\\2\\2 \end{bmatrix}, \begin{bmatrix} 2\\3\\5 \end{bmatrix} \right\}$$

$$N(A^T) = \operatorname{span} \left\{ \begin{bmatrix} -1\\-1\\1\\1 \end{bmatrix} \right\}$$

$$R(A^T) = \operatorname{span} \left\{ \begin{bmatrix} 1\\0\\3\\1 \end{bmatrix}, \begin{bmatrix} 0\\1\\-1\\0 \end{bmatrix} \right\}$$

We can now verify directly that every vector in the basis for N(A) is orthogonal to every vector in the basis for $R(A^T)$, and similarly for $N(A^T)$ and R(A).

Does the equation

$$A\mathbf{x} = \begin{bmatrix} 2\\1\\3 \end{bmatrix}$$

have a solution? We can use the ideas above to answer this question easily. We are really asking

whether $\begin{bmatrix} 2\\1\\3 \end{bmatrix}$ is contained in R(A). But, according to the orthogonality relations, this is the same as asking whether $\begin{bmatrix} 2\\1\\3 \end{bmatrix}$ is contained in $N(A^T)^{\perp}$. This is easy to check. Simply compute the dot product

$$\begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix} \cdot \begin{bmatrix} -1 \\ -1 \\ 1 \end{bmatrix} = -2 - 1 + 3 = 0.$$

Since the result is zero, we conclude that a solution exists.

II.2.9. The formula matrix of a chemical system

The fundamental subspaces of the formula matrix of a chemical system give information about the possible reactions and invariant ratios between quantities of species in the system.

Formula vectors, the formula matrix A and its range R(A)

A chemical system consists of a collection of chemical species, each composed of a number of elements. To each species we associate a *formula vector* which lists the amount of each element in that species. For example, in the chemical system consisting of the species CH_4 , S_2 , CS_2 and H_2S , the components (elements) are C, H and S so that the formula vectors are $[1,4,0]^T$ for CH_4 , $[0,0,2]^T$ for S_2 , $[1,0,2]^T$ for CS_2 and $[0,2,1]^T$ for H_2S . Taking all the formula vectors in the system as columns of a matrix, we obtain the *formula matrix*, A, whose rows are labelled by the elements and whose columns are labelled by the species. In this example

$$A = \begin{array}{cccc} CH_4 & S_2 & CS_2 & H_2S \\ C & 1 & 0 & 1 & 0 \\ 4 & 0 & 0 & 2 \\ S & 0 & 2 & 2 & 1 \end{array}$$

A sample of n_1 moles of CH₄, n_2 moles of S₂, n_3 moles of CS₂ and n_4 moles of H₂S is described by the linear combination

$$\mathbf{b} = n_1 \begin{bmatrix} 1 \\ 4 \\ 0 \end{bmatrix} + n_2 \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} + n_3 \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} + n_4 \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix}$$

The components b_1 , b_2 and b_3 of **b** give the molar amounts of C, H and S in our sample. The vector **b** is called the *element abundance vector*. We can write the equation above as

$$\mathbf{b} = A\mathbf{n}$$

where $\mathbf{n} = [n_1, n_2, n_3, n_4]^T$ is called the *species abundance vector*. The entries of \mathbf{n} (and hence also of \mathbf{b}) are positive numbers. In this context it is natural for them to be integers too.

The element abundance vector **b** is in the range R(A). However, not every vector in R(A) is an element abundance vector, because of the positivity condition.

Chemical reactions and the null space N(A)

In a chemical system, some of the species may react to form other species in the system. We can use the null space N(A) of the formula matrix to find all reactions satisfying the constraints imposed by mass balance.

In the example chemical system system above, a possible reaction is

$$CH_4 + 2S_2 = CS_2 + 2H_2S.$$

This can be written in vector form as

$$\begin{bmatrix} 1 \\ 4 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix} + 2 \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix},$$

$$A\mathbf{n}_1 = A\mathbf{n}_2$$

with $\mathbf{n}_1 = [1, 2, 0, 0]^T$ and $\mathbf{n}_2 = [0, 0, 1, 2]^T$. This equation expresses the mass balance of the reaction, that is, the fact that the number of atoms of each component, C, H and S, is the same on the left and right sides of the equation.

Notice that $\mathbf{n} = \mathbf{n}_1 - \mathbf{n}_2$ is in the null space N(A) since $A\mathbf{n} = A\mathbf{n}_1 - A\mathbf{n}_2 = \mathbf{0}$. In general, given a formula matrix A, an vector \mathbf{n} is called a *reaction vector* if it is contained in N(A) and satisfies an additional non-degeneracy condition.

