

Excursions in Computing Science:

Week 8. Higher Dimensions: 2D Graphics and Internet Search

T. H. Merrett*
McGill University, Montreal, Canada

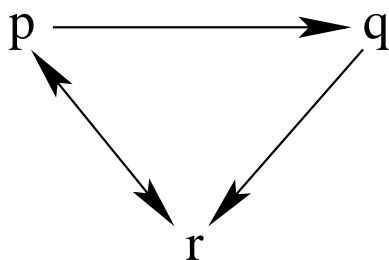
April 20, 2012

I. Prefatory Notes

A. Eigenvectors and Google Page Ranking

1. How do we find out how important a web page is?

We can suppose, circularly, that a page is important if important pages link to it.



Since p has two outgoing links, let's say it divides its importance between q and r .

$$\sqrt{\quad} \begin{array}{c} p \quad q \quad r \\ p \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix} \\ q \\ r \end{array}$$

$$\sqrt{\quad} \begin{array}{c} p \quad q \quad r \\ p \begin{pmatrix} 0 & 0 & 1 \\ \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 1 & 0 \end{pmatrix} \\ q \\ r \end{array}$$

Let's play with this.

Suppose p has importance 1 and q and r have importance 0.

$$\begin{pmatrix} 0 & 0 & 1 \\ 1/2 & 0 & 0 \\ 1/2 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix} \rightarrow \begin{pmatrix} 1/2 \\ 0 \\ 1/2 \end{pmatrix} \rightarrow \begin{pmatrix} 1/2 \\ 1/4 \\ 1/4 \end{pmatrix} \rightarrow \begin{pmatrix} 1/4 \\ 1/4 \\ 1/2 \end{pmatrix} \rightarrow \begin{pmatrix} 1/2 \\ 1/8 \\ 3/8 \end{pmatrix} \rightarrow \begin{pmatrix} 3/8 \\ 1/4 \\ 3/8 \end{pmatrix} \rightarrow \dots$$

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Is this settling down to something?

Try

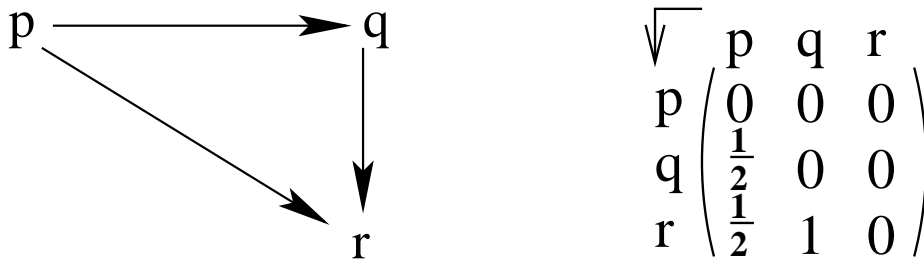
$$\begin{pmatrix} 0 & 0 & 1 \\ 1/2 & 0 & 0 \\ 1/2 & 1 & 0 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix} \rightarrow \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix}$$

or

$$W\vec{R} = w\vec{R}$$

\vec{R} is called an “eigenvector” of W ; w , an ordinary number, is called an “eigenvalue”.

2. But the web doesn't have many cycles.



And now the importance just fades away.

$$\begin{pmatrix} 0 & 0 & 0 \\ 1/2 & 0 & 0 \\ 1/2 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ 1/2 \\ 1/2 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ 0 \\ 1/2 \end{pmatrix} \rightarrow \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

So we need a way to sustain the importance of a page.

Try $W\vec{R} + \vec{S}$ for a “source vector”, \vec{S} , i.e.,

$$\vec{R}' = m(W\vec{R} + \vec{S}), \quad m \stackrel{\text{def}}{=} 1/w$$

If we can get $\vec{R}' = mA\vec{R}$ for some matrix A , we get back to an eigenvector problem:

- make \vec{S} a matrix, $\vec{S}\vec{1}^T = \vec{S}(1, 1, 1)$;
- keep $\|\vec{R}\|_1 \stackrel{\text{def}}{=} \vec{1}^T \vec{R} = R_1 + R_2 + \dots = 1$:

$$\vec{S} = \vec{S} \| R \|_1 = \vec{S}\vec{1}^T \vec{R}$$

So $\vec{R}' = m(W\vec{R} + \vec{S}) = \vec{R}' = m(W + \vec{S}\vec{1}^T)\vec{R}$

and, to find eigenvectors, $\vec{R}' = \vec{R}$.

What should \vec{S} be?

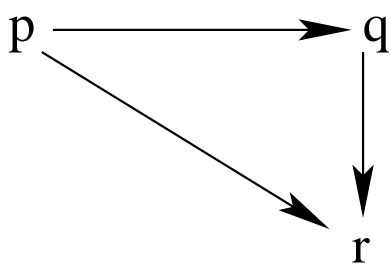
The Google page rank method uses

$$\vec{S} = \alpha\vec{1}; \quad \|\vec{S}\|_1 = 0.15$$

So, for 3D

$$\vec{S} = 0.05 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}; \quad \vec{S}\vec{1}^T = 0.05 \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix}$$

