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VECTORS & MATRICES

1. First steps along the path from arrows to vectors.¹ To say (as beginning physicists are commonly taught to do) that “a vector is a quantity that—like an arrow—has associated with it a magnitude and a direction”² is a bit like saying that “an animal is a creature with long ears and a fluffy tail:” rabbits are animals alright, but not all animals are rabbits. Similarly, vector algebra/calculus does provide a natural language for the description and manipulation of the many arrow-like objects directed to our attention by physics and applied mathematics, but pertains usefully also to many objects—such, for example, as polynomials

$$a(x) = a_0 + a_1x + a_2x^2 + \cdots + a_mx^m$$

—that do not bring arrows spontaneously to mind.

The theory of vectors—**linear algebra**—is an abstract (but for the most part not at all difficult) branch of pure mathematics, which should not be identified with any of its individual applications/manifestations. That said, it must be admitted that arrow-like applications to geometry (especially to Euclidean geometry in spaces of two or three dimensions) and kinematics did serve historically to provide an important motivating force³ (the theory of

¹ It is intended that this material will be read in conjunction with Chapter 7 in K. F. Riley, M. P. Hobson & S.I J. Bence, *Mathematical Methods for Physics and Engineering* (2nd edition 2000 2002).

² See, for example, D. Halliday, R. Resnick & J. Walker, *Fundamentals of Physics* (4th edition 1993), page 46; D. C. Giancoli, *Physics for Scientists & Engineers* (3rd edition 2000), page 45.

³ For a wonderful account of the fascinating history of linear algebra, see M. J. Crowe, *A History of Vector Analysis* (1985).

simultaneous linear equations provided another) and does still provide an admirably transparent introduction to the main ideas. It is therefore without further apology that I will follow a time-worn path to our subject matter.

FIGURE 2—*not* FIGURE 1—provides the image we should have in mind when we think of “vector spaces,” however complicated the context. But vector spaces are of little or no interest in and of themselves: they acquire interest from the things we can do in them. Which are three:

- We can **multiply vectors by constants** (or, as they are often called in this subject area, “scalars” and which will, for the moment, be assumed to be real-valued: see FIGURE 3)
- We can **add vectors** (see FIGURE 4)
- We can **move vectors around** within \mathcal{V} , but discussion of how this is done must be deferred until we have prepared the soil.

The set $\{\mathbf{a}, \mathbf{b}, \mathbf{c}, \dots\}$ is assumed to be **closed** under each of those operations (and in the contrary case does not constitute a vector space).

Scalars (real or complex numbers) can themselves be added *and multiplied*, subject to the familiar associativity, distributivity and commutivity rules. It is, however, **not assumed that vectors can be “multiplied”** (though in some cases they can be).

Multiplication of \mathbf{a} by -1 yields a vector $-\mathbf{a}$ that in arrow language would be represented by a *directionally-reversed copy of \mathbf{a}* . To say the same thing another way, we have

$$\mathbf{a} - \mathbf{a} \equiv \mathbf{a} + (-\mathbf{a}) = (1 - 1)\mathbf{a} = 0\mathbf{a} = \mathbf{0}$$

as a corollary of the primitive statement $(\lambda + \mu)\mathbf{a} = \lambda\mathbf{a} + \mu\mathbf{a}$. Relatedly, we have

$$\lambda(\mathbf{a} + \mathbf{b}) = \lambda\mathbf{a} + \lambda\mathbf{b}$$

which states that scalar multiplication is a **linear operation** (of which we are destined to see many much more interesting examples).

A set of vectors $\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_p\}$ is said to be **linearly independent** if and only if

$$\lambda^1\mathbf{a}_1 + \lambda^2\mathbf{a}_2 + \dots + \lambda^p\mathbf{a}_p = \mathbf{0} \quad \text{requires that all } \lambda^i = 0$$

and otherwise to be linearly dependent. In the latter circumstance one could describe one vector in terms of the others, writing (say)

$$\mathbf{a}^p = \frac{\lambda^1\mathbf{a}_1 + \lambda^2\mathbf{a}_2 + \dots + \lambda^{p-1}\mathbf{a}_{p-1}}{\lambda^p}$$

And if the vectors in the numerator were linearly dependent one could continue the process, until all the vectors were described in terms of some linearly independent subset.

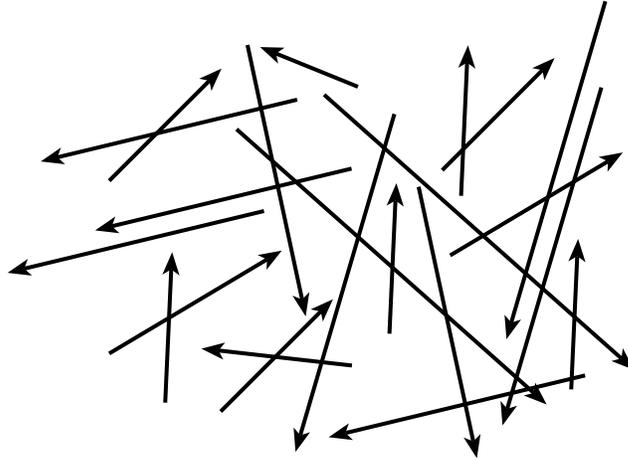


FIGURE 1: Representation of the set of all possible arrows (all lengths, all directions, all points of origin), drawn on the plane. Such objects are called “**space vectors**” by Riley et al, “**displacement vectors**” by most American authors.

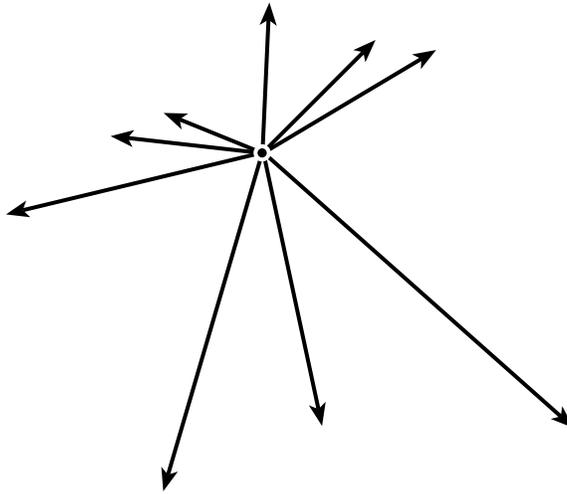


FIGURE 2: “Pincushion” that results from our agreements to identify all arrows that are translates of one another (i.e., to dismiss as irrelevant the “point of application”) and to attach all tails to the same point. That point, thought of as an undirected arrow of zero length, provides a representation of the null vector $\mathbf{0}$. Individual vectors will be denoted \mathbf{a} , \mathbf{b} , \mathbf{c} , . . . Collectively they comprise a **vector space** \mathcal{V} .



FIGURE 3: Representation of the relationship of $\lambda \mathbf{a}$ to \mathbf{a} , in the cases $\lambda = 3$ and $\lambda = -2$. It will be appreciated that while it is possible to construct an arrow that is k times as long as another arrow, it is not possible literally to “multiply an arrow by k ,” though it is possible to multiply by k the vector that represents the arrow.

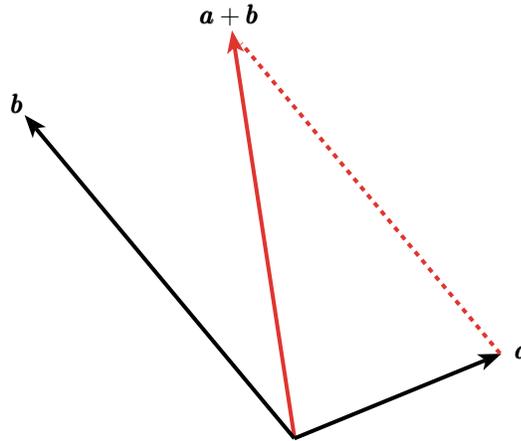


FIGURE 4: Representation of the construction that assigns meaning to $\mathbf{a} + \mathbf{b}$. Again, while it is not possible literally to “add arrows,” it is possible to add the vectors that represent the arrows.

It is clear that any p -tuple of arrows ($p \geq 3$) inscribed on a plane (*i.e.*, any such p -tuple of vectors in \mathcal{V}_2) is necessarily linearly dependent, and that every maximal set of linearly independent plane-arrows has exactly two elements. In 3-space every maximal set has three elements. It is not difficult to show more generally that every maximal set of linearly independent vectors in a given vector space \mathcal{V} has the *same* number n of elements. One writes

$$\dim[\mathcal{V}] = n \quad : \quad n \text{ is the } \mathbf{dimension} \text{ of } \mathcal{V}$$

and—to emphasize that the space is n -dimensional— \mathcal{V}_n in place of \mathcal{V} .

Every such maximal set $\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_n\}$ in \mathcal{V}_n constitutes a **basis** in \mathcal{V}_n , a minimal set in terms of which every $\mathbf{x} \in \mathcal{V}_n$ can be developed

$$\mathbf{x} = x^1 \mathbf{a}_1 + x^2 \mathbf{a}_2 + \dots + x^n \mathbf{a}_n$$

The numbers $\{x^1, x^2, \dots, x^n\}$ are the **coordinates of \mathbf{x} relative to the given basis**. Adopt a different basis and the same \mathbf{x} acquires a different set of coordinates: we must *be careful never to confuse coordinates with the things they describe*. It often proves convenient to display coordinates as stacks of numbers (*i.e.*, as

$n \times 1$ matrices):

$$\begin{pmatrix} x^1 \\ x^2 \\ \vdots \\ x^n \end{pmatrix} : \text{coordinates of } \mathbf{x} \text{ with respect to a given basis}$$

It follows readily from preceding remarks that if (relative to some given basis)

$$\mathbf{x} \text{ and } \mathbf{y} \text{ have coordinates } \begin{pmatrix} x^1 \\ x^2 \\ \vdots \\ x^n \end{pmatrix} \text{ and } \begin{pmatrix} y^1 \\ y^2 \\ \vdots \\ y^n \end{pmatrix}$$

then

$$i) \quad \lambda \mathbf{x} \text{ has coordinates } \begin{pmatrix} \lambda x^1 \\ \lambda x^2 \\ \vdots \\ \lambda x^n \end{pmatrix}$$

$$ii) \quad \mathbf{x} + \mathbf{y} \text{ has coordinates } \begin{pmatrix} x^1 + y^1 \\ x^2 + y^2 \\ \vdots \\ x^n + y^n \end{pmatrix}$$

I have, by the way, decorated coordinates with superscripts rather than with subscripts (and in this respect honored an entrenched convention which Riley *et al* have chosen to violate) for reasons which only much later will I have occasion to explain.

For arrows inscribed on the Euclidean plane (or erected in Euclidean 3-space) we find it quite unproblematic to speak of

- the **length** $a \equiv |\mathbf{a}|$ of any given arrow \mathbf{a}
- the **angle** $\theta \equiv \mathbf{a} \angle \mathbf{b}$ subtended by any given pair of arrows.

