

Linear Algebra Review and Reference

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1 Basic Concepts and Notation

Linear algebra provides a way of compactly representing and operating on sets of linear equations. For example, consider the following system of equations:

$$\begin{array}{rcl} 4x_1 & - & 5x_2 = -13 \\ -2x_1 & + & 3x_2 = 9 \end{array}.$$

This is two equations and two variables, so as you know from high school algebra, you can find a unique solution for x_1 and x_2 (unless the equations are somehow degenerate, for example if the second equation is simply a multiple of the first, but in the case above there is in fact a unique solution). In matrix notation, we can write the system more compactly as:

$$Ax = b$$

with $A = \begin{bmatrix} 4 & -5 \\ -2 & 3 \end{bmatrix}$, $b = \begin{bmatrix} 13 \\ -9 \end{bmatrix}$.

As we will see shortly, there are many advantages (including the obvious space savings) to analyzing linear equations in this form.

1.1 Basic Notation

We use the following notation:

- By $A \in \mathbb{R}^{m \times n}$ we denote a matrix with m rows and n columns, where the entries of A are real numbers.
- By $x \in \mathbb{R}^n$, we denote a vector with n entries. Usually a vector x will denote a **column vector** — i.e., a matrix with n rows and 1 column. If we want to explicitly represent a **row vector** — a matrix with 1 row and n columns — we typically write x^T (here x^T denotes the transpose of x , which we will define shortly).

- The i th element of a vector x is denoted x_i :

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}.$$

- We use the notation a_{ij} (or A_{ij} , $A_{i,j}$, etc) to denote the entry of A in the i th row and j th column:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}.$$

- We denote the j th column of A by a_j or $A_{:,j}$:

$$A = \begin{bmatrix} | & | & \cdots & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & \cdots & | \end{bmatrix}.$$

- We denote the i th row of A by a_i^T or $A_{i,:}$:

$$A = \begin{bmatrix} - & a_1^T & - \\ - & a_2^T & - \\ & \vdots & \\ - & a_m^T & - \end{bmatrix}.$$

- Note that these definitions are ambiguous (for example, the a_1 and a_1^T in the previous two definitions are *not* the same vector). Usually the meaning of the notation should be obvious from its use.

2 Matrix Multiplication

The product of two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$ is the matrix

$$C = AB \in \mathbb{R}^{m \times p},$$

where

$$C_{ij} = \sum_{k=1}^n A_{ik} B_{kj}.$$

Note that in order for the matrix product to exist, the number of columns in A must equal the number of rows in B . There are many ways of looking at matrix multiplication, and we'll start by examining a few special cases.

2.1 Vector-Vector Products

Given two vectors $x, y \in \mathbb{R}^n$, the quantity $x^T y$, sometimes called the **inner product** or **dot product** of the vectors, is a real number given by

$$x^T y \in \mathbb{R} = \sum_{i=1}^n x_i y_i.$$

Note that it is always the case that $x^T y = y^T x$.

Given vectors $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ (they no longer have to be the same size), xy^T is called the **outer product** of the vectors. It is a matrix whose entries are given by $(xy^T)_{ij} = x_i y_j$, i.e.,

$$xy^T \in \mathbb{R}^{m \times n} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & \cdots & x_1 y_n \\ x_2 y_1 & x_2 y_2 & \cdots & x_2 y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_m y_1 & x_m y_2 & \cdots & x_m y_n \end{bmatrix}.$$

2.2 Matrix-Vector Products

Given a matrix $A \in \mathbb{R}^{m \times n}$ and a vector $x \in \mathbb{R}^n$, their product is a vector $y = Ax \in \mathbb{R}^m$. There are a couple ways of looking at matrix-vector multiplication, and we will look at them both.

If we write A by rows, then we can express Ax as,

$$y = \begin{bmatrix} - & a_1^T & - \\ - & a_2^T & - \\ & \vdots & \\ - & a_m^T & - \end{bmatrix} x = \begin{bmatrix} a_1^T x \\ a_2^T x \\ \vdots \\ a_m^T x \end{bmatrix}.$$

In other words, the i th entry of y is equal to the inner product of the i th row of A and x , $y_i = a_i^T x$.

Alternatively, let's write A in column form. In this case we see that,

$$y = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} a_1 \end{bmatrix} x_1 + \begin{bmatrix} a_2 \end{bmatrix} x_2 + \cdots + \begin{bmatrix} a_n \end{bmatrix} x_n.$$

In other words, y is a **linear combination** of the columns of A , where the coefficients of the linear combination are given by the entries of x .

So far we have been multiplying on the right by a column vector, but it is also possible to multiply on the left by a row vector. This is written, $y^T = x^T A$ for $A \in \mathbb{R}^{m \times n}$, $x \in \mathbb{R}^m$, and $y \in \mathbb{R}^n$. As before, we can express y^T in two obvious ways, depending on whether we

express A in terms on its rows or columns. In the first case we express A in terms of its columns, which gives

$$y^T = x^T \begin{bmatrix} | & | & \cdots & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & \cdots & | \end{bmatrix} = [x^T a_1 \quad x^T a_2 \quad \cdots \quad x^T a_n]$$

which demonstrates that the i th entry of y^T is equal to the inner product of x and the i th *column* of A .

Finally, expressing A in terms of rows we get the final representation of the vector-matrix product,

$$\begin{aligned} y^T &= [x_1 \quad x_2 \quad \cdots \quad x_n] \begin{bmatrix} - & a_1^T & - \\ - & a_2^T & - \\ & \vdots & \\ - & a_m^T & - \end{bmatrix} \\ &= x_1 [- \quad a_1^T \quad -] + x_2 [- \quad a_2^T \quad -] + \dots + x_n [- \quad a_n^T \quad -] \end{aligned}$$

so we see that y^T is a linear combination of the *rows* of A , where the coefficients for the linear combination are given by the entries of x .