3. So now W becomes $W + S1^T$

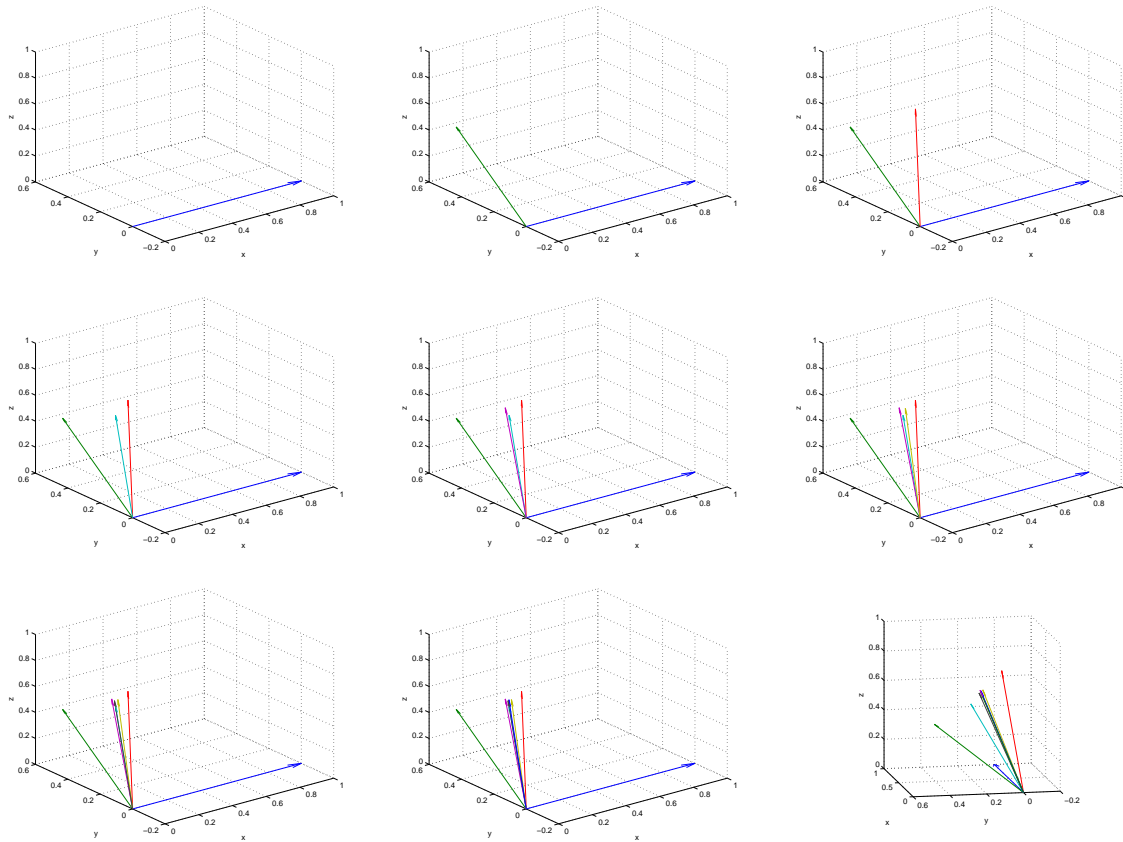


$$\sqrt{\begin{matrix} p & q & r \\ p & \begin{pmatrix} 0.05 & 0.05 & 0.05 \\ 0.55 & 0.05 & 0.05 \\ 0.55 & 1.05 & 0.05 \end{pmatrix} \\ q \\ r \end{matrix}}$$

$$\begin{pmatrix} 0.05 & 0.05 & 0.05 \\ 0.55 & 0.05 & 0.05 \\ 0.55 & 1.05 & 0.05 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \rightarrow \begin{pmatrix} 0.05 \\ 0.55 \\ 0.55 \end{pmatrix} \rightarrow 1.15 \begin{pmatrix} 0.0435 \\ 0.4783 \\ 0.4783 \end{pmatrix} \rightarrow ? \begin{pmatrix} 0.0744 \\ 0.1068 \\ 0.8188 \end{pmatrix} \rightarrow ? \begin{pmatrix} 0.1510 \\ 0.2673 \\ 0.5837 \end{pmatrix} \rightarrow \dots$$

$$\rightarrow ? \begin{pmatrix} 0.1507 \\ 0.2174 \\ 0.6769 \end{pmatrix} \rightarrow ? \begin{pmatrix} 0.1507 \\ 0.2174 \\ 0.6769 \end{pmatrix} \rightarrow \dots$$

Here, the ? indicates the factor that has been removed at each iteration in order that $\|R\|_1 = 1$.



The values have converged to four decimal places after a dozen iterations. (They still keep changing at higher precisions.)

Roughly, $p : q : r = 1 : 2 : 7$.

It is certainly plausible from the web diagram that r should be more important than p or q , both of which supply it with importance, and that p should be of least importance, since nobody else links to it.

B. Linear Equations and Sketchpad

4. Elementary row operations.

1. Multiply row by nonzero constant.
2. Swap two rows.
3. Add multiple of one row to another row.

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$1. \begin{pmatrix} 2x' \\ y' \end{pmatrix} = \begin{pmatrix} 2a & 2c \\ b & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$2. \begin{pmatrix} y' \\ x' \end{pmatrix} = \begin{pmatrix} b & d \\ a & c \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$3. \begin{pmatrix} x' + 2y' \\ y' \end{pmatrix} = \begin{pmatrix} a + 2b & c + 2d \\ b & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

Solving equations: given (x', y') find (x, y) .

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\text{Use (1)} \begin{pmatrix} x'/a \\ y' \end{pmatrix} = \begin{pmatrix} 1 & c/a \\ b & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{“normalize row”}$$

$$\text{Use (3)} \begin{pmatrix} x'/a \\ y' - bx'/a \end{pmatrix} = \begin{pmatrix} 1 & c/a \\ 0 & d - bc/a \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{“zeros below the 1”}$$

$$\text{Use (1)} \begin{pmatrix} x'/a \\ \frac{y' - bx'/a}{d - bc/a} \end{pmatrix} = \begin{pmatrix} 1 & c/a \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{“normalize row”}$$

$$\text{Use (3)} \begin{pmatrix} x'/a - \frac{c}{a} \frac{y' - bx'/a}{d - bc/a} \\ \frac{y' - bx'/a}{d - bc/a} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{ (“zeros above the 1”)}$$

Note. (2) is used to avoid division by zero (or by very small numbers).