I turn now to discussion of the several-step procedure by which those primitive metric concepts can be so abstracted as to become concepts assignable to vectors. All proceeds from the introduction (within Euclidean space) of the **dot product** of a pair of arrows, which is itself not an arrow but a *number*, denoted and defined

$$\mathbf{a} \cdot \mathbf{b} \equiv ab \cos \theta$$

It is natural to construe $\mathbf{a} \angle \mathbf{b}$ —the angle constructed by folding \mathbf{a} into \mathbf{b} —to be the negative of $\mathbf{b} \angle \mathbf{a}$. But $\cos \theta$ is an even function, so that in the present context is a distinction without a difference:

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a}$$

The metric notions that feed into the construction of $\mathbf{a} \cdot \mathbf{b}$ are themselves easily recovered:

$$\mathbf{a} \cdot \mathbf{a} = a^2 \geq 0, \text{ with equality if and only if } \mathbf{a} = \mathbf{0}$$

$$\cos \theta = \frac{\mathbf{a} \cdot \mathbf{b}}{\sqrt{\mathbf{a} \cdot \mathbf{a}} \cdot \sqrt{\mathbf{b} \cdot \mathbf{b}}}$$

Much will be found to hinge upon the **linearity of the dot product**; *i.e.*, upon the fact that

$$\mathbf{a} \cdot (\mathbf{b}_1 + \mathbf{b}_2) = \mathbf{a} \cdot \mathbf{b}_1 + \mathbf{a} \cdot \mathbf{b}_2$$

—the truth of which follows by inspection from the following figure:

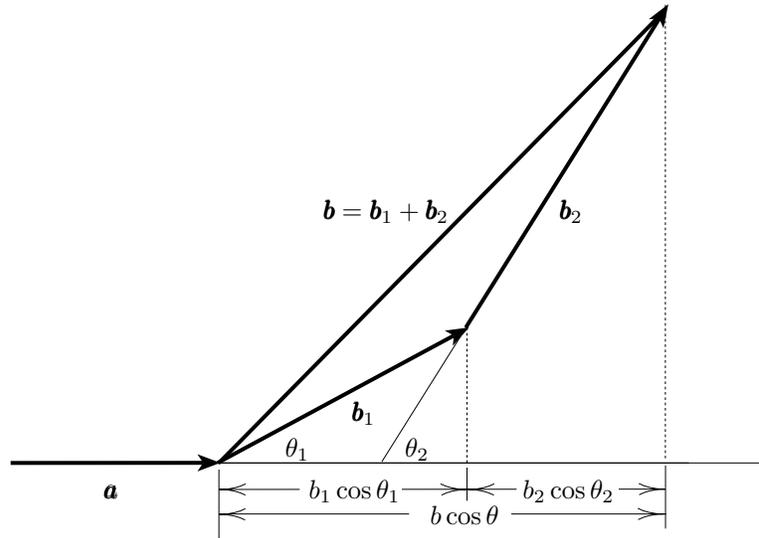


FIGURE 5: Transparently $b \cos \theta = b_1 \cos \theta_1 + b_2 \cos \theta_2$, which when multiplied by \mathbf{a} becomes the condition $\mathbf{a} \cdot \mathbf{b} = \mathbf{a} \cdot \mathbf{b}_1 + \mathbf{a} \cdot \mathbf{b}_2$ claimed in the text.

From the linearity of the dot product (which by symmetry becomes bilinearity) it follows that in two dimensions

$$\begin{aligned} \mathbf{x} \cdot \mathbf{y} &= (x^1 \mathbf{a}_1 + x^2 \mathbf{a}_2) \cdot (y^1 \mathbf{a}_1 + y^2 \mathbf{a}_2) \\ &= x^1 y^1 \mathbf{a}_1 \cdot \mathbf{a}_1 + x^1 y^2 \mathbf{a}_1 \cdot \mathbf{a}_2 + x^2 y^1 \mathbf{a}_2 \cdot \mathbf{a}_1 + x^2 y^2 \mathbf{a}_2 \cdot \mathbf{a}_2 \end{aligned}$$

If the elements of the basis were

- of unit length (or “**normalized**”): $\mathbf{a}_1 \cdot \mathbf{a}_1 = \mathbf{a}_2 \cdot \mathbf{a}_2 = 1$
- and **orthogonal** to each other: $\mathbf{a}_1 \cdot \mathbf{a}_2 = \mathbf{a}_2 \cdot \mathbf{a}_1 = 0$

then the preceding result would assume this much simpler form

$$= x^1 y^1 + x^2 y^2$$

as a special instance of which we recover the Pythagorean theorem:

$$\mathbf{x} \cdot \mathbf{x} = (\text{length of } \mathbf{x})^2 = x_1^2 + x_2^2$$

These results extend straightforwardly to any finite number n of dimensions. They provide first indication of the the computational simplicity/efficiency that

typically follow automatically in the wake of a decision to select an **orthonormal basis** $\{\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n\}$:⁴

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \equiv \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

REMARK: The literal product of two “quaternions” (inventions of the Irish physicist W. R. Hamilton in the 1840s) was found to have a “scalar” part and a “vectorial” part. In the simplified vector algebra devised by the American physicist J. W. Gibbs in the 1890s the former became the “dot product,” the latter the “cross product.” But in the Gibbs’ scheme the “dot product” is not properly a “product” at all: it is meaningless to write $\mathbf{a} \cdot \mathbf{b} \cdot \mathbf{c}$, and while $(\mathbf{a} \cdot \mathbf{b})\mathbf{c}$ and $\mathbf{a}(\mathbf{b} \cdot \mathbf{c})$ each has unambiguous meaning (and, clearly, they are generally not equal). I would prefer to speak of the “dotproduct,” a symmetric bilinear number-valued function of vector pairs in which the final seven letters serve simply to recall some interesting history.

REMARK: The defining properties of the dot product were abstracted from metric aspects of Euclidean geometry, but one can—as we will have occasion to do—turn the procedure around, using the dot product to *assign* metric properties (*i.e.*, to deposit definitions of “length” and “angle” upon) \mathcal{V}_n . Note that in the absence of such definitions it becomes impossible to assign a meaning to “orthonormality,” and impossible therefore to gain access to the advantages that follow therefrom.

I turn now to brief discussion of a couple of the useful applications of the dot product and orthonormality ideas:

PROBLEM 1: Let \mathbf{a} be any vector in \mathcal{V}_n , and let $\hat{\mathbf{n}}$ be any unit vector. Writing $\mathbf{a} = \mathbf{a}_{\parallel} + \mathbf{a}_{\perp}$ with $\mathbf{a}_{\parallel} \equiv (\mathbf{a} \cdot \hat{\mathbf{n}})\hat{\mathbf{n}}$ and $\mathbf{a}_{\perp} \equiv \mathbf{a} - \mathbf{a}_{\parallel}$ show that \mathbf{a}_{\parallel} and \mathbf{a}_{\perp} are orthogonal: $\mathbf{a}_{\parallel} \cdot \mathbf{a}_{\perp} = 0$.

⁴ My \mathbf{e} -notation is intended here and henceforth to signal that the elements of the basis in question are, by assumption, orthonormal. In 3-dimensional contexts—but *only* in those—one frequently sees

$$\begin{aligned} \mathbf{i} & \text{ written for } \mathbf{e}_1 \\ \mathbf{j} & \text{ written for } \mathbf{e}_2 \\ \mathbf{k} & \text{ written for } \mathbf{e}_3 \end{aligned}$$

though this practice entails sacrifice of all the many advantages that indices afford.

Write $\mathbf{a} = \sum_i a^i \mathbf{e}_i$ to describe the development of an arbitrary vector $\mathbf{a} \in \mathcal{V}_n$ with respect to an arbitrary orthonormal basis $\{\mathbf{e}_i\}$. Immediately

$$\mathbf{a} \cdot \mathbf{e}_j = a^j$$

so we have

$$\mathbf{a} = \sum_i (\mathbf{a} \cdot \mathbf{e}_i) \mathbf{e}_i \quad : \quad \text{all } \mathbf{a}$$

This is sometimes called “**Fourier’s identity**” because it is—as we will have occasion to see—an elaboration of this simple idea that lies at the heart of Fourier analysis and all of its generalizations.

PROBLEM 2: Vectors \mathbf{e}_1 and \mathbf{e}_2 , when referred to some unspecified orthonormal basis, can be described

$$\mathbf{e}_1 = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} \quad \text{and} \quad \mathbf{e}_2 = \begin{pmatrix} -\frac{1}{2} \\ \frac{\sqrt{3}}{2} \end{pmatrix}$$

a) Show that \mathbf{e}_1 and \mathbf{e}_2 are orthonormal; *i.e.*, that $\{\mathbf{e}_1, \mathbf{e}_2\}$ itself comprises an orthonormal basis.

b) Evaluate the numbers a^1 and a^2 that permit the vector

$$\mathbf{a} = \begin{pmatrix} 7 \\ 2 \end{pmatrix}$$

to be written $\mathbf{a} = a^1 \mathbf{e}_1 + a^2 \mathbf{e}_2$.

I defer discussion of the “cross product”⁵ $\mathbf{a} \times \mathbf{b}$ because—though arguably a proper “vector-valued product of vectors”—it is meaningful only within \mathcal{V}_3 , and meaningful there only “by accident.”

2. Some vector systems having nothing to do with arrows. Consider the set \mathcal{P}_m of all m^{th} -order polynomials

$$a(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_m x^m$$

with real coefficients. Clearly,

- if $a(x)$ is such a polynomial then so also is every real multiple of $a(x)$;
- if $a(x)$ and $b(x)$ are such polynomials then so also is $a(x) + b(x)$.

Which is all we need to know to assert that \mathcal{P}_m is a vector space. It is clear also that $\{x^0, x^1, x^2, \dots, x^m\}$ are linearly independent elements of \mathcal{P}_m , in which collectively they comprise a basis. We conclude that \mathcal{P}_m is $(m+1)$ -dimensional, a vector space of type \mathcal{V}_{m+1} .

⁵ See §§7.6.3 & 7.6.4 in Riley *et al.*

How might we deposit metric structure upon \mathcal{P}_m ? Here Euclidean geometry provides no guidance, but the *formal properties of the dot product* do. Consider, for example, the construction

$$a(x) \cdot b(x) \equiv \int_{\alpha}^{\beta} a(x)b(x)w(x)dx$$

where the limits of integration are considered to be given/fixed, and where $w(x)$ is taken to be some agreed-upon well-behaved real-valued function. Clearly, the $a(x) \cdot b(x)$ thus defined is a real-valued symmetric bilinear function of its arguments, and if $w(x)$ non-negative on the interval then

$$a(x) \cdot a(x) \geq 0, \text{ with equality if and only if } a(x) \equiv 0$$

We could ask for nothing more: we find ourselves in position to speak of the “length” $\sqrt{a(x) \cdot a(x)}$ of a polynomial, of the “cosine of the angle between” two polynomials

$$\cos \theta \equiv \frac{a(x) \cdot b(x)}{\sqrt{a(x) \cdot a(x)} \sqrt{b(x) \cdot b(x)}}$$

and of the “orthogonality” of polynomials:

$$a(x) \perp b(x) \text{ if and only if } a(x) \cdot b(x) = 0$$

EXAMPLE: Here follows a list of the first five **Hermite polynomials** (as supplied by *Mathematica*’s `HermiteH[n,x]` command):

$$\begin{aligned} H_0(x) &= 1 \\ H_1(x) &= 2x \\ H_2(x) &= 4x^2 - 2 \\ H_3(x) &= 8x^3 - 12x \\ H_4(x) &= 16x^4 - 48x^2 + 12 \end{aligned}$$

Setting $\alpha = -\infty$, $\beta = +\infty$ and $w(x) = e^{-x^2}$ we discover that

$$H_m(x) \cdot H_n(x) = \sqrt{\pi} 2^n n! \delta_{mn}$$

The Hermite polynomials are orthogonal, but (as they stand) not normalized.

EXAMPLE: Here follows a list of the first five **Chebyshev polynomials of the first kind** (as supplied by *Mathematica*’s `ChebyshevT[n,x]` command):

$$\begin{aligned} T_0(x) &= 1 \\ T_1(x) &= x \\ T_2(x) &= 2x^2 - 1 \\ T_3(x) &= 4x^3 - 3x \\ T_4(x) &= 8x^4 - 8x^2 + 1 \end{aligned}$$

Setting $\alpha = -1$, $\beta = +1$ and $w(x) = (1 - x^2)^{-\frac{1}{2}}$ we discover that

$$\begin{aligned} T_0(x) \cdot T_0(x) &= \pi \\ T_m(x) \cdot T_m(x) &= \frac{1}{2}\pi & : & \quad m = 1, 2, 3, \dots \\ T_m(x) \cdot T_n(x) &= 0 & : & \quad m \neq n \end{aligned}$$

The Chebyshev polynomials are orthogonal, but are again not (as they stand) normalized.

The theory of orthogonal polynomials finds many important applications in diverse branches of physics and applied mathematics. The subject is, for some reason, not discussed by Riley *et al*, but see (for example) Chapter 22 in Abramowitz & Stegun.⁶

PROBLEM 3: Develop $a(x) = a + bx + cx^2 + dx^3$ as a weighted sum of Hermite polynomials:

$$a(x) = h^0 H_0(x) + h^1 H_1(x) + h^2 H_2(x) + h^3 H_3(x)$$

Feel free to use *Mathematica* to perform the integrals.

PROBLEM 4 : What, relative to Hermite's definition of the dot product, is the cosine of the angle between $a(x) = x$ and $b(x) = x^2$?