2.3 Matrix-Matrix Products

Armed with this knowledge, we can now look at four different (but, of course, equivalent) ways of viewing the matrix-matrix multiplication $C = AB$ as defined at the beginning of this section. First we can view matrix-matrix multiplication as a set of vector-vector products. The most obvious viewpoint, which follows immediately from the definition, is that the i, j entry of C is equal to the inner product of the i th row of A and the j th row of B . Symbolically, this looks like the following,

$$C = AB = \begin{bmatrix} - & a_1^T & - \\ - & a_2^T & - \\ & \vdots & \\ - & a_m^T & - \end{bmatrix} \begin{bmatrix} | & | & \cdots & | \\ b_1 & b_2 & \cdots & b_p \\ | & | & \cdots & | \end{bmatrix} = \begin{bmatrix} a_1^T b_1 & a_1^T b_2 & \cdots & a_1^T b_p \\ a_2^T b_1 & a_2^T b_2 & \cdots & a_2^T b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^T b_1 & a_m^T b_2 & \cdots & a_m^T b_p \end{bmatrix}.$$

Remember that since $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$, $a_i \in \mathbb{R}^n$ and $b_j \in \mathbb{R}^n$, so these inner products all make sense. This is the most “natural” representation when we represent A by rows and B by columns. Alternatively, we can represent A by columns, and B by rows, which leads to the interpretation of AB as a sum of outer products. Symbolically,

$$C = AB = \begin{bmatrix} | & | & \cdots & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & \cdots & | \end{bmatrix} \begin{bmatrix} - & b_1^T & - \\ - & b_2^T & - \\ & \vdots & \\ - & b_n^T & - \end{bmatrix} = \sum_{i=1}^n a_i b_i^T.$$

Put another way, AB is equal to the sum, over all i , of the outer product of the i th column of A and the i th row of B . Since, in this case, $a_i \in \mathbb{R}^m$ and $b_i \in \mathbb{R}^p$, the dimension of the outer product $a_i b_i^T$ is $m \times p$, which coincides with the dimension of C .

Second, we can also view matrix-matrix multiplication as a set of matrix-vector products. Specifically, if we represent B by columns, we can view the columns of C as matrix-vector products between A and the columns of B . Symbolically,

$$C = AB = A \begin{bmatrix} | & | & \cdots & | \\ b_1 & b_2 & \cdots & b_p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & \cdots & | \\ Ab_1 & Ab_2 & \cdots & Ab_p \\ | & | & & | \end{bmatrix}.$$

Here the i th column of C is given by the matrix-vector product with the vector on the right, $c_i = Ab_i$. These matrix-vector products can in turn be interpreted using both viewpoints given in the previous subsection. Finally, we have the analogous viewpoint, where we represent A by rows, and view the rows of C as the matrix-vector product between the rows of A and C . Symbolically,

$$C = AB = \begin{bmatrix} - & a_1^T & - \\ - & a_2^T & - \\ & \vdots & \\ - & a_m^T & - \end{bmatrix} B = \begin{bmatrix} - & a_1^T B & - \\ - & a_2^T B & - \\ & \vdots & \\ - & a_m^T B & - \end{bmatrix}.$$

Here the i th row of C is given by the matrix-vector product with the vector on the left, $c_i^T = a_i^T B$.

It may seem like overkill to dissect matrix multiplication to such a large degree, especially when all these viewpoints follow immediately from the initial definition we gave (in about a line of math) at the beginning of this section. However, virtually all of linear algebra deals with matrix multiplications of some kind, and it is worthwhile to spend some time trying to develop an intuitive understanding of the viewpoints presented here.

In addition to this, it is useful to know a few basic properties of matrix multiplication at a higher level:

- Matrix multiplication is associative: $(AB)C = A(BC)$.
- Matrix multiplication is distributive: $A(B + C) = AB + AC$.
- Matrix multiplication is, in general, *not* commutative; that is, it can be the case that $AB \neq BA$.

3 Operations and Properties

In this section we present several operations and properties of matrices and vectors. Hopefully a great deal of this will be review for you, so the notes can just serve as a reference for these topics.

3.1 The Identity Matrix and Diagonal Matrices

The **identity matrix**, denoted $I \in \mathbb{R}^{n \times n}$, is a square matrix with ones on the diagonal and zeros everywhere else. That is,

$$I_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

It has the property that for all $A \in \mathbb{R}^{m \times n}$,

$$AI = A = IA$$

where the size of I is determined by the dimensions of A so that matrix multiplication is possible.

A **diagonal matrix** is a matrix where all non-diagonal elements are 0. This is typically denoted $D = \text{diag}(d_1, d_2, \dots, d_n)$, with

$$D_{ij} = \begin{cases} d_i & i = j \\ 0 & i \neq j \end{cases}$$

Clearly, $I = \text{diag}(1, 1, \dots, 1)$.

3.2 The Transpose

The **transpose** of a matrix results from “flipping” the rows and columns. Given a matrix $A \in \mathbb{R}^{m \times n}$, its transpose, written A^T , is defined as

$$A^T \in \mathbb{R}^{n \times m}, (A^T)_{ij} = A_{ji}.$$

We have in fact already been using the transpose when describing row vectors, since the transpose of a column vector is naturally a row vector.