Note. This can be used to find the determinant: keep the product of the denominators,

$$a(d - bc/a) = ad - bc$$

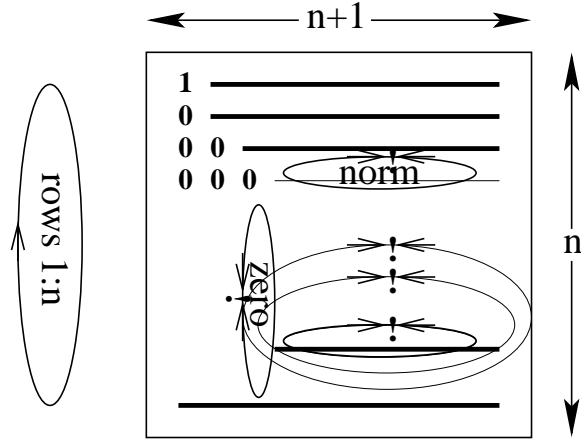
5. Gauss elimination

Do elementary row operations on the “augmented matrix”

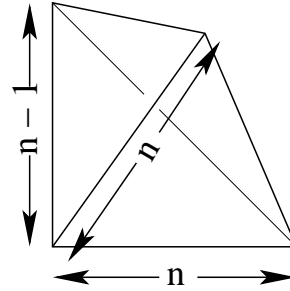
$$\begin{pmatrix} a & b & x' \\ c & d & y' \end{pmatrix}$$

1. Triangularization

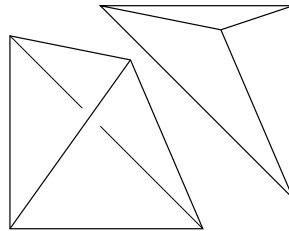
$i = 1:n$
 $\left. \begin{array}{l} n+1-i \\ n-i \end{array} \right\} \begin{array}{l} \bullet \text{ normalize row} \\ \bullet \text{ zeros below the 1} \\ \bullet \text{ rest of the subtractions} \end{array}$
 elements changed: $k(k-1)$ $k = n + 1 - i$



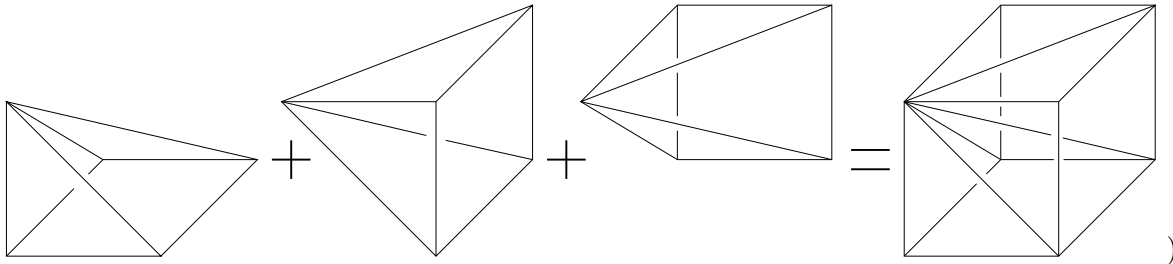
Therefore $\mathcal{O}(n^3)$ elements are changed.
 Or, more precisely, $\frac{1}{3}n^3 + \mathcal{O}(n^2)$,
 which is twice the volume of a tetrahedron:
 $(k(k-1) = 2(k!2)$ elements are changed in
 the innermost loop and $\sum_1^n k!2 = (n+1)!3$,
 which can be presented as a tetrahedron.)



(2 tetrahedra = 1 pyramid)

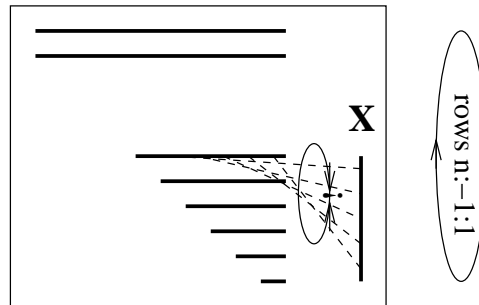
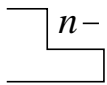


and 3 pyramids = 1 cube:



2. Back-substitution

$$i = n-1: -1: 1$$



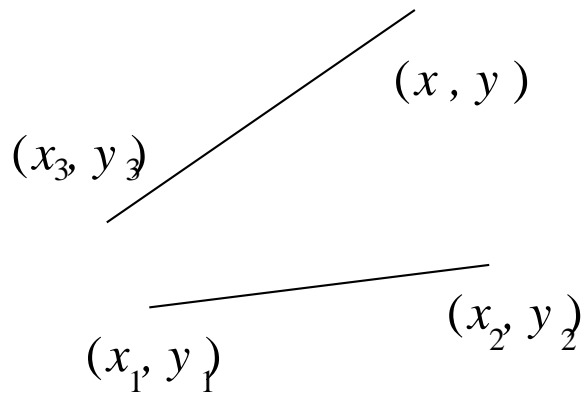
$\mathcal{O}(n^2)$, in fact, $n^2/2$.

6. Sketchpad : 3D for 2D graphics

Drawing program which allows users to specify *constraints*.

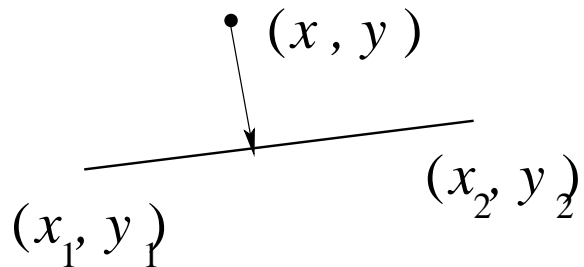
E.g., two lines must have the same length.

$$0 = \text{error} = (x - x_3)^2 + (y - y_3)^2 - ((x_2 - x_1)^2 + (y_2 - y_1)^2)$$



E.g., three points must be collinear.