ADDITIVE COLOR MIXING Consider the set of all colored disks that might be projected onto the wall of a darkened room, or displayed on a computer screen. If **A** identifies such a disk, and **B** identifies another, we write

- $k\mathbf{A}$ to signal that disk **A** has been made k times “brighter” (at $k = 0$ the light source has been turned off);
- $\mathbf{A} + \mathbf{B}$ to signal that disks **A** and **B** have been superimposed.

Additive/subtractive color mixing are complementary subjects that had already a long history⁷ by the time (1860) the 28-year-old J. C. Maxwell entered upon the scene, but it is upon his work that modern color technology mainly rests. Maxwell (who worked not with superimposed disks of light but with spinning tops) found that with only three colors—taken by him to be saturated red **R**, saturated green **G** and saturated blue **B**—he could reproduce *any* color **C**: symbolically

$$\mathbf{C} = r\mathbf{R} + g\mathbf{G} + b\mathbf{B}$$

where $\{r, g, b\}$ real numbers—“color coordinates”—that range on $[0, 1]$. Writing

$$\mathbf{c} \equiv \begin{pmatrix} r \\ g \\ b \end{pmatrix}$$

⁶ M. Abramowitz & I. Stegun, *Handbook of Mathematical Functions* (1965).

⁷ Go to <http://www.handprint.com/HP/WCL/color6.html> for a pretty good survey of the subject and its history.

he found that (trivially)

$$\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \text{ gives } \mathbf{black}$$

while (not at all trivially)

$$\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \text{ gives } \mathbf{white}$$

and (taking k to lie between 0 and 1)

$$\text{at } \begin{pmatrix} k \\ k \\ k \end{pmatrix} \text{ we get various depths of } \mathbf{grey}$$

More particularly (see Figure 6),

$$\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \text{ gives } \mathbf{cyan}$$

$$\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \text{ gives } \mathbf{magenta}$$

$$\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \text{ gives } \mathbf{yellow}$$

The color **orange** presents an interesting problem: any child would tell us to construct **red** + **yellow**, but

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 0 \end{pmatrix}$$

and the 2 falls outside the allowed interval $[0, 1]$. We are obliged to proceed

$$\begin{pmatrix} .5 \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} .5 \\ .5 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ .5 \\ 0 \end{pmatrix} : \text{ gives } \mathbf{orange}$$

as illustrated in FIGURE 7. Evidently “multiplication by scalars” is subject to some idiosyncratic restrictions in the vector theory of colors. That same point emerges also from another consideration. Anyone who has repeated Maxwell’s top experiments has discovered that the colors achieved have typically a washed-out appearance—much less vivid than the primaries from which they

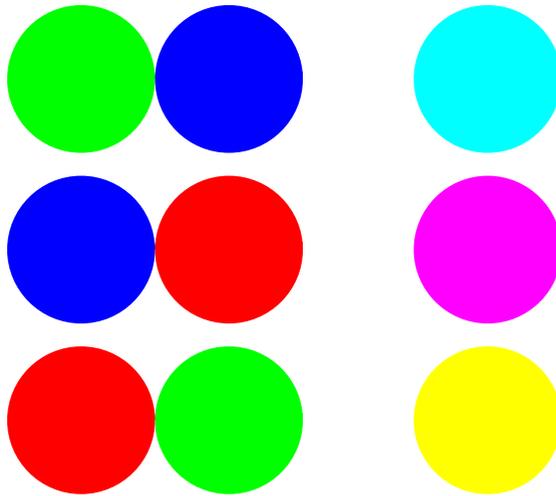


FIGURE 6: *In each row, additive superposition of the colors on the left gives the color on the right. The figure was produced by Mathematica, in response to commands of the design*

```
cyan = Show[Graphics[{
  {RGBColor[0,1,0], Disk[{0,0}, .2]},
  {RGBColor[0,0,1], Disk[ {.4,0}, .2]},
  {RGBColor[0,1,1], Disk[ {1.1,0}, .2]}
}], AspectRatio→Automatic];
```

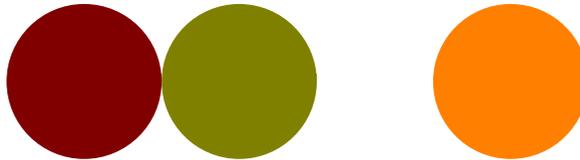


FIGURE 7: *To achieve orange we have been forced to attenuate the red and yellow. The command here read*

```
orange = Show[Graphics[{
  {RGBColor[.5,0,0], Disk[{0,0}, .2]},
  {RGBColor[.5,.5,0], Disk[ {.4,0}, .2]},
  {RGBColor[1,.5,0], Disk[ {1.1,0}, .2]}
}], AspectRatio→Automatic];
```

The attenuated colors would look dimmer in a dark room, but on this white page look blacker.

are constructed. To circumvent this difficulty, Maxwell invoked a strategy that can be described $\mathbf{color} + k \cdot \mathbf{white} = r\mathbf{R} + g\mathbf{G} + b\mathbf{B}$ or again

$$\mathbf{C} + \begin{pmatrix} k \\ k \\ k \end{pmatrix} = r \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + g \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

It seems natural in this light to write

$$\mathbf{C} = \begin{pmatrix} r - k \\ g - k \\ b - k \end{pmatrix}$$

But there are certainly instances in which the vector on the right will have *negative elements*, though there is no such thing as “negative light” of *any* color! The entry of negative coordinates into the theory of vector spaces is an unavoidable consequence of the postulated existence of a zero element $\mathbf{0}$. But in color space the zero is **black**, and (absent of the perfect interference effects that are alien to this discussion) no light can be superimposed upon another light so as to produce black. So it is by a kind of formal trickery that negative coordinates enter into the theory of color space: color space is—if a vector space at all—a vector space with some highly non-standard properties.

“Vector theorists” that we are, and the preceding remark notwithstanding, we find it natural to pose certain questions:

- Can bases alternative to Maxwell’s $\{\mathbf{R}, \mathbf{G}, \mathbf{B}\}$ -basis be used to span the space of colors?
- Why do some color-production processes use 4 or 5-color sets of ink/light?
- How did Edwin Land (go to <http://land.t-a-y-l-o-r.com/>) manage to get along with only *two* colors?
- Can *metric structure* be assigned to color space in a natural/useful way? Here the answer is a qualified “yes.” The matter was first explored by Helmholtz, whose work was taken up and extended by Schrödinger (~1920), but they were concerned with “just noticeable differences” in color. The associated mathematics did borrow from non-Riemannian differential geometry, but made no direct use of the dot product idea. Helmholtz’ involvement (he pioneered the “physics of perception”) and the allusion to “just noticeable differences” underscore the long-recognized fact that the “theory of color (color vision)” lives in the place where physics and neurophysiology intersect.

Mathematica makes it easy to perform certain kinds of experiments in this subject area. Even handier for that purpose is the Color Palette that is accessible from many of the applications that run on Apple computers. One must be aware, however, that an $\{\mathbf{R}, \mathbf{G}, \mathbf{B}\}$ predisposition (circumventable in *Mathematica*) is built into the design of the software, and can introduce bias into some results.

3. Natural occurrences of the “matrix” idea. The formal “theory of matrices” is, like so much else, a 19th Century development, but the basic ideas almost invent themselves as soon as one undertakes to work through certain issues that, pretty obviously, will be central to any “theory of vector spaces.” I will approach the subject from several angles:

FROM ONE BASIS TO ANOTHER Write

$$\mathbf{x} = \sum_{i=1}^n x^i \mathbf{a}_i \quad (1)$$

to describe the development of \mathbf{x} with respect to $\{\mathbf{a}_i\}$, a basis in \mathcal{V}_n . To render explicit the relation between $\{\mathbf{a}_i\}$ and $\{\hat{\mathbf{a}}_j\}$, a second basis in \mathcal{V}_n we write

$$\left. \begin{aligned} \mathbf{a}_1 &= \sum_j M^j_1 \hat{\mathbf{a}}_j \\ \mathbf{a}_2 &= \sum_j M^j_2 \hat{\mathbf{a}}_j \\ &\vdots \\ \mathbf{a}_n &= \sum_j M^j_n \hat{\mathbf{a}}_j \end{aligned} \right\}$$

or more compactly

$$\mathbf{a}_i = \sum_j M^j_i \hat{\mathbf{a}}_j \quad (2)$$

Then

$$\begin{aligned} \mathbf{x} &= \sum_i \sum_j x^i M^j_i \hat{\mathbf{a}}_j \\ &= \sum_j \hat{x}^j \hat{\mathbf{a}}_j \quad \text{with} \quad \hat{x}^j \equiv \sum_i M^j_i x^i \end{aligned} \quad (3)$$

To pass back again to the original basis we write

$$\hat{\mathbf{a}}_j = \sum_k W^k_j \mathbf{a}_k \quad (4)$$

and obtain

$$= \sum_j W^k_j \hat{x}^j \mathbf{a}_k$$

But the coefficient of \mathbf{a}_k is by definition just x^k , so we have

$$\begin{aligned} x^k &= \sum_j W^k_j \hat{x}^j \\ &= \sum_i \left\{ \sum_j W^k_j M^j_i \right\} x^i \end{aligned} \quad (5)$$

which entails

$$\left\{ \sum_j W^k_j M^j_i \right\} = \delta^k_i \tag{6}$$

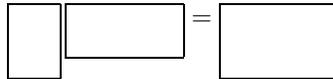
$$\delta^k_i \equiv \begin{cases} 1 & : & k = i \\ 0 & : & k \neq i \end{cases}$$

Matrix notation permits us to surpress the indices and, by elimination of notational clutter, to clarify what is going on. Display the n^2 numbers M^j_i in $n \times n$ tabular array

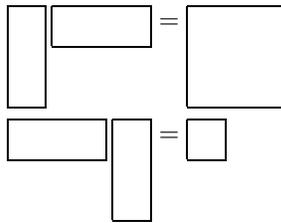
$$\mathbb{M} \equiv \begin{pmatrix} M^1_1 & M^1_2 & \dots & M^1_n \\ M^2_1 & M^2_2 & \dots & M^2_n \\ \vdots & \vdots & & \vdots \\ M^n_1 & M^n_2 & \dots & M^n_n \end{pmatrix} \equiv \|M^{\text{row}}_{\text{column}}\| \tag{7}$$

and—proceeding similarly—from the numbers W^k_j assemble \mathbb{W} . Drawing our inspiration from (6), we will understand $\sum_k W^i_k M^k_j$ to *define* the ij^{th} element of the matrix product $\mathbb{W}\mathbb{M}$. By straightforward extension:

- if $\mathbb{A} = \|A_{ij}\|$ is $m \times n$ and
- if $\mathbb{B} = \|B_{ij}\|$ is $p \times q$ we will
- understand $\|\sum_k A_{ik} B_{kj}\|$, which is meaningful if and only if $n = p$, to define the ij^{th} element of the $m \times q$ matrix product $\mathbb{A}\mathbb{B}$



Notice that the reversed product $\mathbb{B}\mathbb{A}$ will be meaningful if and only if it is also the case that $m = p$, and that—as illustrated below



—it becomes possible to contemplate writing $\mathbb{A}\mathbb{B} = \mathbb{B}\mathbb{A}$ if and only if \mathbb{A} and \mathbb{B} are both square, and of the same dimension. But even then equality is not assured, as the example serves to demonstrate: let

$$\mathbb{A} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \quad \text{and} \quad \mathbb{B} = \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix}$$

Then

$$\mathbb{A}\mathbb{B} = \begin{pmatrix} 19 & 22 \\ 43 & 50 \end{pmatrix} \quad \text{but} \quad \mathbb{B}\mathbb{A} = \begin{pmatrix} 23 & 34 \\ 31 & 46 \end{pmatrix} \neq \mathbb{A}\mathbb{B}$$

The short of it: **matrix multiplication, though invariably associative, is generally non-commutative**.

So we have

$$\begin{aligned}\mathbf{x} &= ax \\ &= \hat{a} \mathbb{M} \mathbb{M}^{-1} \hat{x} \\ &= \hat{a} \hat{x}\end{aligned}$$

which exposes this important fact: **a change of basis stimulates basis elements \mathbf{a}_i and coordinates x^i to transform by distinct but complementary rules:**

$$\begin{array}{ccc} \{\mathbf{a}_i\} & \xrightarrow{\text{mediated by } \mathbb{M}} & \{\hat{\mathbf{a}}_i\} \\ \{x^i\} & \xrightarrow{\text{mediated by } \mathbb{M}^{-1}} & \{\hat{x}^i\} \end{array} \quad (10)$$

It is to distinguish one from the other that we

- decorate objects of the first type with subscripts, and say that they transform “covariantly;”
- decorate objects of the second type with superscripts, and say that they transform “contravariantly.”