The condition $\mathbf{n} \in N(A)$ ensures that a reaction vector \mathbf{n} will contain coefficients for a mass balanced equation. Species corresponding to the positive coefficients are on one side of the reaction equation, while the species corresponding to the negative coefficients are on the other side.

The reaction equation $A\mathbf{n} = \mathbf{0}$ is a linear relation among columns of A for which the corresponding entry in \mathbf{n} is non-zero. The non-degeneracy condition is imposed to ensure that there is no other independent relation among these columns. In other words, up to scaling, there can only be one reaction equation involving a given collection of species. To state the condition, collect all the columns of A for which the corresponding entry in \mathbf{n} is non-zero. If we form a matrix \tilde{A} from these columns then the condition is that $N(\tilde{A})$ is one dimensional. Another way of saying this is that if we drop any one column from our collection the resulting set is linearly independent. Under this condition \mathbf{n} can have at most rank(A) + 1 non-zero entries.

The non-degeneracy condition is automatically satisfied if we compute a basis for N(A) in the standard way from the row reduction of A. This is because exactly one of the non-zero entries of such a basis vector is in a non-pivot position. This implies that the columns in \tilde{A} are a collection of linearly independent columns (the pivot columns) and one additional column. There can only be one independent linear relation in such a collection.

Since a reaction vector remains a reaction vector when multiplied by non-zero constant, we can normalize, for example, to make a particular coefficient equal to one, or to make all the coefficients integers.

Suppose we wish to find what reactions are possible when we add the species H_2 to the collection above. The new formula matrix is

$$A = \begin{array}{ccccc} CH_4 & S_2 & CS_2 & H_2S & H_2 \\ C & 1 & 0 & 1 & 0 & 0 \\ 4 & 0 & 0 & 2 & 2 \\ S & 0 & 2 & 2 & 1 & 0 \end{array} \right).$$

To find the null space we reduce A to reduced row echelon form. Here are the MATLAB/Octave commands to do this.

1> A=[1 0 1 0 0;4 0 0 2 2;0 2 2 1 0];

```
2> rref(A)
ans =
```

1.00000	0.00000	0.00000	0.50000	0.50000
0.00000	1.00000	0.00000	1.00000	0.50000
0.00000	0.00000	1.00000	-0.50000	-0.50000

This shows that the null space is two dimensional and spanned by $[-1, -2, 1, 2, 0]^T$ and $[-1, -1, 1, 0, 2]^T$. Here we have normalized to make the reaction coefficients integers. To write the reaction we collect all the positive coefficients on one side and all the negative coefficients on the other. Then from $[-1, -2, 1, 2, 0]^T$ we recover the reaction

$$CH_4 + 2S_2 = CS_2 + 2H_2S$$

from before. In addition, the vector [-1, -1, 1, 0, 2] yields the new reaction

$$CH_4 + S_2 = CS_2 + 2H_2.$$

The example above is from Smith and Missen [1], where more information on chemical stoiciometry can be found.

Preserved ratios and $N(A^T)$

Non-zero vectors in the nullspace $N(A^T)$ of the transpose of A also give information about the chemical system. Consider the system consisting of only two species CH_4 and H_2S with formula matrix

$$A = \begin{array}{ccc} & CH_4 & H_2S \\ C & 1 & 0 \\ A & 4 & 2 \\ S & 0 & 1 \end{array}$$

Here $N(A^T)$ is one dimensional, spanned by $[4, -1, 2]^T$.

As we saw above, if we combine n_1 moles of CH_4 and n_2 moles of H_2S then the components the corresponding element abundance vector

$$\mathbf{b} = n_1 \begin{bmatrix} 1 \\ 4 \\ 0 \end{bmatrix} + n_2 \begin{bmatrix} 0 \\ 2 \\ 1 \end{bmatrix} = A \begin{bmatrix} n_1 \\ n_2 \end{bmatrix}$$

is in the range R(A). From the orthogonality relation $R(A) = N(A^T)^{\perp}$ we see that **b** must be orthogonal to $[4, -1, 2]^T$. This is true for any choice of n_1 and n_2 , so that for any possible sample,

 $4b_1 - b_2 + 2b_3 = 0$. Thus the molar amounts b_1 , b_2 , and b_3 of C, H and S in any sample of this chemical system have fixed ratio.

$$\frac{4b_1 + 2b_3}{b_2} = 1.$$

For more information about linear algebra applied to petrology see T. Gordon [2].