The following properties of transposes are easily verified:

- $(A^T)^T = A$
- $(AB)^T = B^T A^T$
- $(A + B)^T = A^T + B^T$

3.3 Symmetric Matrices

A square matrix $A \in \mathbb{R}^{n \times n}$ is **symmetric** if $A = A^T$. It is **anti-symmetric** if $A = -A^T$. It is easy to show that for any matrix $A \in \mathbb{R}^{n \times n}$, the matrix $A + A^T$ is symmetric and the matrix $A - A^T$ is anti-symmetric. From this it follows that any square matrix $A \in \mathbb{R}^{n \times n}$ can be represented as a sum of a symmetric matrix and an anti-symmetric matrix, since

$$A = \frac{1}{2}(A + A^T) + \frac{1}{2}(A - A^T)$$

and the first matrix on the right is symmetric, while the second is anti-symmetric. It turns out that symmetric matrices occur a great deal in practice, and they have many nice properties which we will look at shortly. It is common to denote the set of all symmetric matrices of size n as \mathbb{S}^n , so that $A \in \mathbb{S}^n$ means that A is a symmetric $n \times n$ matrix;

3.4 The Trace

The **trace** of a square matrix $A \in \mathbb{R}^{n \times n}$, denoted $\text{tr}(A)$ (or just $\text{tr}A$ if the parentheses are obviously implied), is the sum of diagonal elements in the matrix:

$$\text{tr}A = \sum_{i=1}^n A_{ii}.$$

As described in the CS229 lecture notes, the trace has the following properties (included here for the sake of completeness):

- For $A \in \mathbb{R}^{n \times n}$, $\text{tr}A = \text{tr}A^T$.
- For $A, B \in \mathbb{R}^{n \times n}$, $\text{tr}(A + B) = \text{tr}A + \text{tr}B$.
- For $A \in \mathbb{R}^{n \times n}$, $t \in \mathbb{R}$, $\text{tr}(tA) = t \text{tr}A$.
- For A, B such that AB is square, $\text{tr}AB = \text{tr}BA$.
- For A, B, C such that ABC is square, $\text{tr}ABC = \text{tr}BCA = \text{tr}CAB$, and so on for the product of more matrices.

3.5 Norms

A **norm** of a vector $\|x\|$ is informally measure of the “length” of the vector. For example, we have the commonly-used Euclidean or ℓ_2 norm,

$$\|x\|_2 = \sqrt{\sum_{i=1}^n x_i^2}.$$

Note that $\|x\|_2^2 = x^T x$.

More formally, a norm is any function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ that satisfies 4 properties:

1. For all $x \in \mathbb{R}^n$, $f(x) \geq 0$ (non-negativity).
2. $f(x) = 0$ if and only if $x = 0$ (definiteness).
3. For all $x \in \mathbb{R}^n$, $t \in \mathbb{R}$, $f(tx) = |t|f(x)$ (homogeneity).
4. For all $x, y \in \mathbb{R}^n$, $f(x + y) \leq f(x) + f(y)$ (triangle inequality).

Other examples of norms are the ℓ_1 norm,

$$\|x\|_1 = \sum_{i=1}^n |x_i|$$

and the ℓ_∞ norm,

$$\|x\|_\infty = \max_i |x_i|.$$

In fact, all three norms presented so far are examples of the family of ℓ_p norms, which are parameterized by a real number $p \geq 1$, and defined as

$$\|x\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}.$$

Norms can also be defined for matrices, such as the Frobenius norm,

$$\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n A_{ij}^2} = \sqrt{\text{tr}(A^T A)}.$$

Many other norms exist, but they are beyond the scope of this review.

3.6 Linear Independence and Rank

A set of vectors $\{x_1, x_2, \dots, x_n\}$ is said to be **(linearly) independent** if no vector can be represented as a linear combination of the remaining vectors. Conversely, a vector which *can* be represented as a linear combination of the remaining vectors is said to be **(linearly) dependent**. For example, if

$$x_n = \sum_{i=1}^{n-1} \alpha_i x_i$$

for some $\{\alpha_1, \dots, \alpha_{n-1}\}$ then x_n is dependent on $\{x_1, \dots, x_{n-1}\}$; otherwise, it is independent of $\{x_1, \dots, x_{n-1}\}$.

The **column rank** of a matrix A is the largest number of columns of A that constitute linearly independent set. This is often referred to simply as the number of linearly independent columns, but this terminology is a little sloppy, since it is possible that any vector in some set $\{x_1, \dots, x_n\}$ can be expressed as a linear combination of the remaining vectors, even though some subset of the vectors might be independent. In the same way, the **row rank** is the largest number of rows of A that constitute a linearly independent set.

It is a basic fact of linear algebra, that for any matrix A , $\text{columnrank}(A) = \text{rowrank}(A)$, and so this quantity is simply referred to as the **rank** of A , denoted as $\text{rank}(A)$. The following are some basic properties of the rank:

- For $A \in \mathbb{R}^{m \times n}$, $\text{rank}(A) \leq \min(m, n)$. If $\text{rank}(A) = \min(m, n)$, then A is said to be **full rank**.

- For $A \in \mathbb{R}^{m \times n}$, $\text{rank}(A) = \text{rank}(A^T)$.
- For $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$, $\text{rank}(AB) \leq \min(\text{rank}(A), \text{rank}(B))$.
- For $A, B \in \mathbb{R}^{m \times n}$, $\text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B)$.

3.7 The Inverse

The *inverse* of a square matrix $A \in \mathbb{R}^{n \times n}$ is denoted A^{-1} , and is the unique matrix such that

$$A^{-1}A = I = AA^{-1}.$$

It turns out that A^{-1} may not exist for some matrices A ; we say A is *invertible* or *non-singular* if A^{-1} exists and *non-invertible* or *singular* otherwise. One condition for invertibility we already know: it is possible to show that A^{-1} exists if and only if A is full rank. We will soon see that there are many alternative sufficient and necessary conditions, in addition to full rank, for invertibility. The following are properties of the inverse; all assume that $A, B \in \mathbb{R}^{n \times n}$ are non-singular:

- $(A^{-1})^{-1} = A$
- If $Ax = b$, we can multiply by A^{-1} on both sides to obtain $x = A^{-1}b$. This demonstrates the inverse with respect to the original system of linear equalities we began this review with.
- $(AB)^{-1} = B^{-1}A^{-1}$
- $(A^{-1})^T = (A^T)^{-1}$. For this reason this matrix is often denoted A^{-T} .

3.8 Orthogonal Matrices

Two vectors $x, y \in \mathbb{R}^n$ are *orthogonal* if $x^T y = 0$. A vector $x \in \mathbb{R}^n$ is *normalized* if $\|x\|_2 = 1$. A square matrix $U \in \mathbb{R}^{n \times n}$ is *orthogonal* (note the different meanings when talking about vectors versus matrices) if all its columns are orthogonal to each other and are normalized (the columns are then referred to as being *orthonormal*).