The point just developed acquires special importance in “multilinear algebra” (tensor algebra).⁹

LINEAR TRANSFORMATIONS In the discussion just concluded the vectors \mathbf{x} sat there passively, while the basis vectors moved around within \mathcal{V}_n and the coordinates of \mathbf{x} therefore took on adjusted values. We adopt now a different stance: we assume it to be now the elements $\{\mathbf{a}_i\}$ that sit there passively, while the vectors \mathbf{x} move around under action of an “operator” \mathcal{O} :

$$\mathcal{O} : \mathbf{x} \mapsto \mathbf{x}'$$

Such a viewpoint becomes very natural if one thinks about the vector $\mathbf{x}(t)$ that describes—relative to a fixed reference frame—the (often very complicated) motion of a mass point m in response to prescribed forces $\mathbf{F}(\mathbf{x}, t)$. We restrict our attention here, however, to **linear operators**—operators \mathcal{L} that act subject to the rule

$$\mathcal{L} : \lambda \mathbf{a} + \mu \mathbf{b} \mapsto (\lambda \mathbf{a} + \mu \mathbf{b})' = \lambda \mathbf{a}' + \mu \mathbf{b}'$$

From linearity it follows that if $\mathbf{x} = \sum_j x^j \mathbf{a}_j$ then $\mathbf{x}' = \sum_j x^j \mathbf{a}_j'$, and if

$$\mathbf{a}_j' = \sum_i L^i_j \mathbf{a}_i$$

describes the \mathbf{a}_i' 's in reference to the static original basis then we have

$$\mathbf{x}' = \sum_i x'^i \mathbf{a}_i \quad \text{with} \quad x'^i = \sum_j L^i_j x^j$$

With the clear understanding that the numbers x'^i , L^i_j and x^j all refer to the

⁹ Impatient readers might at this point want to have a look at Chapter 21 in Riley *et al.*

fixed $\{\mathbf{a}_i\}$ -basis, we have in a by-now-obvious matrix notation

$$x' = \mathbb{L}x \quad \text{which is of the design} \quad \boxed{} = \boxed{} \boxed{} \quad (11)$$

Equation (11) is said to provide a (basis dependent) **matrix representation** of the action of \mathcal{L} .

We found on page 6 that if $\mathbf{x} = \sum_i x^i \mathbf{a}_i$ and $\mathbf{y} = \sum_j y^j \mathbf{a}_j$ then

$$\mathbf{x} \cdot \mathbf{y} = \sum_i \sum_j x^i g_{ij} y^j \quad \text{with} \quad g_{ij} \equiv \mathbf{a}_i \cdot \mathbf{a}_j \quad (12)$$

To express the dot product in matrix notation (which is often advantageous) we need a new idea: the **transpose** of a matrix \mathbb{A} , denoted \mathbb{A}^T , is the changing rows into columns, columns into rows. If \mathbb{A} is $m \times n$ then \mathbb{A}^T is $n \times m$:

$$\boxed{}^T = \boxed{}$$

The *symmetry* of a matrix ($\mathbb{A}^T = \mathbb{A}$) clearly requires that it be square. From the trivial identity $\mathbb{A} = \frac{1}{2}(\mathbb{A} + \mathbb{A}^T) + \frac{1}{2}(\mathbb{A} - \mathbb{A}^T)$ we see that every square matrix can be decomposed

$$\mathbb{A} = \mathbb{A}_{\text{symmetric part}} + \mathbb{A}_{\text{antisymmetric part}}$$

Returning now to (12), we have

$$\mathbf{x} \cdot \mathbf{y} = x^T \mathbb{G} y \quad \text{with} \quad \mathbb{G} \equiv \|g_{ij}\| = \mathbb{G}^T$$

With respect to any **orthonormal basis** $\{\mathbf{e}_i\}$ we have $\mathbb{G} = \mathbb{I}$, giving

$$\mathbf{x} \cdot \mathbf{y} = x^T y \quad : \quad \text{number-valued object of type} \quad \boxed{} \boxed{}$$

Linear transformations serve generally to alter the value of dot products:

$$x^T \mathbb{G} y \mapsto x'^T \mathbb{G} y' = x^T \mathbb{L}^T \mathbb{G} \mathbb{L} y$$

Pretty clearly, a linear transformation will preserve all dot products (all lengths and angles)

$$= x^T \mathbb{G} y \quad : \quad \text{all } x, y$$

if and only if it is a property of \mathbb{L} that

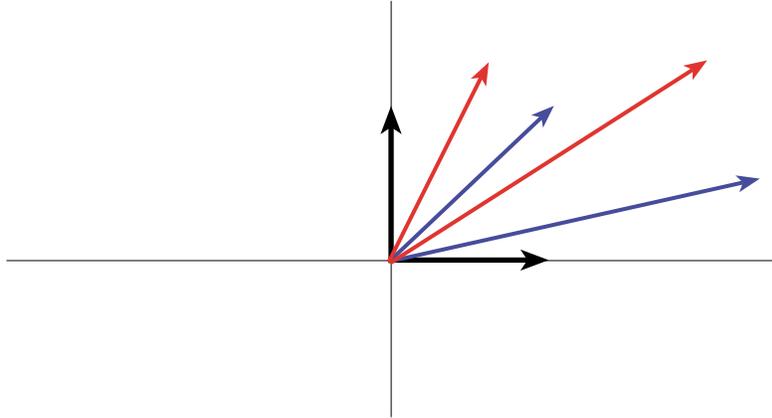


FIGURE 8: The blue vectors \mapsto red vectors under action of the rotation operator \mathcal{L} which, relative to a specified orthonormal basis (black vectors), is represented by the rotation matrix \mathbb{L} .

$$\mathbb{L}^T \mathbb{G} \mathbb{L} = \mathbb{G}$$

which becomes

$$\begin{aligned} &\Downarrow \\ &\mathbb{L}^T \mathbb{L} = \mathbb{I} \quad \text{when the basis is orthonormal} \end{aligned} \quad (13)$$

Matrices with the property (13) are called **rotation matrices**, and have (among many other important properties) the property that *inversion—normally an intricate process, as will emerge—is accomplished by simple transposition*.

EXAMPLE: Look to the 2-dimensional case

$$\mathbb{L} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

The condition (13) is seen by quick calculation to entail

$$\begin{aligned} a^2 + b^2 &= 1 \\ c^2 + d^2 &= 1 \\ ac + bd &= 0 \end{aligned}$$

Conformity with the first pair of requirements is achieved if we set

$$\begin{aligned} a &= \cos \alpha \\ b &= \sin \alpha \\ c &= \sin \beta \\ d &= \cos \beta \end{aligned}$$

The final requirement then becomes

$$\cos \alpha \sin \beta + \sin \alpha \cos \beta = \sin(\alpha + \beta) = 0$$

which in effect forces $\beta = -\alpha$, giving

$$\mathbb{L} = \begin{pmatrix} \cos \alpha & \sin \alpha \\ -\sin \alpha & \cos \alpha \end{pmatrix} \tag{14}$$

For description of an elegant method that permits the argument to be extended to n dimensions ($n \geq 2$) see §4 in “Extrapolated interpolation theory” (1997).

SYSTEMS OF LINEAR EQUATIONS The following system of **inhomogeneous linear equations**¹⁰

$$\left. \begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ &\vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= b_m \end{aligned} \right\} \tag{15.1}$$

is more conveniently notated

$$\mathbb{A}\mathbf{x} = \mathbf{b} \tag{15.2}$$

and, fairly clearly, will be

- underdetermined if $m < n$

$$\left[\begin{array}{ccc|c} & & & \\ & & & \\ & & & \end{array} \right] = \left[\begin{array}{c} \\ \\ \end{array} \right] \tag{16.1}$$

- possibly determined (solvable) if $m = n$

$$\left[\begin{array}{ccc|c} & & & \\ & & & \\ & & & \end{array} \right] = \left[\begin{array}{c} \\ \\ \end{array} \right] \tag{16.2}$$

- overdetermined if $m \geq n$

$$\left[\begin{array}{ccc|c} & & & \\ & & & \\ & & & \end{array} \right] = \left[\begin{array}{c} \\ \\ \end{array} \right] \tag{16.3}$$

As a description of the solution of (15) we expect to have

$$\mathbf{x} = \mathbb{A}^{-1}\mathbf{b} \quad : \quad \text{exists if and only if } \mathbb{A}^{-1} \text{ does}$$

¹⁰ We assume that no equation can be written as a linear combination of the others, for such an equation would be redundant.

Which brings us into direct confrontation with two questions: *Under what conditions does \mathbb{A}^{-1} exist, and when it does exist how is it constructed?* The theory of matrix inversion (which was remarked already on page 15 requires that \mathbb{A} be square) hinges on the

4. Theory of determinants. The history of this subject can be traced back through contributions by Laplace and Vandermonde (1772) to work done by Maclaurin in 1729 but published (posthumously) only in 1748. Maclaurin observed that when

$$\begin{aligned} a_{11}x + a_{12}y + a_{13}z &= b_1 \\ a_{21}x + a_{22}y + a_{23}z &= b_2 \\ a_{31}x + a_{32}y + a_{33}z &= b_1 \end{aligned}$$

is solved for (say) z one gets

$$z = \frac{(a_{21}a_{32} - a_{22}a_{31})b_1 + (a_{12}a_{31} - a_{11}a_{32})b_2 + (a_{11}a_{22} - a_{12}a_{21})b_3}{a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{32}a_{21} - a_{13}a_{22}a_{31} - a_{12}a_{21}a_{33} - a_{11}a_{32}a_{23}}$$

and tried to describe the patterns hidden in this and analogous results. In 1750 Gabriel Cramer rediscovered Maclaurin's result and suggested notational improvements: **Cramer's Rule** would today be written

$$z = \frac{\begin{vmatrix} a_{11} & a_{12} & b_1 \\ a_{21} & a_{22} & b_2 \\ a_{31} & a_{32} & b_3 \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}} \quad : \quad \text{similar constructions supply } x \text{ and } y$$

The formal theory of determinants (which we today think of as number-valued functions of square matrices) was launched by Cauchy's publication of an 84-page memoir in 1812—the interesting point being that this was *prior* to the development of a theory of matrices!

By modern definition

$$\det \mathbb{A} \equiv \sum_P (-)^P a_{1i_1} a_{2i_2} \cdots a_{ni_n}$$

where the sum ranges over all permutations $P \equiv \begin{pmatrix} 1 & 2 & \cdots & n \\ i_1 & i_2 & \cdots & i_n \end{pmatrix}$ and $(-)^P$ is plus or minus according as the permutation is even or odd. Thus¹¹

$$\begin{aligned} \det \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} &= a_{11}a_{22} - a_{12}a_{21} \\ \det \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} &= + a_{11}a_{22}a_{33} - a_{12}a_{21}a_{33} + a_{13}a_{21}a_{32} \\ &\quad - a_{11}a_{23}a_{32} + a_{12}a_{23}a_{31} - a_{13}a_{22}a_{31} \end{aligned}$$

¹¹ Here I used *Mathematica's* `MinimumChangePermutations` command to generate my list of permutations.

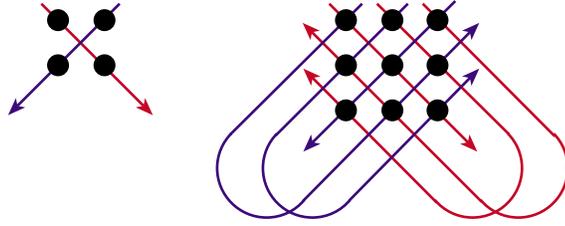


FIGURE 9: *Mnemonics widely used for the evaluation of $\det \mathbb{A}$ in the 2 and 3-dimensional cases: add the products joined by red lines, subtract the products joined by blue lines. From*

$$\det \mathbb{A}_{n \times n} = \text{sum of } n! \text{ terms}$$

and the observation that the construction supplies only $2n$ terms we see that the construction cannot possibly work in cases $n \geq 4$.