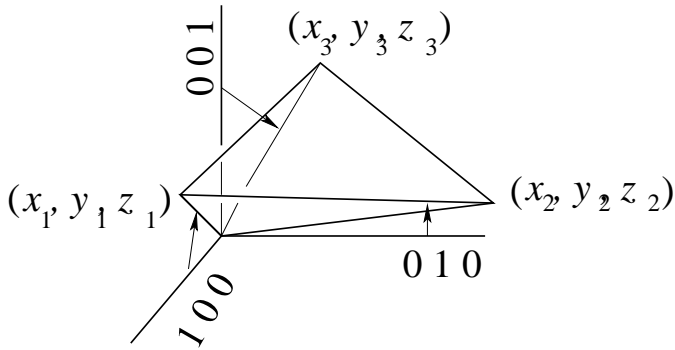
$$0 = \text{error} = \begin{vmatrix} x_1 & x_2 & x \\ y_1 & y_2 & y \\ 1 & 1 & 1 \end{vmatrix}$$



Note. Determinant of 3×3 is volume (by definition):

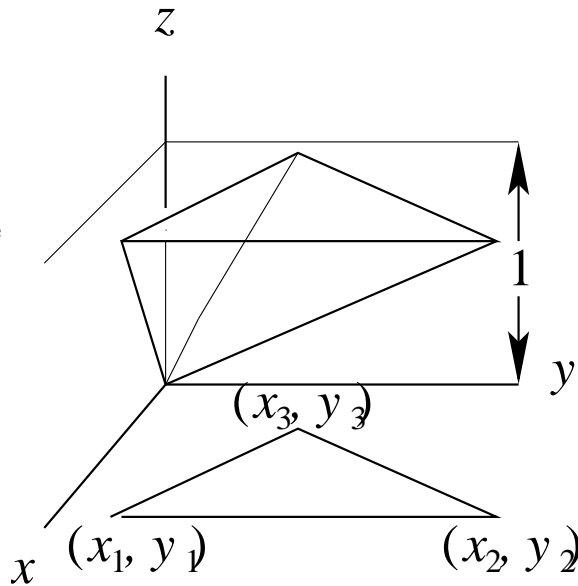
$$\begin{pmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}$$

etc. (The definition of the determinant must also include the requirement that it changes sign whenever any pair of columns is swapped. This is a property of volumes, as suggested by Clifford algebra (Week 7c).)



So, determinant of 3×3 with 1s is triangle area:

$$\frac{1}{2} \begin{vmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ 1 & 1 & 1 \end{vmatrix}$$

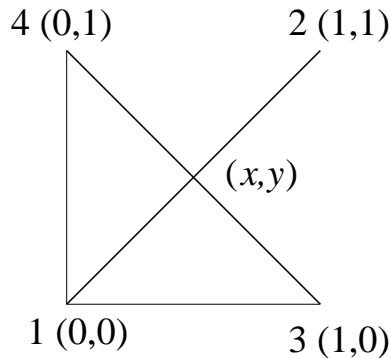


7. Sketchpad example 1 (linear constraint):

Find where two lines intersect.

$$0 = \begin{vmatrix} x_1 & x_2 & x \\ y_1 & y_2 & y \\ 1 & 1 & 1 \end{vmatrix} = \begin{vmatrix} 0 & 1 & x \\ 0 & 1 & y \\ 1 & 1 & 1 \end{vmatrix} = y - x$$

$$0 = \begin{vmatrix} x_3 & x_4 & x \\ y_3 & y_4 & y \\ 1 & 1 & 1 \end{vmatrix} = \begin{vmatrix} 1 & 0 & x \\ 0 & 1 & y \\ 1 & 1 & 1 \end{vmatrix} = 1 - x - y$$



That is

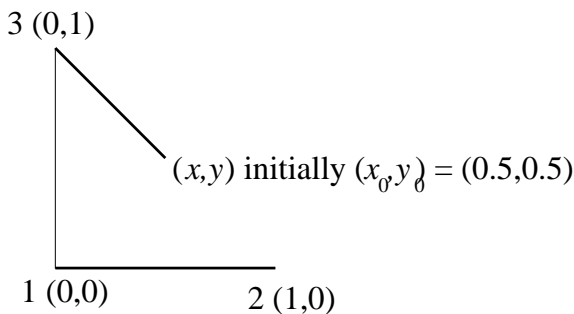
$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

Or, by Gaussian elimination,

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}; \quad \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}; \quad \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1/2 \\ 1/2 \end{pmatrix}$$

8. Sketchpad example 2 (nonlinear constraint):

Let's constrain $((0,1),(x,y))$ to have the same length as $((0,0),(1,0))$, i.e., 1



$$1 = (x - x_3)^2 + (y - y_3)^2 = (x - 0)^2 + (y - 1)^2 = x^2 + (y + 1)^2$$

$$\text{error}_{\text{length}} = x^2 + (y + 1)^2 - 1$$

a) This is underdetermined: (x,y) could be anywhere on a circle of radius 1.

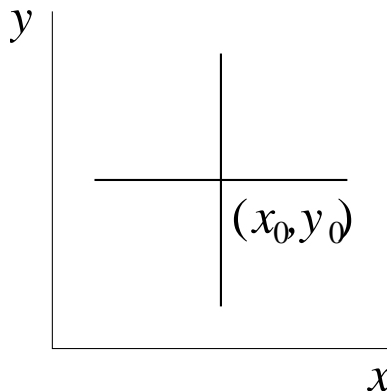
So we'll say that the $((0,1),(x,y))$ line should keep its slope: $x + y = 1$:

$$\text{error}_{\text{slope}} = x + y - 1$$

b) The length constraint is not linear but quadratic. Because we don't always know how to solve nonlinear equations, we'd like to make a *linear approximation* to the nonlinear equation.

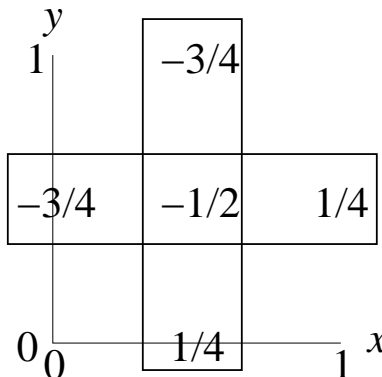
We'll call this a *slope approximation*, because we're going to say that the nonlinear function is approximately equal to its slope at a point under consideration¹.

What does the error look like near $(x_0, y_0) = (0.5, 0.5)$?