It follows immediately from the definition of orthogonality and normality that

$$U^T U = I = U U^T.$$

In other words, the inverse of an orthogonal matrix is its transpose. Note that if U is not square — i.e., $U \in \mathbb{R}^{m \times n}$, $n < m$ — but its columns are still orthonormal, then $U^T U = I$, but $U U^T \neq I$. We generally only use the term orthogonal to describe the previous case, where U is square.

Another nice property of orthogonal matrices is that operating on a vector with an orthogonal matrix will not change its Euclidean norm, i.e.,

$$\|Ux\|_2 = \|x\|_2$$

for any $x \in \mathbb{R}^n$, $U \in \mathbb{R}^{n \times n}$ orthogonal.

3.9 Range and Nullspace of a Matrix

The **span** of a set of vectors $\{x_1, x_2, \dots, x_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{x_1, \dots, x_n\}$. That is,

$$\text{span}(\{x_1, \dots, x_n\}) = \left\{ v : v = \sum_{i=1}^n \alpha_i x_i, \alpha_i \in \mathbb{R} \right\}.$$

It can be shown that if $\{x_1, \dots, x_n\}$ is a set of n linearly independent vectors, where each $x_i \in \mathbb{R}^n$, then $\text{span}(\{x_1, \dots, x_n\}) = \mathbb{R}^n$. In other words, *any* vector $v \in \mathbb{R}^n$ can be written as a linear combination of x_1 through x_n . The **projection** of a vector $y \in \mathbb{R}^m$ onto the span of $\{x_1, \dots, x_n\}$ (here we assume $x_i \in \mathbb{R}^m$) is the vector $v \in \text{span}(\{x_1, \dots, x_n\})$, such that v as close as possible to y , as measured by the Euclidean norm $\|v - y\|_2$. We denote the projection as $\text{Proj}(y; \{x_1, \dots, x_n\})$ and can define it formally as,

$$\text{Proj}(y; \{x_1, \dots, x_n\}) = \underset{v \in \text{span}(\{x_1, \dots, x_n\})}{\text{argmin}} \|y - v\|_2.$$

The **range** (sometimes also called the columnspace) of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{R}(A)$, is the the span of the columns of A . In other words,

$$\mathcal{R}(A) = \{v \in \mathbb{R}^m : v = Ax, x \in \mathbb{R}^n\}.$$

Making a few technical assumptions (namely that A is full rank and that $n < m$), the projection of a vector $y \in \mathbb{R}^m$ onto the range of A is given by,

$$\text{Proj}(y; A) = \underset{v \in \mathcal{R}(A)}{\text{argmin}} \|v - y\|_2 = A(A^T A)^{-1} A^T y.$$

This last equation should look extremely familiar, since it is almost the same formula we derived in class (and which we will soon derive again) for the least squares estimation of parameters. Looking at the definition for the projection, it should not be too hard to convince yourself that this is in fact the same objective that we minimized in our least squares problem (except for a squaring of the norm, which doesn't affect the optimal point) and so these problems are naturally very connected. When A contains only a single column, $a \in \mathbb{R}^m$, this gives the special case for a projection of a vector on to a line:

$$\text{Proj}(y; a) = \frac{aa^T}{a^T a} y.$$

The **nullspace** of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{N}(A)$ is the set of all vectors that equal 0 when multiplied by A , i.e.,

$$\mathcal{N}(A) = \{x \in \mathbb{R}^n : Ax = 0\}.$$

Note that vectors in $\mathcal{R}(A)$ are of size m , while vectors in the $\mathcal{N}(A)$ are of size n , so vectors in $\mathcal{R}(A^T)$ and $\mathcal{N}(A)$ are both in \mathbb{R}^n . In fact, we can say much more. It turns out that

$$\{w : w = u + v, u \in \mathcal{R}(A^T), v \in \mathcal{N}(A)\} = \mathbb{R}^n \text{ and } \mathcal{R}(A^T) \cap \mathcal{N}(A) = \emptyset.$$

In other words, $\mathcal{R}(A^T)$ and $\mathcal{N}(A)$ are disjoint subsets that together span the entire space of \mathbb{R}^n . Sets of this type are called **orthogonal complements**, and we denote this $\mathcal{R}(A^T) = \mathcal{N}(A)^\perp$.

3.10 The Determinant

The **determinant** of a square matrix $A \in \mathbb{R}^{n \times n}$, is a function $\det : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$, and is denoted $|A|$ or $\det A$ (like the trace operator, we usually omit parentheses). The full formula for the determinant gives little intuition about its meaning, so we instead first give three defining properties of the determinant, from which all the rest follow (including the general formula):

1. The determinant of the identity is 1, $|I| = 1$.
2. Given a matrix $A \in \mathbb{R}^{n \times n}$, if we multiply a single row in A by a scalar $t \in \mathbb{R}$, then the determinant of the new matrix is $t|A|$,

$$\left| \begin{bmatrix} - & t a_1^T & - \\ - & a_2^T & - \\ & \vdots & \\ - & a_m^T & - \end{bmatrix} \right| = t|A| \quad .$$

3. If we exchange any two rows a_i^T and a_j^T of A , then the determinant of the new matrix is $-|A|$, for example

$$\left| \begin{bmatrix} - & a_2^T & - \\ - & a_1^T & - \\ & \vdots & \\ - & a_m^T & - \end{bmatrix} \right| = -|A| \quad .$$

These properties, however, also give very little intuition about the nature of the determinant, so we now list several properties that follow from the three properties above:

- For $A \in \mathbb{R}^{n \times n}$, $|A| = |A^T|$.
- For $A, B \in \mathbb{R}^{n \times n}$, $|AB| = |A||B|$.
- For $A \in \mathbb{R}^{n \times n}$, $|A| = 0$ if and only if A is singular (i.e., non-invertible).
- For $A \in \mathbb{R}^{n \times n}$ and A non-singular, $|A|^{-1} = 1/|A|$.