The terms that contribute to $\det \mathbb{A}$ can be grouped in a great variety of ways. Every text describes, for example the recursive **Laplace expansion** procedure, whereby (if one has elected to “expand along the top row”) one writes

$$\det \mathbb{A} = a_{11}A_{11} + a_{12}A_{12} + \cdots + a_{1n}A_{1n} \quad (17)$$

where A_{ij} —the “cofactor” of a_{ij} —is defined

$$A_{ij} \equiv (-1)^{i+j} \cdot \begin{cases} \text{determinant of the } (n-1) \times (n-1) \text{ matrix formed} \\ \text{by striking the } i^{\text{th}} \text{ row and } j^{\text{th}} \text{ column from } \mathbb{A} \end{cases}$$

But specialized monographs¹² describe a great variety of alternative procedures, some of which sometimes prove more efficient/useful. Today one would usually find it most convenient simply to ask *Mathematica* to evaluate

$$\text{Det}[\text{square matrix}]$$

Equation (17) is a special instance of the equation

$$\det \mathbb{A} = \sum_k a_{ik} A_{ik} \quad (18.1)$$

And it is not difficult to show¹³ that

$$\sum_k a_{ik} A_{jk} = 0 \quad : \quad i \neq j \quad (18.2)$$

¹² The classic is Thomas Muir, *A Treatise on the Theory of Determinants* (1882, revised and enlarged by W. H. Metzler in 1933, reissued by Dover in 1960). In 1890 Metzler published a history of the theory of determinants.

¹³ See Chapter 1 page 55 in my *CLASSICAL MECHANICS* (1964/65). The essential point is that if $Q_{\dots i \dots j \dots} = -Q_{\dots j \dots i \dots}$ then $\sum_{i,j} Q_{\dots i \dots j \dots} = 0$.

EXAMPLE: In the 3-dimensional case

$$\mathbb{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

we find, for example, that

$$\begin{aligned} & a_{11}A_{11} + a_{12}A_{12} + a_{13}A_{13} \\ &= a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix} \\ &= \text{sum of 6 terms encountered at the bottom of page 21} \\ &= \det \mathbb{A} \end{aligned}$$

while

$$\begin{aligned} & a_{21}A_{11} + a_{22}A_{12} + a_{23}A_{13} \\ &= a_{21} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{22} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{23} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix} \\ &= \text{sum of 6 terms that cancel pairwise} \\ &= 0 \end{aligned}$$

Equations (18) can be combined to read

$$\begin{aligned} \sum_k a_{ik} A_{jk} &= \det \mathbb{A} \cdot \delta_{ij} \\ &\Downarrow \\ \|a_{ij}\| \cdot \|A_{ij}\|^T &= \det \mathbb{A} \cdot \mathbb{I} \end{aligned}$$

which is not simply a collection of formulæ for the evaluation of $\det \mathbb{A}$: it permits us to write

$$\|a_{ij}\|^{-1} \equiv \mathbb{A}^{-1} = \frac{\|A_{ij}\|^T}{\det \mathbb{A}} = \frac{\text{transposed matrix of cofactors}}{\text{determinant}} \quad (19)$$

and to observe that

$$\mathbb{A}^{-1} \text{ exists if and only if } \det \mathbb{A} \neq 0: \mathbb{A} \text{ is } \mathbf{\text{non-singular}} \quad (20)$$

It is by now apparent that matrix inversion is generally a complicated business. In practice we are usually content to leave the labor to *Mathematica*: the command

`Inverse[square matrix]`

quickly supplies the inverses of matrices that are far too large to be managed by pen-&-paper computation.

REMARK: We would be remiss not to take notice of several **general properties** of determinants. Clearly

$$\begin{aligned}\det \mathbf{0} &= 0 \\ \det \mathbf{I} &= 1 \\ \det(\lambda \mathbf{A}) &= \lambda^n \det \mathbf{A}\end{aligned}$$

That

$$\begin{aligned}\det(\mathbf{A}\mathbf{B}) &= \det \mathbf{A} \cdot \det \mathbf{B} \\ &= \det(\mathbf{B}\mathbf{A})\end{aligned}\tag{21}$$

can with patience be demonstrated by low-dimensional example (or in higher dimension tested with the assistance of *Mathematica*)—let \mathbf{A} and \mathbf{B} be 2×2 : then

$$\begin{aligned}\det(\mathbf{A}\mathbf{B}) &= (a_{11}b_{11} + a_{12}b_{21})(a_{21}b_{12} + a_{22}b_{22}) \\ &\quad - (a_{11}b_{12} + a_{12}b_{22})(a_{21}b_{11} + a_{22}b_{21}) \\ &= (a_{11}a_{22} - a_{12}a_{21})(b_{11}b_{22} - b_{12}b_{21}) \\ &\quad + 8 \text{ terms that cancel pairwise} \\ &= \det \mathbf{A} \cdot \det \mathbf{B}\end{aligned}$$

From (21) it follows in particular that

$$\det(\mathbf{A}^{-1}) = (\det \mathbf{A})^{-1}\tag{22}$$

I will not attempt to prove (21) in the general case: all proofs known to me require the development of a certain amount of support apparatus, and none is elementary (for a relatively simple proof see page 49 in the old class notes¹² mentioned just above). Nothing useful can be said about $\det(\mathbf{A} + \mathbf{B})$ in the general case, but $\det(\mathbf{A} - \lambda \mathbf{I})$ will presently assume a persistent major importance.

We are in position now to state exactly what we mean when we write $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$ to describe the solution of (15: case $m = n$). We are in position also to assert that such a solution will exist if and only if $\det \mathbf{A} \neq 0$. Or, to say the same thing another way: if and only if the column vectors

$$\boldsymbol{\alpha}_1 \equiv \begin{pmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{pmatrix}, \boldsymbol{\alpha}_2 \equiv \begin{pmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{n2} \end{pmatrix}, \dots, \boldsymbol{\alpha}_n \equiv \begin{pmatrix} a_{1n} \\ a_{2n} \\ \vdots \\ a_{nn} \end{pmatrix}$$

are linearly independent.¹⁴

¹⁴ The argument here runs as follows: $\boldsymbol{\alpha}_1 x_1 + \boldsymbol{\alpha}_2 x_2 + \dots + \boldsymbol{\alpha}_n x_n = \mathbf{A}\mathbf{x} = \mathbf{0}$ supplies the linear independence condition $\mathbf{x} = \mathbf{A}^{-1}\mathbf{0} = \mathbf{0}$ if and only if \mathbf{A}^{-1} exists (*i.e.*, if and only if $\det \mathbf{A} \neq 0$).

PROBLEM 5 : While it is not particularly difficult to establish quite generally that

$$\det(\mathbb{A}^\top) = \det \mathbb{A}$$

I ask you to demonstrate the point in the 3-dimensional case.

PROBLEM 6 : Let \mathbb{A} be diagonal

$$\mathbb{A} = \begin{pmatrix} a_1 & 0 & 0 & \dots & 0 \\ 0 & a_2 & 0 & \dots & 0 \\ 0 & 0 & a_3 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & a_n \end{pmatrix}$$

and let b_k denote the natural logarithm of a_k :

$$a_k = e^{b_k} = \sum_p \frac{1}{p!} (b_k)^p$$

Write

$$\mathbb{B} = \begin{pmatrix} b_1 & 0 & 0 & \dots & 0 \\ 0 & b_2 & 0 & \dots & 0 \\ 0 & 0 & b_3 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & b_n \end{pmatrix}$$

i) Discuss why it is sensible to write $\mathbb{A} = e^{\mathbb{B}}$.

The **trace** of a square matrix is by definition the *sum of the diagonal elements*:

$$\text{tr } \mathbb{A} \equiv a_{11} + a_{22} + \dots + a_{nn}$$

ii) Argue that

$$\det \mathbb{A} = e^{\text{tr} \mathbb{B}} \tag{23.1}$$

Remarkably, this striking result—which can be expressed

$$\log \det \mathbb{A} = \text{tr } \log \mathbb{A} \tag{23.2}$$

is valid also for a very wide class of *non*-diagonal matrices.¹⁵

iii) If \mathbb{B} were antisymmetric, what would be the value of $\det \mathbb{A}$?

¹⁵ **EXAMPLE:** Let

$$\mathbb{B} = \begin{pmatrix} 0.8 & 0.2 \\ 0.4 & 0.5 \end{pmatrix}$$

Mathematica's `MatrixExp[square matrix]` command supplies

$$\mathbb{A} = \begin{pmatrix} 2.306582 & 0.389687 \\ 0.779373 & 1.722290 \end{pmatrix}$$

and we verify that indeed $\det \mathbb{A} = e^{0.8+0.5}$ (= 3.6693).

PROBLEM 7: Arguing from the definition (page 21), establish that upon the interchange of any two columns a determinant changes sign

$$\begin{vmatrix} \dots p_1 \dots \dots q_1 \dots \dots \\ \dots p_2 \dots \dots q_2 \dots \dots \\ \dots p_n \dots \dots q_n \dots \dots \end{vmatrix} = - \begin{vmatrix} \dots q_1 \dots \dots p_1 \dots \dots \\ \dots q_2 \dots \dots p_2 \dots \dots \\ \dots q_n \dots \dots p_n \dots \dots \end{vmatrix}$$

and that the same is true of rows. Note that it follows from this fact that if any two columns or rows are the same (or proportional) then the determinant necessarily vanishes.

We have been concerned with the inversion of *square* matrices, taking our motivation from a classic problem—the solution of systems of type (16.2). But we will on occasion be confronted also with under/overdetermined systems (types (16.1) and (16.3)). What can be said in such cases? The question leads to a **generalized theory of matrix inversion** that permits the inversion of *rectangular* matrices. But before we can approach that theory we must acquire familiarity with

5. Some aspects of the eigenvalue problem. Though we approach this topic for a fairly arcane practical reason, it is fundamental to the physics of many-particle oscillatory systems, to quantum mechanics and to many other subjects, and therefore has a strong independent claim to our attention.

Supposing \mathbb{A} to be an $n \times n$ square matrix, we ask—as many physical (also many geometrical/algebraic) considerations might lead us to ask—for solutions of

$$\mathbb{A}\mathbf{x} = \lambda\mathbf{x}$$

i.e., for vectors \mathbf{x} upon which the action of \mathbb{A} is purely “dilatational.” Clearly, the equivalent equation

$$(\mathbb{A} - \lambda\mathbb{I})\mathbf{x} = \mathbf{0}$$

will possess non-trivial solutions if and only if

$$\det(\mathbb{A} - \lambda\mathbb{I}) = 0$$

(for otherwise $(\mathbb{A} - \lambda\mathbb{I})^{-1}$ would exist, and we would have $\mathbf{x} = (\mathbb{A} - \lambda\mathbb{I})^{-1}\mathbf{0} = \mathbf{0}$). We are therefore forced to set λ equal to one or another of the roots of the “characteristic polynomial”

$$\det(\mathbb{A} - \lambda\mathbb{I}) = a_0 + a_1\lambda + a_2\lambda^2 + \dots + a_n\lambda^n$$

These, by the fundamental theorem of algebra, are n in number, and may be real or complex even though our tacit assumption that \mathbb{A} be real forces the coefficients $\{a_0, a_1, a_2, \dots, a_n\}$ to be real (and forces the complex roots to occur in conjugate pairs).

EXAMPLE: Looking to the x -parameterized class of cases

$$\mathbb{A}(x) = \begin{pmatrix} 1 & 2 \\ -2 & x \end{pmatrix}$$

we obtain

$$\det \mathbb{A}(x) = (4 - x) - (1 + x)\lambda + \lambda^2$$

giving

$$\lambda = \frac{1}{2} \left[1 + x \pm \sqrt{(x+3)(x-5)} \right]$$

which are

- in real if $x < -3$ or $x > 5$;
- conjugate complex in all cases;
- equal to one another (degenerate) if $x = -3$ or $x = 5$.

Those roots—call them $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ —are the **eigenvalues** (collectively, the **spectrum**) of \mathbb{A} , and their discovery is the first half of “the eigenvalue problem.” The second half is to discover/display the associated **eigenvectors**, the vectors $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ that are defined by the equations

$$\mathbb{A}\mathbf{x}_i = \lambda_i\mathbf{x}_i \quad : \quad i = 1, 2, \dots, n$$

Notice that if \mathbb{A} is real but λ_i is complex then the associated eigenvector \mathbf{x}_i will of necessity be also complex: to accommodate such a development we would have to move beyond our theory of real vector spaces to a theory of complex vector spaces. I introduce now an assumption that will permit us to delay that inevitable effort:

The matrices to which applications draw our attention are very often **symmetric**, a circumstance which I will emphasize by writing \mathbb{S} instead of \mathbb{A} :

$$\mathbb{S}^T = \mathbb{S}$$

THEOREM: The eigenvalues of any real symmetric matrix \mathbb{S} are necessarily and invariably *real*.