1. $y = y_0 = 0.5$; vary x :
 $\text{error}_{\text{length}}^x = x^2 + y_0^2 - 2y_0 = x^2 - 3/4$

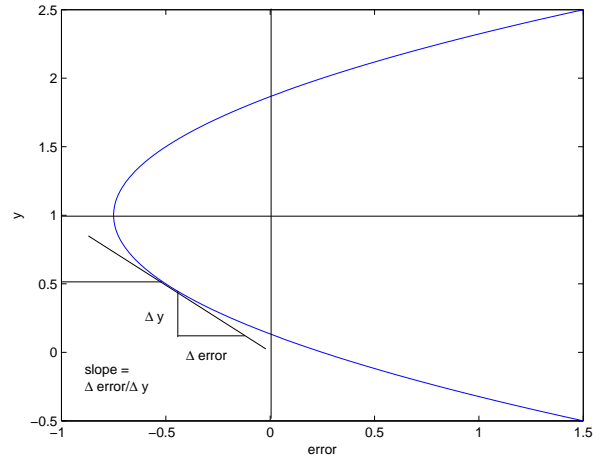
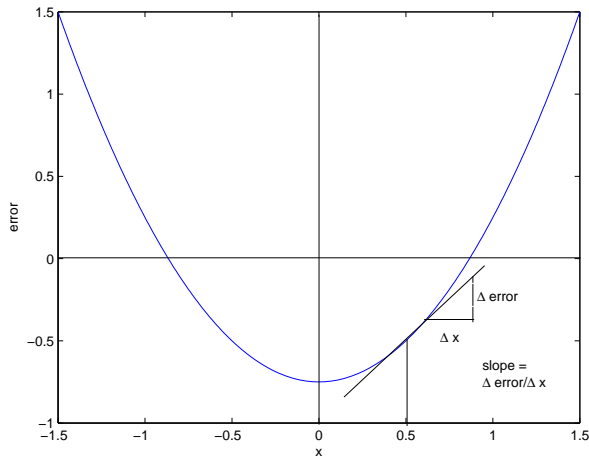
2. $x = x_0 = 0.5$; vary y :
 $\text{error}_{\text{length}}^y = x_0^2 + y^2 - 2y = y(y-2) + 1/4$



¹Sorry, this is the abstract slope of the non-linear function, *not* the concrete slope of the line $(0,1)-(x,y)$ in the paragraph before

$$\text{error}_{\text{length}}^x = x^2 - 3/4$$

$$\text{error}_{\text{length}}^y = y(y - 2) + 1/4$$



$$\begin{aligned} \text{slope}_x |_{(x_0, y_0)} &= \frac{\Delta \text{error}}{\Delta x} \\ &= \frac{1/4 - (-3/4)}{1} \\ &= 1 \\ \text{error}_{\text{length}}^x &\simeq 1 * (x - 0.5) \end{aligned}$$

$$\begin{aligned} \text{slope}_y |_{(x_0, y_0)} &= \frac{\Delta \text{error}}{\Delta y} \\ &= \frac{-3/4 - 1/4}{1} \\ &= -1 \\ \text{error}_{\text{length}}^y &\simeq -1 * (y - 0.5) \end{aligned}$$

So we try

$$\begin{aligned} \text{error}_{\text{length}} &\simeq \text{error}_{\text{length}}^x + \text{error}_{\text{length}}^y + \text{length} \quad \text{where } x = x_0, y = y_0 \\ &\simeq 1 * (x - 0.5) + (-1 * (y - 0.5)) + (-1/2) \\ &= x - y - 1/2 \end{aligned}$$

We now have two linear equations to solve.

$$\begin{aligned} \text{error}_{\text{length}} &= x - y - 1/2 \\ \text{error}_{\text{slope}} &= x + y - 1 \end{aligned}$$

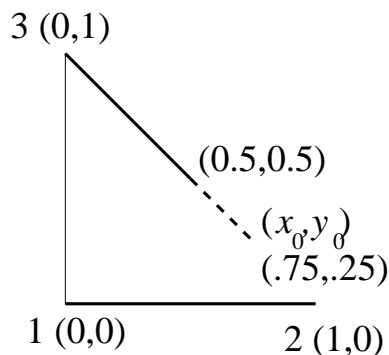
That is

$$\begin{aligned} 0 &= \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} -1 \\ -1/2 \end{pmatrix} \\ \begin{pmatrix} 1 \\ 1/2 \end{pmatrix} &= \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \end{aligned}$$

Gaussian elimination gives

$$\begin{aligned} \begin{pmatrix} 1 \\ -1/2 \end{pmatrix} &= \begin{pmatrix} 1 & 1 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \\ \begin{pmatrix} x \\ y \end{pmatrix} &= \begin{pmatrix} 3/4 \\ 1/4 \end{pmatrix} \end{aligned}$$

So (x_0, y_0) changes position from $(1/2, 1/2)$ to $(3/4, 1/4)$.



This keeps the slope at -1 , but the length is not equal to 1.
 In fact we can figure out that (x_0, y_0) should be at $(1/\sqrt{2}, 1 - 1/\sqrt{2}) = (0.707, 0.293)$.

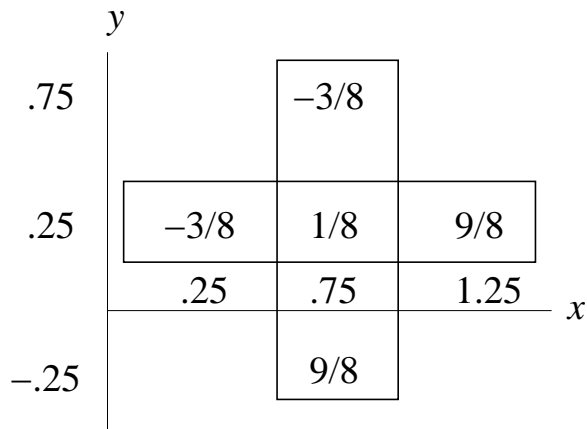
9. Iterate!

Since the first step did not get all the way, we take another step.
 It will get us closer. (No amount of steps will ever get us all the way because each step will give numbers which are fractions, i.e., rational, while $\sqrt{2}$ is irrational.)

But we can go on taking steps until we are close enough.