Before given the general definition for the determinant, we define, for $A \in \mathbb{R}^{n \times n}$, $A_{\setminus i, \setminus j} \in \mathbb{R}^{(n-1) \times (n-1)}$ to be the *matrix* that results from deleting the i th row and j th column from A . The general (recursive) formula for the determinant is

$$\begin{aligned} |A| &= \sum_{i=1}^n (-1)^{i+j} a_{ij} |A_{\setminus i, \setminus j}| \quad (\text{for any } j \in 1, \dots, n) \\ &= \sum_{j=1}^n (-1)^{i+j} a_{ij} |A_{\setminus i, \setminus j}| \quad (\text{for any } i \in 1, \dots, n) \end{aligned}$$

with the initial case that $|A| = a_{11}$ for $A \in \mathbb{R}^{1 \times 1}$. If we were to expand this formula completely for $A \in \mathbb{R}^{n \times n}$, there would be a total of $n!$ (n factorial) different terms. For this reason, we hardly even explicitly write the complete equation of the determinant for matrices bigger than 3×3 . However, the equations for determinants of matrices up to size 3×3 are fairly common, and it is good to know them:

$$\begin{aligned} |[a_{11}]| &= a_{11} \\ \left| \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \right| &= a_{11}a_{22} - a_{12}a_{21} \\ \left| \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \right| &= a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} \\ &\quad - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} - a_{13}a_{22}a_{31} \end{aligned}$$

The **classical adjoint** (often just called the adjoint) of a matrix $A \in \mathbb{R}^{n \times n}$, is denoted $\text{adj}(A)$, and defined as

$$\text{adj}(A) \in \mathbb{R}^{n \times n}, \quad (\text{adj}(A))_{ij} = (-1)^{i+j} |A_{\setminus j, \setminus i}|$$

(note the switch in the indices $A_{\setminus j, \setminus i}$). It can be shown that for any nonsingular $A \in \mathbb{R}^{n \times n}$,

$$A^{-1} = \frac{1}{|A|} \text{adj}(A) .$$

While this is a nice “explicit” formula for the inverse of matrix, we should note that, numerically, there are in fact much more efficient ways of computing the inverse.

3.11 Quadratic Forms and Positive Semidefinite Matrices

Given a matrix square $A \in \mathbb{R}^{n \times n}$ and a vector $x \in \mathbb{R}^n$, the scalar value $x^T A x$ is called a **quadratic form**. Written explicitly, we see that

$$x^T A x = \sum_{i=1}^n \sum_{j=1}^n A_{ij} x_i x_j .$$

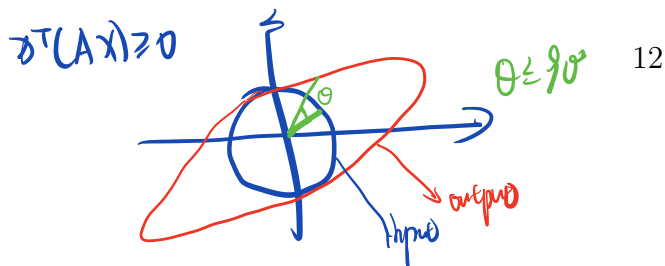
Note that,

$$x^T A x = (x^T A x)^T = x^T A^T x = x^T \left(\frac{1}{2} A + \frac{1}{2} A^T \right) x$$

i.e., only the symmetric part of A contributes to the quadratic form. For this reason, we often implicitly assume that the matrices appearing in a quadratic form are symmetric.

We give the following definitions:

- A symmetric matrix $A \in \mathbb{S}^n$ is **positive definite** (PD) if for all non-zero vectors $x \in \mathbb{R}^n$, $x^T A x > 0$. This is usually denoted $A \succ 0$ (or just $A > 0$), and often times the set of all positive definite matrices is denoted \mathbb{S}_{++}^n .



- A symmetric matrix $A \in \mathbb{S}^n$ is **positive semidefinite** (PSD) if for all vectors $x^T Ax \geq 0$. This is written $A \succeq 0$ (or just $A \geq 0$), and the set of all positive semidefinite matrices is often denoted \mathbb{S}_+^n .
- Likewise, a symmetric matrix $A \in \mathbb{S}^n$ is **negative definite** (ND), denoted $A \prec 0$ (or just $A < 0$) if for all non-zero $x \in \mathbb{R}^n$, $x^T Ax < 0$.
- Similarly, a symmetric matrix $A \in \mathbb{S}^n$ is **negative semidefinite** (NSD), denoted $A \preceq 0$ (or just $A \leq 0$) if for all $x \in \mathbb{R}^n$, $x^T Ax \leq 0$.
- Finally, a symmetric matrix $A \in \mathbb{S}^n$ is **indefinite**, if it is neither positive semidefinite nor negative semidefinite — i.e., if there exists $x_1, x_2 \in \mathbb{R}^n$ such that $x_1^T Ax_1 > 0$ and $x_2^T Ax_2 < 0$.

It should be obvious that if A is positive definite, then $-A$ is negative definite and vice versa. Likewise, if A is positive semidefinite then $-A$ is negative semidefinite and vice versa. If A is indefinite, then so is $-A$. It can also be shown that positive definite and negative definite matrices are always invertible.

Finally, there is one type of positive definite matrix that comes up frequently, and so deserves some special mention. Given any matrix $A \in \mathbb{R}^{m \times n}$ (not necessarily symmetric or even square), the matrix $G = A^T A$ (sometimes called a **Gram matrix**) is always positive semidefinite. Further, if $m \geq n$ (and we assume for convenience that A is full rank), then $G = A^T A$ is positive definite.