Proof: Starting from $\mathbb{S}\mathbf{x}_i = \lambda_i\mathbf{x}_i$ and proceeding in the recognition that \mathbf{x}_i may be complex, construct $\mathbf{x}_i^* \mathbb{S} \mathbf{x}_i = \lambda_i(\mathbf{x}_i^* \cdot \mathbf{x}_i)$. Clearly, the number $\mathbf{x}_i^* \cdot \mathbf{x}_i$ is (since, by the symmetry of the dot product, equal to its own conjugate) is real in all cases. Appealing first to the symmetry and then to the reality of \mathbb{S} we have

$$\mathbf{x}_i^* \cdot \mathbb{S} \mathbf{x}_i = \mathbf{x}_i \cdot \mathbb{S} \mathbf{x}_i^* = (\mathbf{x}_i^* \cdot \mathbb{S} \mathbf{x}_i)^*$$

So

$$\lambda_i = \frac{\mathbf{x}_i^* \cdot \mathbb{S} \mathbf{x}_i}{\mathbf{x}_i^* \cdot \mathbf{x}_i} = \text{ratio of two real numbers} \quad \text{QED}$$

From the reality of \mathbb{S} and λ_i it follows that, without loss of generality, one can assume \mathbf{x}_i to be real.

THEOREM: Eigenvectors associated with *distinct* eigenvalues of any real symmetric matrix \mathbb{S} are necessarily and invariably *orthogonal*.

Proof: Starting from

$$\mathbb{S} \mathbf{x}_i = \lambda_i \mathbf{x}_i$$

$$\mathbb{S} \mathbf{x}_j = \lambda_j \mathbf{x}_j$$

construct

$$\mathbf{x}_j \cdot \mathbb{S} \mathbf{x}_i = \lambda_i \mathbf{x}_j \cdot \mathbf{x}_i$$

$$\mathbf{x}_i \cdot \mathbb{S} \mathbf{x}_j = \lambda_j \mathbf{x}_i \cdot \mathbf{x}_j$$

From the symmetry of \mathbb{S} it follows that the expressions on the left (therefore also those on the right) are equal. Which by the symmetry of the dot product means that

$$(\lambda_i - \lambda_j) \mathbf{x}_i \cdot \mathbf{x}_j = 0$$

But by assumption $(\lambda_i - \lambda_j) \neq 0$, so

$$\mathbf{x}_i \cdot \mathbf{x}_j = 0 \quad : \quad i \neq j \quad \text{QED}$$

We can without loss of generality assume the \mathbf{x}_i to have been normalized (which we emphasize by writing \mathbf{e}_i in place of \mathbf{x}_i). This done, we have (or, in cases of spectral degeneracy, can “by hand” *arrange* to have)

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} \quad (24)$$

We conclude that implicit in the design of every such \mathbb{S} is an \mathbb{S} -adapted orthonormal basis in the vector space upon which \mathbb{S} acts.

THEOREM: Every real symmetric matrix \mathbb{S} can be “rotated to diagonal form,” with its eigenvalues strung along the diagonal. To say the same thing another way: There always exists a real rotation matrix \mathbb{R} ($\mathbb{R}^T \mathbb{R} = \mathbb{I}$: see again page19) such that

$$\mathbb{R}^T \mathbb{S} \mathbb{R} = \begin{pmatrix} \lambda_1 & 0 & 0 & \dots & 0 \\ 0 & \lambda_2 & 0 & \dots & 0 \\ 0 & 0 & \lambda_3 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & \lambda_n \end{pmatrix} \quad (25.1)$$

Proof: From the normalized eigenvectors

$$\mathbf{e}_i = \begin{pmatrix} e_{i1} \\ e_{i2} \\ \vdots \\ e_{in} \end{pmatrix}$$

construct $\mathbb{R} \equiv (\mathbf{e}_1 \quad \mathbf{e}_2 \quad \dots \quad \mathbf{e}_n)$. Then

$$\mathbb{R}^T = \begin{pmatrix} \mathbf{e}_1^T \\ \mathbf{e}_2^T \\ \vdots \\ \mathbf{e}_n^T \end{pmatrix}$$

and that $\mathbb{R}^T \mathbb{R} = \mathbb{I}$ is seen to be simply a restatement of the orthonormality conditions (24): $\mathbf{e}_i^T \mathbf{e}_j = \delta_{ij}$. Equally immediate are the statements

$$\begin{aligned} \mathbb{S} \mathbb{R} &= \mathbb{S} \cdot (\mathbf{e}_1 \quad \mathbf{e}_2 \quad \dots \quad \mathbf{e}_n) \\ &= (\lambda_1 \mathbf{e}_1 \quad \lambda_2 \mathbf{e}_2 \quad \dots \quad \lambda_n \mathbf{e}_n) \end{aligned}$$

which entail

$$\begin{aligned} \mathbb{R}^T \mathbb{S} \mathbb{R} &= \begin{pmatrix} \lambda_1 \mathbf{e}_1^T \mathbf{e}_1 & \lambda_2 \mathbf{e}_1^T \mathbf{e}_2 & \dots & \lambda_n \mathbf{e}_1^T \mathbf{e}_n \\ \lambda_1 \mathbf{e}_2^T \mathbf{e}_1 & \lambda_2 \mathbf{e}_2^T \mathbf{e}_2 & \dots & \lambda_n \mathbf{e}_2^T \mathbf{e}_n \\ \vdots & \vdots & & \vdots \\ \lambda_1 \mathbf{e}_n^T \mathbf{e}_1 & \lambda_2 \mathbf{e}_n^T \mathbf{e}_2 & \dots & \lambda_n \mathbf{e}_n^T \mathbf{e}_n \end{pmatrix} \\ &= \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix} \text{ by orthonormality} \quad QED \end{aligned}$$

6. Singular value decomposition (SVD). It has been known for a long time to mathematicians,¹⁵ and is a fact that for several decades has been known to and heavily exploited by experts in numerical computation¹⁶—but that remains generally unfamiliar to physicists—that the “spectral representation”

$$\mathbb{S} = \mathbb{R} \begin{pmatrix} \lambda_1 & 0 & 0 & \dots & 0 \\ 0 & \lambda_2 & 0 & \dots & 0 \\ 0 & 0 & \lambda_3 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & \lambda_n \end{pmatrix} \mathbb{R}^T \quad (25.2)$$

of the real symmetric (square) matrix \mathbb{S} is simply the most familiar instance of a vastly more general representation theorem that pertains **to all—even to rectangular—matrices** \mathbb{S} . I refer to what has come to be called the “singular value decomposition” (or SVD)—of which, by the way, earlier versions of *Mathematica* knew nothing, but *Mathematica5* provides an implementation that is very sweet, and upon which I will draw heavily.

¹⁵ The subject originates in papers published by Eugenio Beltrami (1873) and Camille Jordan (1874), the substance of which was independently reinvented a bit later by J. J. Sylvester and elaborated a generation later by E. Schmidt and Hermann Weyl. See “On the early history of the singular value decomposition” by G. W. Stewart, *SIAM Review* **35**, 551 (1993).

¹⁶ See J. C. Nash, “The singular-value decomposition and its use to solve least squares problems,” in *Compact Numerical Methods for Computers: Linear Algebra & Function Minimization* (2nd edition 1990), pages 30–48; G. H. Golub & C. F. Van Loan, “The singular value decomposition” in *Matrix Computations* (3rd edition 1996), pages 70–71; and J. E. Gentle, “The singular value factorization” in *Numerical Linear Algebra for Applications in Statistics* (1998), pages 102–103.

Let \mathbb{A} be a real¹⁷ $m \times n$ matrix. Construct

$$\begin{aligned}\mathbb{A} \cdot \mathbb{A}^T &: m \times m \text{ real symmetric matrix} \\ \mathbb{A}^T \cdot \mathbb{A} &: n \times n \text{ real symmetric matrix}\end{aligned}$$

Both of these are matrices to which the theory developed in the preceding section directly pertains: the eigenvalues of each will assuredly be real, and (because each is a “square” of sorts) we will not be surprised if the eigenvalues turn out to be non-negative.

EXAMPLE: Let

$$\mathbb{A} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 2 & 3 & 4 \\ 5 & 6 & 7 \\ 3 & 4 & 5 \end{pmatrix}$$

The commands `Eigenvalues[$\mathbb{A} \cdot \mathbb{A}^T$]` & `Eigenvalues[$\mathbb{A}^T \cdot \mathbb{A}$]` provide

$$\{278.924, 1.07556, 0, 0, 0\}$$

and $\{278.924, 1.07556, 0\}$

respectively. The “singular values”¹⁸ are the positive square roots of the latter numbers, and are (as here) conventionally presented in descending order:

$$\sigma_1 = \sqrt{278.924} = 16.7010$$

$$\sigma_2 = \sqrt{1.07556} = 1.03709$$

$$\sigma_3 = 0$$

The command `SingularValueDecomposition[N[\mathbb{A}]]`¹⁹ produces a list of three matrices

$$\mathbb{U} = \begin{pmatrix} -0.219 & -0.743 & -0.615 & -0.140 & -0.049 \\ -0.525 & +0.155 & +0.196 & -0.757 & -0.298 \\ -0.321 & -0.444 & +0.582 & +0.443 & -0.407 \\ -0.627 & +0.454 & -0.422 & +0.459 & -0.103 \\ -0.423 & -0.144 & +0.259 & -0.005 & +0.856 \end{pmatrix}$$

¹⁷ The theory is usually presented as it pertains to *complex* matrices. It is only for expository simplicity that I have assumed reality.

¹⁸ The obscure terminology is reported to derive from aspects of the work of Schmidt and Weyl, who approached this subject not from linear algebra but from the theory of integral equations.

¹⁹ *Mathematica* would read (say) 3 in this context as an implicit demand that it work in higher precision than its algorithm is designed to achieve: it insists that we instead write `N[3]=3.0`, *etc.*

$$\mathbb{D} = \begin{pmatrix} 16.70 & 0. & 0. \\ 0. & 1.037 & 0. \\ 0. & 0. & 0. \\ 0. & 0. & 0. \\ 0. & 0. & 0. \end{pmatrix}$$

$$\mathbb{V} = \begin{pmatrix} -0.441 & +0.799 & +0.408 \\ -0.568 & +0.103 & -0.816 \\ -0.695 & -0.592 & +0.408 \end{pmatrix}$$

Executing the commands

```
Transpose[U].U//Chop//MatrixForm
Transpose[V].V//Chop//MatrixForm
```

(//Chop discards artifacts of the order 10^{-16} , and I have abandoned most of the decimal detail that *Mathematica* carries in its mind) we discover that \mathbb{U} and \mathbb{V} are both *rotation matrices*, while \mathbb{D} is “diagonal” in the lopsided sense that the example serves to define. Finally we execute the command

```
A-U.D.Transpose[V]//Chop//MatrixForm
```

and discover that, in this instance,

$$\mathbb{A} = \mathbb{U}\mathbb{D}\mathbb{V}^T \quad (26)$$

The remarkable fact—the upshot of the **singular value decomposition theorem**, which I will not attempt to prove—is that decompositions of the form (26) are available *in all cases*. When \mathbb{A} is square and symmetric (26) gives back precisely (25.2) or (when one or more of the eigenvalues of \mathbb{A} are negative) to a slight variant thereof.

PROBLEM 8: a) Look to the case

$$\mathbb{A} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 5 & 6 \\ 3 & 6 & 9 \end{pmatrix} \quad : \quad \text{real symmetric}$$

Compare the lists produced by the commands `Eigenvalues[A]//N` and `SingularValueList[N[A]]//Chop`. Write out in matrix form the matrices \mathbb{U} , \mathbb{D} , and \mathbb{V} that are produced by the command `SingularValueDecomposition[N[A]]//Chop`. Compare \mathbb{U} and \mathbb{V} . Demonstrate that \mathbb{U} and \mathbb{V} are rotation matrices, and discuss the relationship in this instance between (26) and (25.2).

b) Repeat those steps in the case

$$\mathbb{B} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 5 & 6 \\ 3 & 6 & 7 \end{pmatrix} \quad : \quad \text{real symmetric}$$

and state your conclusions.