Iteration is the essence of nonlinearity.

$$\begin{aligned}
 \text{error}_{\text{length}}^x &= x^2 + y_0(y_0 - 2) & \text{error}_{\text{length}}^y &= x_0^2 + y(y - 2) \\
 &= x^2 + 1/4(1/4 - 2) & &= (3/4)^2 + y(y - 2) \\
 &= x^2 - 7/16 & &= y(y - 2) + 9/16
 \end{aligned}$$



$$\begin{aligned}
 \text{error}_{\text{length}} &\simeq \frac{9 - (-3)}{8}(x - 3/4) + \frac{-3 - 9}{8}(y - 1/4) + 1/8 \\
 &= 3/2(x - 3/4) - 3/2(y - 1/4) + 1/8 \\
 &= 3/2x - 3/2y - 5/8
 \end{aligned}$$

Again, two linear equations.

$$\begin{aligned}
 \text{error}_{\text{length}} &= 3/2x - 3/2y - 5/8 \\
 \text{error}_{\text{slope}} &= x + y - 1
 \end{aligned}$$

That is

$$0 = \begin{pmatrix} 1 & 1 \\ 3/2 & -3/2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} -1 \\ -5/8 \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ 5/8 \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 3/2 & -3/2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

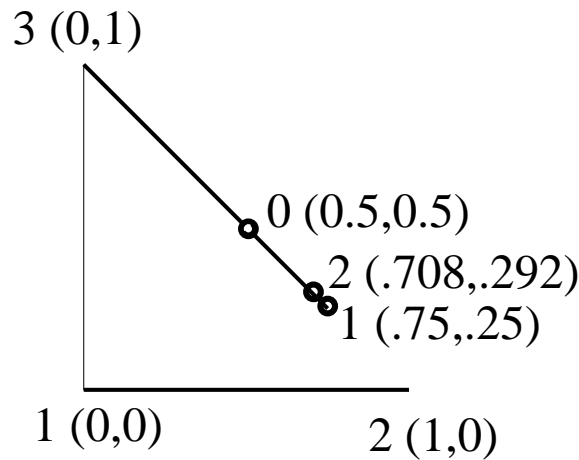
Gaussian elimination gives

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 17/24 \\ 7/24 \end{pmatrix} = \begin{pmatrix} 0.708 \\ 0.292 \end{pmatrix}$$

This answer is wrong by only 1 in the third decimal place.

Not enough to show on the drawing.

So two iterations were enough this time, although we could keep going.

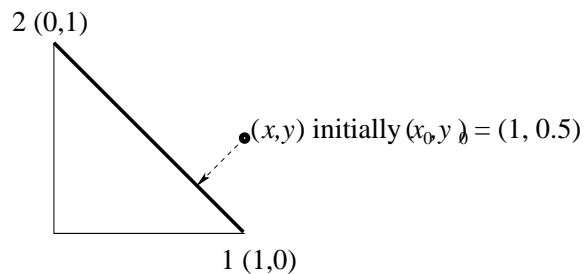


10. Underdetermined equations

Sketchpad example 3 (point collinear with line):

$$0 = \begin{vmatrix} x_1 & x_2 & x \\ y_1 & y_2 & y \\ 1 & 1 & 1 \end{vmatrix} = \begin{vmatrix} 1 & 0 & x \\ 0 & 1 & y \\ 1 & 1 & 1 \end{vmatrix}$$

$$= 1 - x - y = (-1, -1) \begin{pmatrix} x \\ y \end{pmatrix} + 1$$



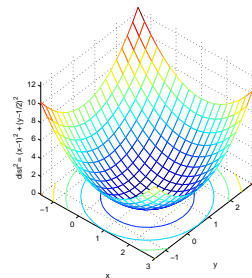
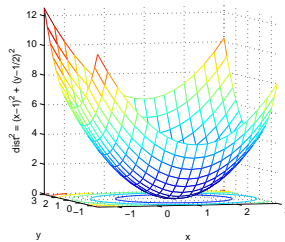
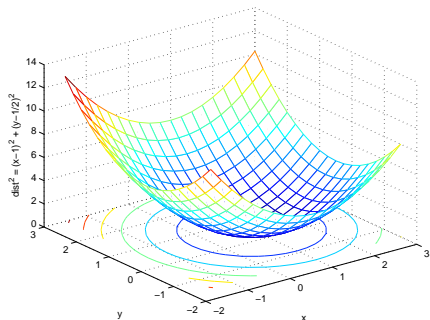
One equation, two unknowns

$$(1, 1) \begin{pmatrix} x \\ y \end{pmatrix} = 1$$

Let's minimize how far (x, y) moves from (x_0, y_0) .

$$\begin{aligned} \text{dist}^2 &= (x - x_0)^2 + (y - y_0)^2 \\ &= (x - 1)^2 + (y - 1/2)^2 \\ &= x^2 - 2x + y^2 - y + 5/4 \end{aligned}$$

On minimizing: slope = 0 means slope_x = 0 and slope_y = 0



On slopes:

$$\begin{aligned} \text{slope } x^2 &= \frac{(x + \Delta x)^2 - x^2}{\Delta x} = \frac{(x^2 + 2x\Delta x + \dots) - x^2}{\Delta x} \simeq 2x \\ \text{slope } x &= \frac{(x + \Delta x) - x}{\Delta x} = 1 \\ \text{slope } c &= \frac{c - c}{\Delta x} = 0 \end{aligned}$$

So

$$0 = \begin{pmatrix} \text{slope}_x \\ \text{slope}_y \end{pmatrix} \text{dist}^2 = \begin{pmatrix} \text{slope}_x \\ \text{slope}_y \end{pmatrix} (x^2 - 2x + y^2 - y + 5/4) = \begin{pmatrix} 2x - 2 \\ 2y - 1 \end{pmatrix}$$

and so $x = 1, y = 1/2$.