3.12 Eigenvalues and Eigenvectors

Given a square matrix $A \in \mathbb{R}^{n \times n}$, we say that $\lambda \in \mathbb{C}$ is an **eigenvalue** of A and $x \in \mathbb{C}^n$ is the corresponding **eigenvector**¹ if

$$Ax = \lambda x, \quad x \neq 0.$$

Intuitively, this definition means that multiplying A by the vector x results in a new vector that points in the same direction as x , but scaled by a factor λ . Also note that for any eigenvector $x \in \mathbb{C}^n$, and scalar $t \in \mathbb{C}$, $A(cx) = cAx = c\lambda x = \lambda(cx)$, so cx is also an eigenvector. For this reason when we talk about “the” eigenvector associated with λ , we usually assume that the eigenvector is normalized to have length 1 (this still creates some ambiguity, since x and $-x$ will both be eigenvectors, but we will have to live with this).

We can rewrite the equation above to state that (λ, x) is an eigenvalue-eigenvector pair of A if,

$$(\lambda I - A)x = 0, \quad x \neq 0.$$

¹Note that λ and the entries of x are actually in \mathbb{C} , the set of complex numbers, not just the reals; we will see shortly why this is necessary. Don’t worry about this technicality for now, you can think of complex vectors in the same way as real vectors.

But $(\lambda I - A)x = 0$ has a non-zero solution to x if and only if $(\lambda I - A)$ has a non-empty nullspace, which is only the case if $(\lambda I - A)$ is singular, i.e.,

$$|(\lambda I - A)| = 0 \quad .$$

We can now use the previous definition of the determinant to expand this expression into a (very large) polynomial in λ , where λ will have maximum degree n . We then find the n (possibly complex) roots of this polynomial to find the n eigenvalues $\lambda_1, \dots, \lambda_n$. To find the eigenvector corresponding to the eigenvalue λ_i , we simply solve the linear equation $(\lambda_i I - A)x = 0$. It should be noted that this is not the method which is actually used in practice to numerically compute the eigenvalues and eigenvectors (remember that the complete expansion of the determinant has $n!$ terms); it is rather a mathematical argument.

The following are properties of eigenvalues and eigenvectors (in all cases assume $A \in \mathbb{R}^{n \times n}$ has eigenvalues $\lambda_1, \dots, \lambda_n$ and associated eigenvectors x_1, \dots, x_n):

- The trace of a A is equal to the sum of its eigenvalues,

$$\text{tr} A = \sum_{i=1}^n \lambda_i \quad .$$

- The determinant of A is equal to the product of its eigenvalues,

$$|A| = \prod_{i=1}^n \lambda_i \quad .$$

- The rank of A is equal to the number of non-zero eigenvalues of A .
- If A is non-singular then $1/\lambda_i$ is an eigenvalue of A^{-1} with associated eigenvector x_i , i.e., $A^{-1}x_i = (1/\lambda_i)x_i$.
- The eigenvalues of a diagonal matrix $D = \text{diag}(d_1, \dots, d_n)$ are just the diagonal entries d_1, \dots, d_n .

We can write all the eigenvector equations simultaneously as

$$AX = X\Lambda$$

where the columns of $X \in \mathbb{R}^{n \times n}$ are the eigenvectors of A and Λ is a diagonal matrix whose entries are the eigenvalues of A , i.e.,

$$X \in \mathbb{R}^{n \times n} = \begin{bmatrix} | & | & \cdots & | \\ x_1 & x_2 & \cdots & x_n \\ | & | & & | \end{bmatrix}, \quad \Lambda = \text{diag}(\lambda_1, \dots, \lambda_n) \quad .$$

If the eigenvectors of A are linearly independent, then the matrix X will be invertible, so $A = X\Lambda X^{-1}$. A matrix that can be written in this form is called **diagonalizable**.

3.13 Eigenvalues and Eigenvectors of Symmetric Matrices

Two remarkable properties come about when we look at the eigenvalues and eigenvectors of a symmetric matrix $A \in \mathbb{S}^n$. First, it can be shown that all the eigenvalues of A are real. Secondly, the eigenvectors of A are orthonormal, i.e., the matrix X defined above is an orthogonal matrix (for this reason, we denote the matrix of eigenvectors as U in this case). We can therefore represent A as $A = U\Lambda U^T$, remembering from above that the inverse of an orthogonal matrix is just its transpose.

Using this, we can show that the definiteness of a matrix depends entirely on the sign of its eigenvalues. Suppose $A \in \mathbb{S}^n = U\Lambda U^T$. Then

$$x^T A x = x^T U \Lambda U^T x = y^T \Lambda y = \sum_{i=1}^n \lambda_i y_i^2$$

where $y = U^T x$ (and since U is full rank, any vector $y \in \mathbb{R}^n$ can be represented in this form). Because y_i^2 is always positive, the sign of this expression depends entirely on the λ_i 's. If all $\lambda_i > 0$, then the matrix is positive definite; if all $\lambda_i \geq 0$, it is positive semidefinite. Likewise, if all $\lambda_i < 0$ or $\lambda_i \leq 0$, then A is negative definite or negative semidefinite respectively. Finally, if A has both positive and negative eigenvalues, it is indefinite.

An application where eigenvalues and eigenvectors come up frequently is in maximizing some function of a matrix. In particular, for a matrix $A \in \mathbb{S}^n$, consider the following maximization problem,

$$\max_{x \in \mathbb{R}^n} x^T A x \quad \text{subject to } \|x\|_2^2 = 1$$

i.e., we want to find the vector (of norm 1) which maximizes the quadratic form. Assuming the eigenvalues are ordered as $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$, the optimal x for this optimization problem is x_1 , the eigenvector corresponding to λ_1 . In this case the maximal value of the quadratic form is λ_1 . Similarly, the optimal solution to the minimization problem,

$$\min_{x \in \mathbb{R}^n} x^T A x \quad \text{subject to } \|x\|_2^2 = 1$$

is x_n , the eigenvector corresponding to λ_n , and the minimal value is λ_n . This can be proved by appealing to the eigenvector-eigenvalue form of A and the properties of orthogonal matrices. However, in the next section we will see a way of showing it directly using matrix calculus.