- [1] William R. Smith and Ronald W. Missen, What is Chemical Stoichiometry?, Chemical Engineering Education, Winter 1979, 26–32.
- [2] T. Gordon, Vector subspace analysis applied to inverse geochemical mass transfer problems, at people.ucalgary.ca/~gordon/InverseMassTransferProblems/GAC-MAC2000Slides.pdf

II.3. Graphs and Networks

Prerequisites and Learning Goals

From your work in previous courses you should be able to

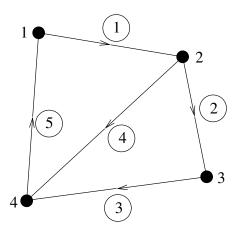
- State Ohm's law for a resistor.
- State Kirchhoff's laws for a resistor network.

After completing this section, you should be able to

- Write down the incidence matrix of a directed graph, and draw the graph given the incidence matrix.
- Define the Laplace operator L, or Laplacian, for a graph; given a graph, determine the entries of L and describe how they are related to the nodes and edges of the graph.
- When the edges of a graph represent resistors or batteries in a circuit, you should be able to
 - define voltage, voltage difference, current, and loop vectors;
 - interpret each of the four subspaces associated with the incidence matrix D and their dimensions in terms of voltage, current, and loop vectors; relate the dimension of N(D) to the number of connected components in a graph; find bases for each subspace of D and verify the orthogonality relations between such subspaces;
 - interpret the range and the nullspace of the Laplacian in terms of voltage and current vectors, and give a physical justification of such interpretation;
 - explain what happens to L if two nodes in the graph are renamed and why and when it is useful to do so;
 - construct the voltage-to-current map for a pair of nodes and use it to calculate voltages, currents, or effective resistances; perform all necessary computations in MAT-LAB/Octave.

II.3.1. Directed graphs and their incidence matrix

A directed graph is a collection of vertices (or nodes) connected by edges with arrows. Here is a graph with 4 vertices and 5 edges.



Graphs come up in many applications. For example, the nodes could represent computers and the arrows internet connections. Or the nodes could be factories and the arrows represent movement of goods. We will mostly focus on a single interpretation where the edges represent resistors or batteries hooked up in a circuit.

In this interpretation we will be assigning a number to each edge to indicate the amount of current flowing through that edge. This number can be positive or negative. The arrows indicate the direction associated to a positive current.

The incidence matrix of a graph is an $n \times m$ matrix, where n is the number of edges and m is the number of vertices. We label the rows by the edges in the graph and the columns by the vertices. Each row of the matrix corresponds to an edge in the graph. It has a -1 in the place corresponding to the vertex where the arrow starts and a 1 in the place corresponding to the vertex where the arrow ends.

Here is the incidence matrix for the illustrated graph.

The columns of the matrix have the following interpretation. The column representing a given vertex has a +1 for each arrow coming in to that vertex and a -1 for each arrow leaving the vertex.

Given an incidence matrix, the corresponding graph can easily be drawn. What is the graph for

$$\begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 1 & 0 & -1 \end{bmatrix}$$
?

(Answer: a triangular loop.)

II.3.2. Nullspace and range of incidence matrix and its transpose

We now wish to give an interpretation of the fundamental subspaces associated with the incidence matrix of a graph. Let's call the matrix D. In our example D acts on vectors $\mathbf{v} \in \mathbb{R}^4$ and produces

a vector $D\mathbf{v}$ in \mathbb{R}^5 . We can think of the vector $\mathbf{v} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix}$ as an assignment of a voltage to each of the nodes in the graph. Then the vector $D\mathbf{v} = \begin{bmatrix} v_2 - v_1 \\ v_3 - v_2 \\ v_4 - v_3 \\ v_4 - v_2 \\ v_4 - v_3 \\ v_4 - v_2 \\ v_4 - v_2 \\ v_4 - v_3 \\ v_4 - v_4 \\ v_5 - v_4 \\ v_5 - v_5 \\ v_6 - v_6 \\ v$

across that edge. The matrix D is similar to the derivative matrix when we studied finite difference approximations. It can be thought of as the derivative matrix for a graph.