Of course: (x, y) is closest to (x_0, y_0) when $(x, y) = (x_0, y_0) = (1, 1/2)$

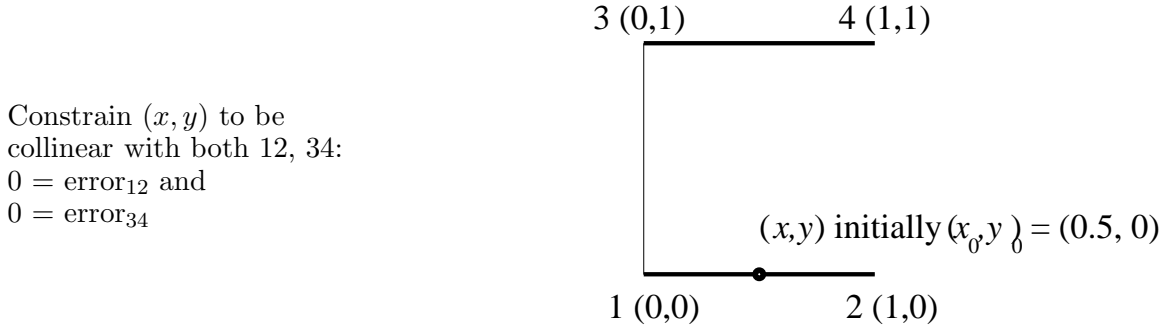
11. Now let's minimize *subject to the constraint* $x + y = 1$

$$\begin{aligned} 0 &= \begin{pmatrix} \text{slope}_x \\ \text{slope}_y \\ \text{slope}_\lambda \end{pmatrix} (\text{dist}^2 + \lambda * (x + y - 1)) \\ &= \begin{pmatrix} \text{slope}_x \\ \text{slope}_y \\ \text{slope}_\lambda \end{pmatrix} (x^2 - 2x + y^2 - y + 5/4 + \lambda * (x + y - 1)) \\ &= \begin{pmatrix} 2x - 2 + \lambda \\ 2y - 1 + \lambda \\ x + y - 1 \end{pmatrix} \\ &= \begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ \lambda \end{pmatrix} + \begin{pmatrix} -2 \\ -1 \\ -1 \end{pmatrix} \\ \begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix} &= \begin{pmatrix} 2 & 0 & 1 \\ 0 & 2 & 1 \\ 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ \lambda \end{pmatrix} \\ \begin{pmatrix} x \\ y \\ \lambda \end{pmatrix} &= \begin{pmatrix} 3/4 \\ 1/4 \\ 1/2 \end{pmatrix} \end{aligned}$$

The λ is called a “Lagrange multiplier”, and the trick makes sense if you think about it.
 (3/4,1/4) is where the arrow points in the figure: (x, y) moved perpendicularly towards the line.

12. Overdetermined equations

Sketchpad example 4 (point collinear with two lines):



We’ll start simply, by constraining (x, y) to be collinear with 12

$$0 = \text{error}'_{12} = \begin{vmatrix} x_1 & x_2 & x \\ y_1 & y_2 & y \\ 1 & 1 & 1 \end{vmatrix} = \begin{vmatrix} 0 & 1 & x \\ 0 & 0 & y \\ 1 & 1 & 1 \end{vmatrix} = y$$

This is underdetermined: x is not specified at all.

So instead we minimize how far (x, y) moves from (x_0, y_0) , as before, subject to the constraint $y = 0$.

$$(x - x_0)^2 + (y - y_0)^2 + \lambda_1 y = x^2 - x + y^2 + 1/4 + \lambda_1 y$$

$$\begin{aligned} 0 &= \text{error}_{12} \\ &= \begin{pmatrix} \text{slope}_x \\ \text{slope}_y \\ \text{slope}_{\lambda_1} \end{pmatrix} (x^2 - x + y^2 + \lambda_1 y + 1/4) \\ &= \begin{pmatrix} 2x - 1 \\ 2y + \lambda_1 \\ y \end{pmatrix} \\ &= \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ \lambda_1 \end{pmatrix} + \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix} \end{aligned}$$

Similarly we minimize how far (x, y) moves from (x_0, y_0) , to get to line 34: i.e., subject to the constraint given by the determinant below. Minimize

$$(x - x_0)^2 + (y - y_0)^2 + \lambda_2 \begin{vmatrix} x_3 & x_4 & x \\ y_3 & y_4 & y \\ 1 & 1 & 1 \end{vmatrix} = (x - 0.5)^2 + (y - 0)^2 + \lambda_2 \begin{vmatrix} 0 & 1 & x \\ 1 & 1 & y \\ 1 & 1 & 1 \end{vmatrix} = x^2 - x + y^2 + 1/4 + \lambda_2 * (y - 1)$$

$$\begin{aligned} 0 &= \text{error}_{34} \\ &= \begin{pmatrix} \text{slope}_x \\ \text{slope}_y \\ \text{slope}_{\lambda_2} \end{pmatrix} (x^2 - x + y^2 + 1/4 + \lambda_2 * (y - 1)) \end{aligned}$$

$$\begin{aligned}
&= \begin{pmatrix} 2x - 1 \\ 2y + \lambda_2 \\ y - 1 \end{pmatrix} \\
&= \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ \lambda_2 \end{pmatrix} + \begin{pmatrix} -1 \\ 0 \\ -1 \end{pmatrix}
\end{aligned}$$

13. This gives six equations in four unknowns, which thus are overdetermined.

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ \lambda_1 \\ \lambda_2 \end{pmatrix}$$

To avoid getting confused with all these numbers, let's call this

$$B = AX$$

If we minimize

$$(AX - B)^T(AX - B)$$

we will get a "least squares" solution: error² is minimized (that is, the error that we get by forcing X to be the solution given by choosing any four elements of B and the corresponding rows of A).

It is plausible that $\text{slope}_X((AX - B)^T(AX - B))$ is proportional to

$$A^T(AX - B)$$

so I am going to suppose it (but it really needs to be shown).

This slope must be set to zero for the minimization: so we must solve

$$A^TAX = A^TB$$

$$\begin{aligned}
A^TA &= \begin{pmatrix} 2 & 0 & 0 & 2 & 0 & 0 \\ 0 & 2 & 1 & 0 & 2 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 8 & 0 & 0 & 0 \\ 0 & 10 & 2 & 2 \\ 0 & 2 & 1 & 0 \\ 0 & 2 & 0 & 1 \end{pmatrix} \\
A^TB &= \begin{pmatrix} 2 & 0 & 0 & 2 & 0 & 0 \\ 0 & 2 & 1 & 0 & 2 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 4 \\ 1 \\ 0 \\ 0 \end{pmatrix}
\end{aligned}$$

MATLAB:

```
A = [8,0,0,0;0,10,2,2;0,2,1,0;0,2,0,1];  
B = [4;1;0;0];  
X = A\B
```

X =

```
0.5000  
0.5000  
-1.0000  
-1.0000
```

This gives $(x, y) = (1/2, 1/2)$, halfway between the two lines.