4 Matrix Calculus

While the topics in the previous sections are typically covered in a standard course on linear algebra, one topic that does not seem to be covered very often (and which we will use extensively) is the extension of calculus to the vector setting. Despite the fact that all the actual calculus we use is relatively trivial, the notation can often make things look much more difficult than they are. In this section we present some basic definitions of matrix calculus and provide a few examples.

4.1 The Gradient

Suppose that $f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ is a function that takes as input a matrix A of size $m \times n$ and returns a real value. Then the **gradient** of f (with respect to $A \in \mathbb{R}^{m \times n}$) is the matrix of partial derivatives, defined as:

$$\nabla_A f(A) \in \mathbb{R}^{m \times n} = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \cdots & \frac{\partial f(A)}{\partial A_{1n}} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \cdots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix}$$

i.e., an $m \times n$ matrix with

$$(\nabla_A f(A))_{ij} = \frac{\partial f(A)}{\partial A_{ij}}.$$

Note that the size of $\nabla_A f(A)$ is always the same as the size of A . So if, in particular, A is just a vector $x \in \mathbb{R}^n$,

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}.$$

It is very important to remember that the gradient of a function is *only* defined if the function is real-valued, that is, if it returns a scalar value. We can not, for example, take the gradient of Ax , $A \in \mathbb{R}^{n \times n}$ with respect to x , since this quantity is vector-valued.

It follows directly from the equivalent properties of partial derivatives that:

- $\nabla_x(f(x) + g(x)) = \nabla_x f(x) + \nabla_x g(x)$.
- For $t \in \mathbb{R}$, $\nabla_x(t f(x)) = t \nabla_x f(x)$.

It is a little bit trickier to determine what the proper expression is for $\nabla_x f(Ax)$, $A \in \mathbb{R}^{n \times n}$, but this is doable as well (in fact, you'll have to work this out for a homework problem).

4.2 The Hessian

Suppose that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a function that takes a vector in \mathbb{R}^n and returns a real number. Then the **Hessian** matrix with respect to x , written $\nabla_x^2 f(x)$ or simply as H is the $n \times n$ matrix of partial derivatives,

$$\nabla_x^2 f(x) \in \mathbb{R}^{n \times n} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix}.$$

In other words, $\nabla_x^2 f(x) \in \mathbb{R}^{n \times n}$, with

$$(\nabla_x^2 f(x))_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}.$$

Note that the Hessian is always symmetric, since

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} = \frac{\partial^2 f(x)}{\partial x_j \partial x_i}.$$

Similar to the gradient, the Hessian is defined only when $f(x)$ is real-valued.

It is natural to think of the gradient as the analogue of the first derivative for functions of vectors, and the Hessian as the analogue of the second derivative (and the symbols we use also suggest this relation). This intuition is generally correct, but there are a few caveats to keep in mind.

First, for real-valued functions of one variable $f : \mathbb{R} \rightarrow \mathbb{R}$, it is a basic definition that the second derivative is the derivative of the first derivative, i.e.,

$$\frac{\partial^2 f(x)}{\partial x^2} = \frac{\partial}{\partial x} \frac{\partial}{\partial x} f(x).$$

However, for functions of a vector, the gradient of the function is a vector, and we cannot take the gradient of a vector — i.e.,

$$\nabla_x \nabla_x f(x) = \nabla_x \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}$$

and this expression is not defined. Therefore, it is *not* the case that the Hessian is the gradient of the gradient. However, this is *almost* true, in the following sense: If we look at the i th entry of the gradient $(\nabla_x f(x))_i = \partial f(x)/\partial x_i$, and take the gradient with respect to x we get

$$\nabla_x \frac{\partial f(x)}{\partial x_i} = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_i \partial x_1} \\ \frac{\partial^2 f(x)}{\partial x_i \partial x_2} \\ \vdots \\ \frac{\partial^2 f(x)}{\partial x_i \partial x_n} \end{bmatrix}$$

which is the i th column (or row) of the Hessian. Therefore,

$$\nabla_x^2 f(x) = \begin{bmatrix} \nabla_x(\nabla_x f(x))_1 & \nabla_x(\nabla_x f(x))_2 & \cdots & \nabla_x(\nabla_x f(x))_n \end{bmatrix}.$$

If we don't mind being a little bit sloppy we can say that (essentially) $\nabla_x^2 f(x) = \nabla_x(\nabla_x f(x))^T$, so long as we understand that this really means taking the gradient of each entry of $(\nabla_x f(x))^T$, not the gradient of the whole vector.

Finally, note that while we can take the gradient with respect to a matrix $A \in \mathbb{R}^n$, for the purposes of this class we will only consider taking the Hessian with respect to a vector $x \in \mathbb{R}^n$. This is simply a matter of convenience (and the fact that none of the calculations we do require us to find the Hessian with respect to a matrix), since the Hessian with respect to a matrix would have to represent all the partial derivatives $\partial^2 f(A)/(\partial A_{ij} \partial A_{kl})$, and it is rather cumbersome to represent this as a matrix.

4.3 Gradients and Hessians of Quadratic and Linear Functions

Now let's try to determine the gradient and Hessian matrices for a few simple functions. It should be noted that all the gradients given here are special cases of the gradients given in the CS229 lecture notes.

For $x \in \mathbb{R}^n$, let $f(x) = b^T x$ for some known vector $b \in \mathbb{R}^n$. Then

$$f(x) = \sum_{i=1}^n b_i x_i$$

so

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^n b_i x_i = b_k.$$

From this we can easily see that $\nabla_x b^T x = b$. This should be compared to the analogous situation in single variable calculus, where $\partial/(\partial x) ax = a$.