II.3.3. The null space N(D)

This is the set of voltages \mathbf{v} for which the voltage differences in $D\mathbf{v}$ are all zero. This means that any two nodes connected by an edge will have the same voltage. In our example, this implies all

the voltages are the same, so every vector in N(D) is of the form $\mathbf{v} = s \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$ for some s. In other

words, the null space is one dimensional with basis $\left\{ \begin{bmatrix} 1\\1\\1\\1 \end{bmatrix} \right\}$.

For a graph that has several disconnected pieces, $D\mathbf{v} = \mathbf{0}$ will force \mathbf{v} to be constant on each connected component of the graph. Each connected component will contribute one basis vector to N(D). This is the vector that is equal to 1 on that component and zero everywhere else. Thus $\dim(N(D))$ will be equal to the number of connected components (i.e., connected pieces that are disconnected from each other) in the graph.

II.3.4. The range R(D)

The range of D consists of all vectors \mathbf{b} in \mathbb{R}^5 that are voltage differences, i.e., $\mathbf{b} = D\mathbf{v}$ for some \mathbf{v} . We know that the dimension of R(D) is $4 - \dim(N(D)) = 4 - 1 = 3$. So the set of voltage difference vectors must be restricted in some way. In fact a voltage difference vector will have the property that the sum of the differences around a closed loop is zero. In the example the edges (1), (4), (5) form

a loop, so if
$$\mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$
 is a voltage difference vector then $b_1 + b_4 + b_5 = 0$ We can check this directly

in the example. Since
$$\mathbf{b} = D\mathbf{v} = \begin{bmatrix} v_2 - v_1 \\ v_3 - v_2 \\ v_4 - v_3 \\ v_4 - v_2 \\ v_1 - v_4 \end{bmatrix}$$
 we check that $(v_2 - v_1) + (v_4 - v_2) + (v_1 - v_4) = 0$.

In the example graph there are three loops, namely 1, 4, 5 and 2, 3, 4 and 1, 2, 3, 5. The corresponding equations that the components of a vector \mathbf{b} must satisfy to be in the range of D are

$$b_1 + b_4 + b_5 = 0$$
$$b_2 + b_3 - b_4 = 0$$
$$b_1 + b_2 + b_3 + b_5 = 0$$

Notice the minus sign in the second equation corresponding to a backwards arrow. However these equations are not all independent, since the third is obtained by adding the first two. There are two independent equations that the components of \mathbf{b} must satisfy. Since R(D) is 3 dimensional, there can be no additional constraints.

Now we wish to find interpretations for the null space and the range of D^T . Let $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix}$ be

a vector in \mathbb{R}^5 which we interpret as being an assignment of a current to each edge in the graph.

Then
$$D^T \mathbf{y} = \begin{bmatrix} y_5 - y_1 \\ y_1 - y_2 - y_4 \\ y_2 - y_3 \\ y_3 + y_4 - y_5 \end{bmatrix}$$
. This vector assigns to each node the amount of current collecting at

that node.

II.3.5. The null space $N(D^T)$

This is the set of current vectors $\mathbf{y} \in \mathbb{R}^5$ which do not result in any current building up (or draining away) at any of the nodes. We know that the dimension of this space must be $5 - \dim(R(D^T)) =$

 $5 - \dim(R(D)) = 5 - 3 = 2$. We can guess at a basis for this space by noting that current running

around a loop will not build up at any of the nodes. The loop vector $\begin{bmatrix} 1\\0\\0\\1\\1 \end{bmatrix}$ represents a current

running around the loop 1, 4, 5. We can verify that this vector lies in the null space of D^T :

$$\begin{bmatrix} -1 & 0 & 0 & 0 & 1 \\ 1 & -1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The current vectors corresponding to the other two loops are $\begin{bmatrix} 0 \\ 1 \\ 1 \\ -1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 1 \end{bmatrix}$. However these three

vectors are not linearly independent. Any choice of two of these vectors are independent, and form a basis.

II.3.6. The range $R(D^T)$

This is the set of vectors in \mathbb{R}^4 of the form $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = D^T \mathbf{y}$. With our interpretation these are vectors

which measure how the currents in y are building up or draining away from each node. Since the current that is building up at one node must have come from some other nodes, it must be that

$$x_1 + x_2 + x_3 + x_4 = 0$$

In our example, this can be checked directly. This one condition in \mathbb{R}^4 results in a three dimensional subspace.