PROBLEM 9: Repeat those steps as they pertain to the extreme case

$$\mathbb{A} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix}$$

and demonstrate that indeed

$$\mathbb{U}\mathbb{D}\mathbb{V}^T = \begin{pmatrix} 1. \\ 2. \\ 3. \\ 4. \end{pmatrix}$$

This exercise serves to underscore the *universality* of the SVD.

PROBLEM 10: a) Show that if the $n \times n$ matrix \mathbb{A} is *antisymmetric* then

$$\begin{aligned} \det \mathbb{A} &= \det \mathbb{A}^T = (-1)^n \det \mathbb{A} \\ &= 0 \quad \text{if } n \text{ is odd} \end{aligned}$$

b) Repeat the now-familiar sequence of steps in the case

$$\mathbb{A} = \begin{pmatrix} 0 & -3 & 4 \\ 3 & 0 & -5 \\ -4 & 5 & 0 \end{pmatrix} \quad : \quad \text{real } \textit{antisymmetric}$$

What's funny about the eigenvalues? Comment on the relation of the eigenvalue list to the singular value list, and on the relation of \mathbb{V} to \mathbb{U} .

c) Use the command `MatrixExp[A]` to construct $\mathbb{R} \equiv e^{\mathbb{A}}$ and show (in anticipation of things to come) that \mathbb{R} is a rotation matrix.

Assume for the moment (as the founding fathers of this subject *always* assumed) that the real matrix $\mathbb{A} = \mathbb{U}\mathbb{D}\mathbb{V}^T$ is square. Then so also with the diagonal matrix

$$\mathbb{D} \equiv \begin{pmatrix} \sigma_1 & 0 & \dots & 0 \\ 0 & \sigma_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & \sigma_n \end{pmatrix}$$

and the rotation matrices \mathbb{U} and \mathbb{V} be square. Clearly

$$\mathbb{D}^{-1} = \begin{pmatrix} 1/\sigma_1 & 0 & \dots & 0 \\ 0 & 1/\sigma_2 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 1/\sigma_n \end{pmatrix}$$

is (when it exists) the left/right inverse of \mathbb{D} , and it will exist if and only if none of singular values σ_i vanishes: $\sigma_1\sigma_2 \cdots \sigma_n \neq 0$. It is clear also that

$$\mathbb{A}^{-1} \equiv \mathbb{V} \mathbb{D}^{-1} \mathbb{U}^{\top} \quad (27)$$

serves to describe (when it exists) the left/right inverse of \mathbb{A} , and that it will exist if and only if \mathbb{D}^{-1} does. We have here a matrix inversion that makes no use of determinants. We will not be terribly surprised, therefore, to discover (recall that $\det \mathbb{A}$ is defined only for square matrices) that (27) has valuable things to say **even when \mathbb{A} is rectangular** (which is to say: **not square**).

We look now to an illustrative case in which \mathbb{A} —still assumed to be square—is **singular** ($\det \mathbb{A} = 0$). The remarkable fact is that we are not in such cases stopped cold in our tracks. We are placed by the SVD in position to salvage all that can be salvaged. Consider the example

$$\mathbb{A} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

which is found to have

$$\begin{aligned} \text{eigenvalues} & : \{16.12, -1.117, 0\} \\ \text{singular values} & : \{16.85, 1.068\} \end{aligned}$$

The command `MatrixRank[\mathbb{A}]` answers the question “How many linearly independent vectors can be constructed from (*i.e.*, what is the dimension of the space spanned by) the rows of \mathbb{A} ? Which in this case turns out to be 2. The command `RowReduce[\mathbb{A}]` produces

$$\mathbb{A}_{\text{row reduced}} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 2 \\ 0 & 0 & 0 \end{pmatrix}$$

which is in effect a list of linearly independent vectors

$$\mathbf{m}_1 \equiv \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{m}_2 \equiv \begin{pmatrix} 0 \\ 1 \\ 2 \end{pmatrix}$$

that are **not annihilated by \mathbb{A}** (nor, indeed, is any linear combination of those vectors). The command `NullSpace[\mathbb{A}]` responds, on the other hand, with a list—here a list with a single entry

$$\mathbf{n}_1 = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

—of linearly independent vectors that **are annihilated by \mathbb{A}** . Generally, the vectors $\{\mathbf{n}_1, \mathbf{n}_2, \dots, \mathbf{n}_q\}$ span the “null space” of \mathbb{A} , a q -dimensional subspace \mathcal{N} of the vector space \mathcal{V} upon which \mathbb{A} acts, while the $\{\mathbf{m}_1, \mathbf{m}_2, \dots, \mathbf{m}_p\}$ span

the $p = n - q = \text{Rank}[\mathbb{A}]$ -dimensional complement \mathcal{N}^* of \mathcal{N} . Elements of \mathcal{N}^* are orthogonal to elements of \mathcal{N} : in the present instance we verify that indeed

$$\mathbf{m}_1 \cdot \mathbf{n}_1 = \mathbf{m}_2 \cdot \mathbf{n}_1 = 0$$

For $\mathbf{x} \in \mathcal{N}$ we have $\mathbb{A}\mathbf{x} = \mathbf{0}$ and it is unreasonable to expect to be able to write $\mathbf{x} = \mathbb{A}^{-1}\mathbf{0}$, for such an \mathbb{A}^{-1} would recreate \mathbf{x} out of nothing. On the other hand, or \mathbf{x} in \mathcal{N}^* we have $\mathbb{A}\mathbf{x} = \mathbf{y} \neq \mathbf{0}$ and it seems reasonable that we might expect to be able to write $\mathbf{x} = \mathbb{A}^{-1}\mathbf{y}$. The SVD supplies means to do so.

Returning to our example, we have²⁰

$$\mathbb{A} = \mathbb{U}\mathbb{D}\mathbb{V}^T$$

$$\mathbb{D} = \begin{pmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \\ 0 & 0 & \sigma_3 \end{pmatrix} \quad \text{with } \sigma_1 > \sigma_2 > \sigma_3 = \mathbf{0}$$

and construct

$$\mathbb{A}^* \equiv \mathbb{V}\mathbb{D}^*\mathbb{U}^T$$

with (note the 0 in the σ_3 place, where one might have expected to find an ∞)

$$\mathbb{D}^* \equiv \begin{pmatrix} (\sigma_1)^{-1} & 0 & 0 \\ 0 & (\sigma_2)^{-1} & 0 \\ 0 & 0 & \mathbf{0} \end{pmatrix}$$

and verify by computation that

$$\left. \begin{aligned} \mathbb{A}^* \cdot \mathbb{A}\mathbf{m}_1 &= \mathbf{m}_1 \\ \mathbb{A}^* \cdot \mathbb{A}\mathbf{m}_2 &= \mathbf{m}_2 \\ \mathbb{A}^* \cdot \mathbb{A}\mathbf{n}_1 &= \mathbf{0} \end{aligned} \right\} \quad (27)$$

Evidently \mathbb{A}^* acts as an inverse on \mathcal{N}^* , but acts passively on \mathcal{N} .

The wonderful fact—at which I hinted already on the preceding page—is that this basic strategy works even when \mathbb{A} is rectangular. Consider the example

$$\mathbb{B} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \\ 3 & 5 & 7 \end{pmatrix}$$

which has rank 2. Such a matrix cannot be said to have eigenvalues, but its singular values are well defined: they are $\{19.10, 1.818\}$ (always equal in number to the rank). The space \mathcal{N}^* is again 2 dimensional, and spanned by the same vectors \mathbf{m}_1 and \mathbf{m}_2 as were encountered in the preceding example. The

²⁰ It would be distracting and not very informative to write out the numeric details, which I will be content to allow to remain in the mind of the computer.

null space \mathcal{N} is again 1-dimensional, and spanned again by \mathbf{n}_1 . But \mathbb{U} is now 4×4 , \mathbb{V} is now 3×3 and \mathbb{D} given now by

$$\mathbb{D} = \begin{pmatrix} 19.10 & 0 & 0 \\ 0 & 1.818 & 0 \\ 0 & 0 & \mathbf{0} \\ 0 & 0 & 0 \end{pmatrix}$$

From

$$\mathbb{D}^* = \begin{pmatrix} (19.10)^{-1} & 0 & 0 & 0 \\ 0 & (1.811)^{-1} & 0 & 0 \\ 0 & 0 & \mathbf{0} & 0 \end{pmatrix}$$

we construct $\mathbb{A}^* \equiv \mathbb{V}\mathbb{D}^*\mathbb{U}^\top$ —which was 3×3 but is now 3×4 —and again recover (27).

Look finally to the case

$$\mathbb{C} = \begin{pmatrix} 1 & 4 & 7 & 3 \\ 2 & 5 & 8 & 5 \\ 3 & 6 & 9 & 7 \end{pmatrix} = \mathbb{B}^\top$$

which has rank 2 and the same singular values as \mathbb{B} . \mathcal{N}^* is again 2-dimensional, and spanned by

$$\mathbf{m}_1 = \begin{pmatrix} 3 \\ 0 \\ -3 \\ 5 \end{pmatrix}, \quad \mathbf{m}_2 = \begin{pmatrix} 0 \\ 3 \\ 6 \\ 1 \end{pmatrix}$$

But the null space \mathcal{N} is now also 2-dimensional, spanned by

$$\mathbf{n}_1 = \begin{pmatrix} -5 \\ -1 \\ 0 \\ 3 \end{pmatrix}, \quad \mathbf{n}_2 = \begin{pmatrix} 1 \\ -2 \\ 1 \\ 0 \end{pmatrix}$$

We verify again that $\mathcal{N}^* \perp \mathcal{N}$. From

$$\mathbb{D} = \begin{pmatrix} 19.10 & 0 & 0 & 0 \\ 0 & 1.811 & 0 & 0 \\ 0 & 0 & \mathbf{0} & 0 \end{pmatrix}$$

we construct

$$\mathbb{D}^* = \begin{pmatrix} (19.10)^{-1} & 0 & 0 \\ 0 & (1.818)^{-1} & 0 \\ 0 & 0 & \mathbf{0} \\ 0 & 0 & 0 \end{pmatrix}$$

and proceed as before to the same satisfactory conclusion.

Thus are we able to assign a useful interpretation to the statement that “**every real matrix—whether square or rectangular—is invertible.**” We find ourselves in position to discuss sensibly the solution of *any* linear system (16), even those that are under/overdetermined. We have in hand what Riley *et al* (their page 307) call “the method of choice in analyzing any set of simultaneous linear equations.”

EXAMPLE: Suppose we had interest in the overdetermined system

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 2 & 3 & 4 \\ 5 & 6 & 7 \\ 3 & 4 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{pmatrix} \quad : \quad \text{more compactly } \mathbb{A}\mathbf{x} = \mathbf{b}$$

where \mathbb{A} figured already in the example on page 30. \mathbb{A} is of rank 2, and its 1-dimensional null space is spanned once again by

$$\mathbf{n} = \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

By computation

$$\mathbb{A}^* = \frac{1}{30} \begin{pmatrix} -17 & 4 & -10 & 11 & -3 \\ -2 & 1 & -1 & 2 & 0 \\ 13 & -2 & 8 & -7 & 3 \end{pmatrix}$$

Writing

$$\mathbf{b} = \mathbf{b}_{\text{non-null}} + \mathbf{b}_{\text{null}}$$

we compute

$$\mathbb{A}\mathbf{b} = \mathbb{A}\mathbf{b}_{\text{non-null}} = \frac{1}{6} \begin{pmatrix} -2 \\ 1 \\ 4 \end{pmatrix} \equiv \mathbf{m} \perp \mathbf{n}$$

giving

$$\mathbf{b}_{\text{non-null}} = \mathbb{A}^*\mathbf{m} = \frac{1}{2} \begin{pmatrix} 4 \\ 7 \\ 5 \\ 8 \\ 6 \end{pmatrix}$$

$$\mathbf{b}_{\text{null}} = \mathbf{b} - \mathbf{b}_{\text{non-null}} = \frac{1}{2} \begin{pmatrix} -2 \\ -3 \\ 1 \\ 0 \\ 4 \end{pmatrix}$$

and with these statements we can explicitly verify that

$$\begin{aligned} \mathbb{A}\mathbf{b}_{\text{non-null}} &= \mathbf{m}, & \mathbb{A}^*\mathbf{m} &= \mathbf{b}_{\text{non-null}} \\ \mathbb{A}\mathbf{b}_{\text{null}} &= \mathbf{0}, & \mathbb{A}^*\mathbf{0} &= \mathbf{0} \end{aligned}$$