Now consider the quadratic function $f(x) = x^T A x$ for $A \in \mathbb{S}^n$. Remember that

$$f(x) = \sum_{i=1}^n \sum_{j=1}^n A_{ij} x_i x_j$$

so

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^n \sum_{j=1}^n A_{ij} x_i x_j = \sum_{i=1}^n A_{ik} x_i + \sum_{j=1}^n A_{kj} x_j = 2 \sum_{i=1}^n A_{ki} x_i$$

where the last equality follows since A is symmetric (which we can safely assume, since it is appearing in a quadratic form). Note that the k th entry of $\nabla_x f(x)$ is just the inner product of the k th row of A and x . Therefore, $\nabla_x x^T A x = 2Ax$. Again, this should remind you of the analogous fact in single-variable calculus, that $\partial/(\partial x) ax^2 = 2ax$.

Finally, let's look at the Hessian of the quadratic function $f(x) = x^T A x$ (it should be obvious that the Hessian of a linear function $b^T x$ is zero). This is even easier than determining the gradient of the function, since

$$\frac{\partial^2 f(x)}{\partial x_k \partial x_\ell} = \frac{\partial^2}{\partial x_k \partial x_\ell} \sum_{i=1}^n \sum_{j=1}^n A_{ij} x_i x_j = A_{k\ell} + A_{\ell k} = 2A_{k\ell}.$$

Therefore, it should be clear that $\nabla_x^2 x^T A x = 2A$, which should be entirely expected (and again analogous to the single-variable fact that $\partial^2/(\partial x^2) ax^2 = 2a$).

To recap,

- $\nabla_x b^T x = b$
- $\nabla_x x^T A x = 2Ax$ (if A symmetric)
- $\nabla_x^2 x^T A x = 2A$ (if A symmetric)

4.4 Least Squares

Lets apply the equations we obtained in the last section to derive the least squares equations. Suppose we are given matrices $A \in \mathbb{R}^{m \times n}$ (for simplicity we assume A is full rank) and a vector $b \in \mathbb{R}^m$ such that $b \notin \mathcal{R}(A)$. In this situation we will not be able to find a vector $x \in \mathbb{R}^n$, such that $Ax = b$, so instead we want to find a vector x such that Ax is as close as possible to b , as measured by the square of the Euclidean norm $\|Ax - b\|_2^2$.

Using the fact that $\|x\|_2^2 = x^T x$, we have

$$\begin{aligned}\|Ax - b\|_2^2 &= (Ax - b)^T (Ax - b) \\ &= x^T A^T A x - 2b^T A x + b^T b\end{aligned}$$

Taking the gradient with respect to x we have, and using the properties we derived in the previous section

$$\begin{aligned}\nabla_x (x^T A^T A x - 2b^T A x + b^T b) &= \nabla_x x^T A^T A x - \nabla_x 2b^T A x + \nabla_x b^T b \\ &= 2A^T A x - 2A^T b\end{aligned}$$

Setting this last expression equal to zero and solving for x gives the normal equations

$$x = (A^T A)^{-1} A^T b$$

which is the same as what we derived in class.

4.5 Gradients of the Determinant

Now lets consider a situation where we find the gradient of a function with respect to a matrix, namely for $A \in \mathbb{R}^{n \times n}$, we want to find $\nabla_A |A|$. Recall from our discussion of determinants that

$$|A| = \sum_{i=1}^n (-1)^{i+j} A_{ij} |A_{\setminus i, \setminus j}| \quad (\text{for any } j \in 1, \dots, n)$$

so

$$\frac{\partial}{\partial A_{k\ell}} |A| = \frac{\partial}{\partial A_{k\ell}} \sum_{i=1}^n (-1)^{i+j} A_{ij} |A_{\setminus i, \setminus j}| = (-1)^{k+\ell} |A_{\setminus k, \setminus \ell}| = (\text{adj}(A))_{\ell k}.$$

From this it immediately follows from the properties of the adjoint that

$$\nabla_A |A| = (\text{adj}(A))^T = |A| A^{-T}.$$

preliminary lemma
 $\sum_i \sum_j A_{ij} B_{ji} = \text{trace}(A^T B)$

Now let's consider the function $f : \mathbb{S}_{++}^n \rightarrow \mathbb{R}$, $f(A) = \log |A|$. Note that we have to restrict the domain of f to be the positive definite matrices, since this ensures that $|A| > 0$, so that the log of $|A|$ is a real number. In this case we can use the chain rule (nothing fancy, just the ordinary chain rule from single-variable calculus) to see that

$$\frac{\partial \log |A|}{\partial A_{ij}} = \frac{\partial \log |A|}{\partial |A|} \frac{\partial |A|}{\partial A_{ij}} = \frac{1}{|A|} \frac{\partial |A|}{\partial A_{ij}}.$$

From this it should be obvious that

$$\nabla_A \log |A| = \frac{1}{|A|} \nabla_A |A| = A^{-1}$$

where we can drop the transpose in the last expression because A is symmetric. Note the similarity to the single-valued case, where $\partial/(\partial x) \log x = 1/x$.

4.6 Eigenvalues as Optimization

Finally, we use matrix calculus to solve an optimization problem in a way that leads directly to eigenvalue/eigenvector analysis. Consider the following, equality constrained optimization problem:

$$\max_{x \in \mathbb{R}^n} x^T A x \quad \text{subject to } \|x\|_2^2 = 1$$

for a symmetric matrix $A \in \mathbb{S}^n$. A standard way of solving optimization problems with equality constraints is by forming the **Lagrangian**, an objective function that includes the equality constraints.² The Lagrangian in this case can be given by

$$\mathcal{L}(x, \lambda) = x^T A x - \lambda x^T x$$

where λ is called the Lagrange multiplier associated with the equality constraint. It can be established that for x^* to be an optimal point to the problem, the gradient of the Lagrangian has to be zero at x^* (this is not the only condition, but it is required). That is,

$$\nabla_x \mathcal{L}(x, \lambda) = \nabla_x (x^T A x - \lambda x^T x) = 2A^T x - 2\lambda x = 0.$$

Notice that this is just the linear equation $Ax = \lambda x$. This shows that the only points which can possibly maximize (or minimize) $x^T A x$ assuming $x^T x = 1$ are the eigenvectors of A .

²Don't worry if you haven't seen Lagrangians before, as we will cover them in greater detail later in CS229.