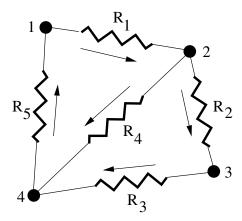
II.3.7. Summary and Orthogonality relations

The two subspaces R(D) and $N(D^T)$ are subspaces of \mathbb{R}^5 . The subspace $N(D^T)$ contains all linear combination of loop vectors, while R(D) contains all vectors whose dot product with loop vectors is zero. This verifies the orthogonality relation $R(D) = N(D^T)^{\perp}$.

The two subspaces N(D) and $R(D^T)$ are subspaces of \mathbb{R}^4 . The subspace N(D) contains constant vectors, while $R(D^T)$ contains all vectors orthogonal to constant vectors. This verifies the other orthogonality relation $N(D) \perp R(D^T)$.

II.3.8. Resistors and the Laplacian

Now we suppose that each edge of our graph represents a resistor. This means that we associate with the *i*th edge a resistance R_i . Sometimes it is convenient to use conductances γ_i which are defined to be the reciprocals of the resistances, that is, $\gamma_i = 1/R_i$.



If we begin by an assignment of voltage to every node, and put these numbers in a vector $\mathbf{v} \in \mathbb{R}^4$. Then $D\mathbf{v} \in \mathbb{R}^5$ represents the vector of voltage differences for each of the edges.

Given the resistance R_i for each edge, we can now invoke Ohm's law to compute the current flowing through each edge. For each edge, Ohm's law states that

$$(\Delta V)_i = j_i R_i$$

where $(\Delta V)_i$ is the voltage drop across the edge, j_i is the current flowing through that edge, and R_i is the resistance. Solving for the current we obtain

$$j_i = R_i^{-1}(\Delta V)_i.$$

Notice that the voltage drop $(\Delta V)_i$ in this formula is exactly the *i*th component of the vector $D\mathbf{v}$. So if we collect all the currents flowing along each edge in a vector \mathbf{j} indexed by the edges, then Ohm's law for all the edges can be written as

$$\mathbf{j} = R^{-1}D\mathbf{v}$$

where

$$R = \begin{bmatrix} R_1 & 0 & 0 & 0 & 0 \\ 0 & R_2 & 0 & 0 & 0 \\ 0 & 0 & R_3 & 0 & 0 \\ 0 & 0 & 0 & R_4 & 0 \\ 0 & 0 & 0 & 0 & R_5 \end{bmatrix}$$

is the diagonal matrix with the resistances on the diagonal.

Finally, if we multiply **j** by the matrix D^T the resulting vector

$$\mathbf{J} = D^T \mathbf{j} = D^T R^{-1} D \mathbf{v}$$

has one entry for each node, representing the total current flowing in or out of that node along the edges that connect to it.

The matrix

$$L = D^T R^{-1} D$$

appearing in this formula is called the *Laplacian*. It is similar to the second derivative matrix that appeared when we studied finite difference approximations.

One important property of the Laplacian is symmetry, that is the fact that $L^T = L$. To see this recall that the transpose of a product of matrices is the product of the transposes in reverse order $((ABC)^T = C^T B^T A^T)$. This implies that

$$L^{T} = (D^{T}R^{-1}D)^{T} = D^{T}R^{-1}D = L$$

Here we used that $D^{TT} = D$ and that R^{-1} , being a diagonal matrix, satisfies $R^{-1T} = R^{-1}$.

Let's determine the entries of L. To start we consider the case where all the resistances have the same value 1 so that $R = R^{-1} = I$. In this case $L = D^T D$. Let's start with the example graph above. Then

$$L = \begin{bmatrix} -1 & 0 & 0 & 0 & 1 \\ 1 & -1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 & -1 \end{bmatrix} \begin{bmatrix} -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix}$$

Notice that the *i*th diagonal entry is the total number of edges connected to the *i*th node. The i, j entry is -1 if the *i*th node is connected to the *j*th node, and 0 otherwise.

This pattern describes the Laplacian L for any graph. To see this, write

$$D = [\mathbf{d}_1 | \mathbf{d}_2 | \mathbf{d}_3 | \cdots | \mathbf{d}_m]$$

Then the i, j entry of D^TD is $\mathbf{d}_i^T\mathbf{d}_j$. Recall that \mathbf{d}_i has an entry of -1 for every edge leaving the ith node, and a 1 for every edge coming in. So $\mathbf{d}_i^T\mathbf{d}_i$, the diagonal entries of D^TD , are the sum of $(\pm 1)^2$, with one term for each edge connected to the ith node. This sum gives the total number of edges connected to the ith node. To see this in the example graph, let's consider the first node. This node has two edges connected to it and