For a useful brief discussion of the preceding subject matter one might inquire after “linear systems” in the *Mathematica5* Help Browser, which opens an electronic version of §3.7.8 in the most recent edition of S. Wolfram’s text. Google (ask for SVD) leads also to a great many sources, some of which are quite informative. See also §8.18.3 in Riley *et al.*

7. Alternative approach to the same material. Imagine that you have in front of you a device the output b of which is controlled by n adjustable precision dials. In the i^{th} of a series of m experiments you set the dials to read

$$\{a_{i1}, a_{i2}, \dots, a_{in}\} \quad : \quad i = 1, 2, \dots, m$$

and measure as best you can the output

$$x_i = X_i + e_i \quad : \quad \begin{cases} X_i \text{ is the “true value” for that dial setting} \\ e_i \text{ is error} \end{cases}$$

You conjecture that the output depends *linearly* on the dial settings

$$X_i = a_{i1}k_1 + a_{i2}k_2 + \dots + a_{in}k_n = x_i - e_i$$

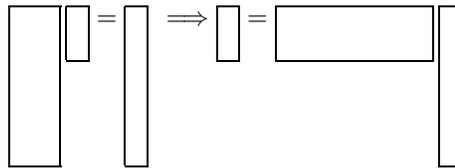
and seek “best estimated values” of the constants $\{k_1, k_2, \dots, k_n\}$. With Gauss, you interpret “best” to mean “the k -values that minimize $\sum_i (e_i)^2$ ”. In an obvious matrix notation, your problem is to minimize the length of the “error vector” $\mathbf{e} = \mathbb{A}\mathbf{k} - \mathbf{x}$; *i.e.*, to discover the \mathbf{k} that serves to

$$\begin{aligned} \text{MINIMIZE} \quad : \quad (\mathbb{A}\mathbf{k} - \mathbf{x})^\top (\mathbb{A}\mathbf{k} - \mathbf{x}) &= \mathbf{k}^\top \mathbb{A}^\top \mathbb{A} \mathbf{k} - \mathbf{k}^\top \mathbb{A}^\top \mathbf{x} - \mathbf{x}^\top \mathbb{A} \mathbf{k} + \mathbf{x}^\top \mathbf{x} \\ &= \mathbf{k}^\top (\mathbb{A}^\top \mathbb{A} \mathbf{k} - 2\mathbb{A}^\top \mathbf{x}) + \mathbf{x}^\top \mathbf{x} \end{aligned}$$

Differentiating with respect to each of the components of \mathbf{k} , then setting all derivatives equal to zero, we find $\mathbf{k} = (\mathbb{A}^\top \mathbb{A})^{-1} \mathbb{A}^\top \mathbf{x}$. In short: were it the case that $\mathbf{e} = \mathbf{0}$ we would be proceeding

$$\begin{aligned} \text{from } \mathbb{A}\mathbf{k} = \mathbf{x} \quad \text{to} \quad \mathbf{k} &= \mathbb{A}_{\text{pseudo inverse}} \mathbf{x} \\ \mathbb{A}_{\text{pseudo inverse}} &\equiv (\mathbb{A}^\top \mathbb{A})^{-1} \mathbb{A}^\top \end{aligned}$$

In practice a good experimentalist would, in an effort to achieve high accuracy, make many measurements ($m \gg n$) and confront the situation of illustrated below:



The train of thought sketched above appears to have occurred first to E. H. Moore, whose remarks at a regional meeting in 1920 of the American

Mathematical Society are summarized in that society's Bulletin²¹ but attracted little attention. The subject was independently reinvented in the mid-1950s by Roger Penrose, whose initial publication²² lacked clear motivation and was phrased quite abstractly, but was followed promptly by a paper²³ intended to establish "relevance to the statistical problem of finding 'best' approximate solutions of inconsistent systems of equations by the method of least squares." The matrix that I have denoted $\mathbb{A}_{\text{pseudo inverse}}$ is often called the "generalized left inverse" or "Moore-Penrose inverse," and is constructed by *Mathematica5* in response to the command "PseudoInverse[A]." The remarkable fact is that

\mathbb{A}^* and $\mathbb{A}_{\text{pseudo inverse}}$ refer to the **same object**

I will not belabor the demonstration, but offer a single example to illustrate the point: let

$$\mathbb{A} = \begin{pmatrix} 1 & 2 \\ 2 & 3 \\ 3 & 4 \\ 4 & 5 \\ 5 & 6 \end{pmatrix}$$

Looking first to \mathbb{A}^* and then to $\mathbb{A}_{\text{pseudo inverse}}$ we find that

$$\mathbb{A}^* = \mathbb{A}_{\text{pseudo inverse}} = \begin{pmatrix} -1.0 & -0.6 & -0.2 & 0.2 & 0.6 \\ 0.8 & 0.5 & 0.2 & -0.1 & -0.4 \end{pmatrix}$$

and that the pseudo inverse is (with *Mathematica5*'s indispensable assistance) much *easier* to evaluate.

PROBLEM 11: Evaluate the pseudo inverse of

$$\mathbb{A} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{pmatrix}$$

What do you make of the denominators? What do you guess would be the pseudo inverse of an *arbitrary* single-column matrix (or vector)?

8. A clever application of the SVD. I turn finally to discussion of an application of SVD-related ideas that was brought to my attention by Joel Franklin, and that originated in some of his own work having to do with the mechanics of many-body systems. Let N points be interconnected by $\nu \leq N(N-1)$ rigid

²¹ Bull. Amer. Math. Soc. (2) **26**, 394 (1920).

²² "A generalized inverse for matrices," Proc. Camb. Phil. Soc. **51**, 406 (1955).

²³ "On best approximate solutions of linear matrix equations," Proc. Camb. Phil. Soc. **52**, 17 (1956).

linkages. Our problem is to decide whether or not the linkages render the point system rigid. The problem could be posed in any number of dimensions: I will, for expository convenience, assume that the points lie in a plane. Let vectors $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\}$ mark the positions of the points, and let vectors $\{\mathbf{a}_1, \mathbf{a}_2, \dots, \mathbf{a}_\nu\}$ describe the linkages:

$$\mathbf{a}_\alpha = \mathbf{x}_{j(\alpha)} - \mathbf{x}_{i(\alpha)} \quad : \quad \text{links } i^{\text{th}} \text{ point to the } j^{\text{th}}$$

The assumed inextensibility of the linkages means that point-adjustment is allowed only to the extent that it preserves each of the numbers

$$\varphi_\alpha(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N) \equiv \frac{1}{2} \mathbf{a}_\alpha \cdot \mathbf{a}_\alpha$$

Writing $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N\} \mapsto \{\mathbf{x}_1 + \delta\mathbf{x}_1, \mathbf{x}_2 + \delta\mathbf{x}_2, \dots, \mathbf{x}_N + \delta\mathbf{x}_N\}$ to describe an infinitesimal adjustment, we find that the $\delta\mathbf{x}$'s are constrained to satisfy

$$\sum_{k=1}^N \nabla_k \varphi_\alpha(\mathbf{x}) \cdot \delta\mathbf{x}_k = 0$$

EXAMPLE: Reading from the FIGURE 10 we have

$$\begin{aligned} \mathbf{a}_1 &= \mathbf{x}_2 - \mathbf{x}_1 \\ \mathbf{a}_2 &= \mathbf{x}_3 - \mathbf{x}_2 \\ \mathbf{a}_3 &= \mathbf{x}_1 - \mathbf{x}_3 \\ \mathbf{a}_4 &= \mathbf{x}_4 - \mathbf{x}_1 \end{aligned}$$

giving

$$\begin{aligned} \delta\varphi_1 &= (\mathbf{x}_2 - \mathbf{x}_1) \cdot (\delta\mathbf{x}_2 - \delta\mathbf{x}_1) = 0 \\ \delta\varphi_2 &= (\mathbf{x}_3 - \mathbf{x}_2) \cdot (\delta\mathbf{x}_3 - \delta\mathbf{x}_2) = 0 \\ \delta\varphi_3 &= (\mathbf{x}_1 - \mathbf{x}_3) \cdot (\delta\mathbf{x}_1 - \delta\mathbf{x}_3) = 0 \\ \delta\varphi_4 &= (\mathbf{x}_4 - \mathbf{x}_1) \cdot (\delta\mathbf{x}_4 - \delta\mathbf{x}_1) = 0 \end{aligned}$$

which when spelled out in detail can be written²⁴

$$\begin{pmatrix} -X_{21} & -Y_{21} & +X_{21} & +Y_{21} & 0 & 0 & 0 & 0 \\ 0 & 0 & -X_{32} & -Y_{32} & +X_{32} & +Y_{32} & 0 & 0 \\ +X_{13} & +Y_{13} & 0 & 0 & -X_{13} & -Y_{13} & 0 & 0 \\ -X_{41} & -Y_{41} & 0 & 0 & 0 & 0 & +X_{41} & +Y_{41} \end{pmatrix} \begin{pmatrix} \delta x_1 \\ \delta y_1 \\ \delta x_2 \\ \delta y_2 \\ \delta x_3 \\ \delta y_3 \\ \delta x_4 \\ \delta y_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

and abbreviated $\mathbb{J} \boldsymbol{\delta} = \mathbf{0}$. To see more clearly past the notational

²⁴ Here $X_{ij} \equiv x_i - x_j$, $Y_{ij} \equiv y_i - y_j$.

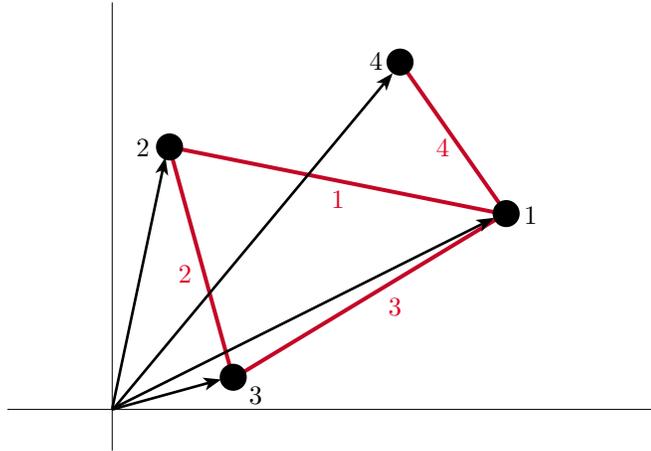


FIGURE 10: A system of 4 points interconnected by four linkages.

clutter we observe that \mathbb{J} possesses the design

$$\mathbb{J} = \begin{pmatrix} -a & -b & a & b & 0 & 0 & 0 & 0 \\ 0 & 0 & -c & -d & c & d & 0 & 0 \\ e & f & 0 & 0 & -e & -f & 0 & 0 \\ -g & -h & 0 & 0 & 0 & 0 & g & h \end{pmatrix}$$

We are informed by *Mathematica5* that

$$\text{MatrixRank}[\mathbb{J}] = 4$$

(this is, after all, obvious to the unaided eye) which means that the associated null space \mathcal{N} is $8 - 4 = 4$ dimensional. But rigid objects on the plane have only 3 degrees of freedom: two translational and one rotational. We conclude that the object shown in the figure has one “floppy degree of freedom,” and it is easy to see what it is: point #4 is not tied down. If we link that point to point #2 then

$$\mathbb{J} \mapsto \mathbb{K} = \begin{pmatrix} -a & -b & a & b & 0 & 0 & 0 & 0 \\ 0 & 0 & -c & -d & c & d & 0 & 0 \\ e & f & 0 & 0 & -e & -f & 0 & 0 \\ -g & -h & 0 & 0 & 0 & 0 & g & h \\ 0 & 0 & m & n & 0 & 0 & -m & -n \end{pmatrix}$$

\mathbb{K} is seen to have rank 5, the associated null space \mathcal{N} is only 3-dimensional, the system has become rigid. The command

$$\text{NullSpace}[\mathbb{K}]$$

works—even though \mathbb{K} is symbolic (not numerical)—to produce a triple of symbolic vectors that comprise a basis in \mathcal{N} . One readily verifies that, in particular, the vectors

$$\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}$$

that serve respectively to describe x -translation and y -translation lie in \mathcal{N} . Orthogonal to them (and more difficult to describe) is the vector that generates infinitesimal rotations.