$$\mathbf{d}_1 = \begin{bmatrix} -1\\0\\0\\0\\1 \end{bmatrix}$$

Thus the 1,1 entry of the Laplacian is

$$\mathbf{d}_1^T \mathbf{d}_1 = (-1)^2 + 1^2 = 2$$

On the other hand, if $i \neq j$ then the vectors \mathbf{d}_i and \mathbf{d}_j have a non-zero entry in the same position only if one of the edges leaving the *i*th node is coming in to the *j*th node or vice versa. For a graph with at most one edge connecting any two nodes (we usually assume this) this means that $\mathbf{d}_i^T \mathbf{d}_j$ will equal -1 if the *i*th and *j*th nodes are connected by an edge, and zero otherwise. For example, in the graph above the first edge leaves the first node, so that \mathbf{d}_1 has a -1 in the first position. This first edge comes in to the second node so \mathbf{d}_2 has a +1 in the first position. Otherwise, there is no overlap in these vectors, since no other edges touch both these nodes. Thus

$$\mathbf{d}_{1}^{T}\mathbf{d}_{2} = \begin{bmatrix} -1 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -1 \\ 0 \\ -1 \\ 0 \end{bmatrix} = -1$$

What happens if the resistances are not all equal to one? In this case we must replace D with $R^{-1}D$ in the calculation above. This multiplies the kth row of D with $\gamma_k = 1/R_k$. Making this change in the calculations above leads to the following prescription for calculating the entries of L. The diagonal entries are given by

$$L_{i,i} = \sum_{k} \gamma_k$$

Where the sum goes over all edges touching the ith node. When $i \neq j$ then

$$L_{i,j} = \begin{cases} -\gamma_k & \text{if nodes } i \text{ and } j \text{ are connected with edge } k \\ 0 & \text{if nodes } i \text{ and } j \text{ are not connected} \end{cases}$$

II.3.9. Kirchhoff's law and the null space of L

Kirchhoff's law states that currents cannot build up at any node. If \mathbf{v} is the voltage vector for a circuit, then we saw that $L\mathbf{v}$ is the vector whose *i*th entry is the total current building up at the *i*th node. Thus, for an isolated circuit that is not hooked up to any batteries, Kirchhoff's law can be written as

$$L\mathbf{v} = \mathbf{0}$$

By definition, the solutions are exactly the vectors in the nullspace N(L) of L. It turns out that N(L) is the same as N(D), which contains all constant voltage vectors. This is what we should expect. If there are no batteries connected to the circuit the voltage will be the same everywhere and no current will flow.

To see N(L) = N(D) we start with a vector $\mathbf{v} \in N(D)$. Then $D\mathbf{v} = \mathbf{0}$ implies $L\mathbf{v} = D^T R^{-1}D\mathbf{v} = D^T R^{-1}\mathbf{0} = \mathbf{0}$. This show that $\mathbf{v} \in N(L)$ too, that is, $N(D) \subseteq N(L)$

To show the opposite inclusion we first note that the matrix R^{-1} can be factored into a product of invertible matrices $R^{-1} = R^{-1/2}R^{-1/2}$ where $R^{-1/2}$ is the diagonal matrix with diagonal entries $1/\sqrt{R_i}$. This is possible because each R_i is a positive number. Also, since $R^{-1/2}$ is a diagonal matrix it is equal to its transpose, that is, $R^{-1/2} = (R^{-1/2})^T$.

Now suppose that $L\mathbf{v} = \mathbf{0}$. This can be written $D^T(R^{-1/2})^T R^{-1/2} D\mathbf{v} = \mathbf{0}$. Now we multiply on the left with \mathbf{v}^T . This gives

$$\mathbf{v}^T D^T (R^{-1/2})^T R^{-1/2} D \mathbf{v} = (R^{-1/2} D \mathbf{v})^T R^{-1/2} D \mathbf{v} = 0$$

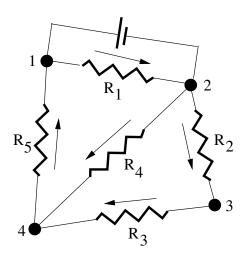
But for any vector \mathbf{w} , the number $\mathbf{w}^T\mathbf{w}$ is the dot product of \mathbf{w} with itself which is equal to the length of \mathbf{w} squared. Thus the equation above can be written

$$||R^{-1/2}D\mathbf{v}||^2 = 0$$

This implies that $R^{-1/2}D\mathbf{v} = \mathbf{0}$. Finally, since $R^{-1/2}$ is invertible, this yields $D\mathbf{v} = \mathbf{0}$. We have shown that any vector in N(L) also is contained in N(D). Thus $N(L) \subseteq N(D)$ and together with the previous inclusion this yields N(L) = N(D).

II.3.10. Connecting a battery

To see more interesting behaviour in a circuit, we pick two nodes and connect them to a battery. For example, let's take our example circuit above and connect the nodes 1 and 2.



The terminals of a battery are kept at a fixed voltage. Thus the voltages v_1 and v_2 are now known, say,

$$v_1 = b_1$$
$$v_2 = b_2$$

Of course, it is only voltage differences that have physical meaning, so we could set $b_1 = 0$. Then b_2 would be the voltage of the battery.

At the first and second nodes there now will be current flowing in and out from the battery. Let's call these currents J_1 and J_2 . At all the other nodes the total current flowing in and out is still zero, as before.

How are the equations for the circuit modified? For simplicity let's set all the resistances $R_i = 1$. The new equations are

$$\begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} J_1 \\ J_2 \\ 0 \\ 0 \end{bmatrix}$$

Two of the voltages v_1 and v_2 have changed their role in these equations from being unknowns to being knowns. On the other hand, the first two currents, which were originally known quantities (namely zero) are now unknowns.

Since the current flowing into the network should equal the current flowing out, we expect that

 $J_1 = -J_2$. This follows from the orthogonality relations for L. The vector $\begin{bmatrix} J_1 \\ J_2 \\ 0 \\ 0 \end{bmatrix}$ is contained in

R(L). But $R(L) = N(L^T)^{\perp} = N(L)^{\perp}$ (since $L = L^T$). But we know that N(L) consists of all constant vectors. Hence

$$\begin{bmatrix} J_1 \\ J_2 \\ 0 \\ 0 \end{bmatrix} \cdot \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = J_1 + J_2 = 0$$

To solve this system of equations we write it in block matrix form

$$\begin{bmatrix} A & B^T \\ B & C \end{bmatrix} \begin{bmatrix} \mathbf{b} \\ \mathbf{v} \end{bmatrix} = \begin{bmatrix} \mathbf{J} \\ \mathbf{0} \end{bmatrix}$$

where

$$A = \begin{bmatrix} 2 & -1 \\ -1 & 3 \end{bmatrix} \quad B = \begin{bmatrix} 0 & -1 \\ -1 & -1 \end{bmatrix} \quad C = \begin{bmatrix} 2 & -1 \\ -1 & 3 \end{bmatrix}$$

and

$$\mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \quad \mathbf{v} = \begin{bmatrix} v_3 \\ v_4 \end{bmatrix} \quad \mathbf{J} = \begin{bmatrix} J_1 \\ J_2 \end{bmatrix} \quad \mathbf{0} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Our system of equations can then be written as two 2×2 systems.

$$A\mathbf{b} + B^T \mathbf{v} = \mathbf{J}$$
$$B\mathbf{b} + C\mathbf{v} = \mathbf{0}$$

We can solve the second equation for \mathbf{v} . Since C is invertible

$$\mathbf{v} = -C^{-1}B\mathbf{b}$$

Using this value of \mathbf{v} in the first equation yields

$$\mathbf{J} = (A - B^T C^{-1} B) \mathbf{b}$$

The matrix $A-B^TC^{-1}B$ is the voltage-to-current map. In our example

$$A - B^T C^{-1} B = (8/5) \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

In fact, for any circuit the voltage to current map is given by

$$A - B^T C^{-1} B = \gamma \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

This can be deduced from two facts: (i) $A - B^T C^{-1} B$ is symmetric and (ii) $R(A - B^T C^{-1} B) = \operatorname{span} \left(\begin{bmatrix} 1 \\ -1 \end{bmatrix} \right)$. You are asked to carry this out in a homework problem.

Notice that this form of the matrix implies that if $b_1 = b_2$ then the currents are zero. Another way of seeing this is to notice that if $b_1 = b_2$ then $\begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$ is orthogonal to the range of $A - B^T C^{-1} B$ by (ii) and hence in the nullspace $N(A - B^T C^{-1} B)$.

The number

$$R = \frac{1}{\gamma}$$

is the ratio of the applied voltage to the resulting current, is the effective resistance of the network between the two nodes.

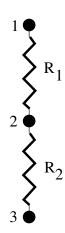
So in our example circuit, the effective resistance between nodes 1 and 2 is 5/8.

If the battery voltages are $b_1 = 0$ and $b_2 = b$ then the voltages at the remaining nodes are

$$\begin{bmatrix} v_3 \\ v_4 \end{bmatrix} = -C^{-1}B \begin{bmatrix} 0 \\ b \end{bmatrix} = \begin{bmatrix} 4/5 \\ 3/5 \end{bmatrix} b$$

II.3.11. Two resistors in series

Let's do a trivial example where we know the answer. If we connect two resistors in series, the resistances add, and the effective resistance is $R_1 + R_2$. The graph for this example looks like



The Laplacian for this circuit is

$$L = \begin{bmatrix} \gamma_1 & -\gamma_1 & 0 \\ -\gamma_1 & \gamma_1 + \gamma_2 & -\gamma_2 \\ 0 & -\gamma_2 & \gamma_2 \end{bmatrix}$$

with $\gamma_i = 1/R_i$, as always. We want the effective resistance between nodes 1 and 3. Although it is not strictly necessary, it is easier to see what the submatrices A, B and C are if we reorder the vertices so that the ones we are connecting, namely 1 and 3, come first. This reshuffles the rows and columns of L yielding

$$\begin{array}{cccc}
1 & 3 & 2 \\
1 & \gamma_1 & 0 & -\gamma_1 \\
3 & \gamma_2 & -\gamma_2 \\
-\gamma_1 & -\gamma_2 & \gamma_1 + \gamma_2
\end{array}$$

Here we have labelled the re-ordered rows and columns with the nodes they represent. Now the desired submatrices are

$$A = \begin{bmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{bmatrix} \quad B = \begin{bmatrix} -\gamma_1 & -\gamma_2 \end{bmatrix} \quad C = \begin{bmatrix} \gamma_1 + \gamma_2 \end{bmatrix}$$

and

$$A - B^T C^{-1} B = \begin{bmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{bmatrix} - \frac{1}{\gamma_1 + \gamma_2} \begin{bmatrix} \gamma_1^2 & \gamma_1 \gamma_2 \\ \gamma_1 \gamma_2 & \gamma_2^2 \end{bmatrix} = \frac{\gamma_1 \gamma_2}{\gamma_1 + \gamma_2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

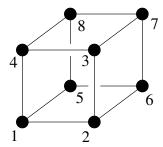
This gives an effective resistance of

$$R = \frac{\gamma_1 + \gamma_2}{\gamma_1 \gamma_2} = \frac{1}{\gamma_1} + \frac{1}{\gamma_2} = R_1 + R_2$$

as expected.

II.3.12. Example: a resistor cube

Hook up resistors along the edges of a cube. If each resistor has resistance $R_i = 1$, what is the effective resistance between opposite corners of the cube?



We will use MATLAB/Octave to solve this problem. To begin we define the Laplace matrix L. Since each node has three edges connecting it, and all the resistances are 1, the diagonal entries are all 3. The off-diagonal entries are -1 or 0, depending on whether the corresponding nodes are connected or not.

```
>L=[3 -1 0 -1 -1 0 0 0; -1 3 -1 0 0 -1 0 0;
0 -1 3 -1 0 0 -1 0; -1 0 -1 3 0 0 0 -1;
-1 0 0 0 3 -1 0 -1; 0 -1 0 0 -1 3 -1 0;
0 0 -1 0 0 -1 3 -1; 0 0 0 -1 -1 0 -1 3];
```

We want to find the effective resistance between 1 and 7. To compute the submatrices A, B and C it is convenient to re-order the nodes so that 1 and 7 come first. In MATLAB/Octave, this can be achieved with the following statement.

```
>L=L([1,7,2:6,8],[1,7,2:6,8]);
```

In this statement the entries in the first bracket [1,7,2:6,8] indicates the new ordering of the rows. Here 2:6 stands for 2,3,4,5,6. The second bracket indicates the re-ordering of the columns, which is the same as for the rows in our case.

Now it is easy to extract the submatrices A, B and C and compute the voltage-to-current map DN

```
>N = length(L);
>A = L(1:2,1:2);
>B = L(3:N,1:2);
>C = L(3:N,3:N);
>DN = A - B'*C^(-1)*B;
```

The effective resistance is the reciprocal of the first entry in DN. The command format rat gives the answer in rational form. (Note: this is just a rational approximation to the floating point answer, not an exact rational arithmetic as in Maple or Mathematica.)

```
>format rat
>R = 1/DN(1,1)
R = 5/6
```