This seems a good compromise. It minimizes the error² from both lines if we put the point closer to one than the other line (or even right on it).

14. Summary

(These notes show the trees. Try to see the forest!)

- A. • A Web page is considered to have some importance, which it shares equally among all the web pages it links to.
- A Web page derives its importance from the importance of the Web pages that link to it.
 - Some preliminary importance may be assigned to each Web page in a way that sustains some sort of importance even though no other page may link to it.
 - The importances of all pages can be thought of as a vector over the Web the sum of whose terms is 1, taken to be the overall importance of the Web.
 - The links of the Web can be thought of as a matrix, which includes both the sharing of importance and the sustaining importance.
 - The final importances of the Web pages are in the vector that is unchanged by operating on it with the matrix: the eigenvector of the matrix.
 - Iteration is one way to find the eigenvector associated with the largest eigenvalue.
- B. • Elementary row operations on the matrix and the target vector in a matrix equation do not change the meaning of the equation.
- They can be used systematically to solve matrix equations by “gaussian elimination”.
 - Gaussian elimination has a “triangularization” step costing $n^3/3$ operations, (+,*), and a “back-substitution” step costing $n^2/2$.
 - Sketchpad uses matrix equations to enforce constraints on a drawing.
 - Linear constraints, such as requiring that a point lie on the intersection of two lines, give simple matrix (“linear”) equations.
 - Nonlinear constraints, such as requiring a line of a given slope to have the same length as another line, require linear approximation to the nonlinear equation, which is iterated until the solution is close enough.
 - Underdetermined constraints, such as requiring a point to be collinear with one line, are solved by also minimizing how far the point must move from its initial position.

- Distance, which is quadratic, can be minimized by setting its slope, which is linear, to zero, giving a linear constraint.
- Minimization subject to a constraint can be done by multiplying the error from this constraint by a “Lagrange multiplier”, adding it all to the expression to be minimized, and minimizing as before and also with respect to the Lagrange multiplier.
- Overdetermined constraints, such as requiring a point to be collinear with two parallel lines, can be solved by minimizing the sum of squares of all the measures of how wrong any particular position of the point might be, all subject to the constraint.

II. The Excursions

You’ve seen lots of ideas. Now *do* something with them!

1. Do the relative importances of documents p , q and r make sense in the first, cyclic Web example? What strikes you most? If the link from q to r is removed, what changes? Why?
2. Why does repeating $\mathbf{b} = \mathbf{A}\mathbf{b}$ eventually find the eigenvector of A with the largest eigenvalue for almost any starting value for b ? Which starting value for b would fail to give this eigenvector?
3. Using a source vector, S , with 1-norm 0.15, what are the final ranks of p, q and r given the Web

$$\begin{array}{c} \sqrt{} \\ \mathbf{p} \quad \mathbf{q} \quad \mathbf{r} \\ \mathbf{p} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\ \mathbf{q} \\ \mathbf{r} \end{array}$$

(This matrix describes the Web, but is not necessarily W : check this!) Don’t forget to normalize R before each iteration. (Write a MATLAB script to do an iteration.) Is there a cycle? What would happen if $S = 0$?

4. Are R and S *really* vectors? (Week 7c)
5. Look up Page, Brin, Motwani & Winograd, 1999 *The PageRank Citation Ranking: Bringing Order to the Web* [PBMW99]. What other forms do they suggest for the source vector?
6. Use the same iteration technique to find an eigenvector of

$$\frac{5}{3} \begin{pmatrix} 1 & -4/5 \\ -4/5 & 1 \end{pmatrix}$$

How fast does it converge? (If you got convergence on the first iteration, try it again with some other starting vector.) Once you have figured out the eigenvector, find a vector orthogonal to it and use that as the starting vector. What are the eigenvalues? What is their product? (You do not need to normalise before each iteration for this question. In fact, you should not.) In MATLAB, run `characteristic = poly(A)`, where A is the above matrix, then run `roots(characteristic)`. Make connections! NB `poly(A)` gives a polynomial in e which is $\det(A - e\mathbf{I})$. Try the code `syms e; det(A - e*eye(2))`. Then try `solve(ans)`.

7. Try the iteration technique on the Hadamard matrix,

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

Comment! Explore as in the previous excursion.

8. Try the iteration technique on

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \quad \text{How about} \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} ?$$

Comment! Explore as in the previous excursion.

9. What are the two eigenvectors of the Lorentz transformation shown in the first diagram of Note 9, Week 3? How do the two eigenvalues compare with 1? Show how an arbitrary vector, repeatedly transformed, converges to the eigenvector with the larger eigenvalue. Which is the one vector that will not converge to this eigenvector? Why?

10. (Factor analysis/Principle components analysis in the measurement of personality)

(This is a long discussion which you can follow by plotting the points, and doing the calculations. Factor analysis is widely used, not just in psychology.)

A “social attitude inventory” asks psych. test subjects if, on a scale of 1 to 5, they strongly agree (1), agree (2), don’t care (3), disagree (4) or strongly disagree (5) with statements such as the following.

x *Birth control, except when recommended by a doctor, should be made illegal*

y *It is immoral for men and women to find out whether they are sexually suited before marriage (e.g., by trial marriage).*

z *Conscientious objectors (pacifists) should be excused military service without stigma and certainly not treated as traitors to their country.*

(These questions are adapted from chapter 7 of [Eys58], published in 1957. How should this questionnaire have changed in the intervening fifty years to capture the same aspects of personality today?)

Suppose that five subjects responded as follows to the above three questions.

Question\Subject	a	b	c	d	e
x	1	5	3	2	4
y	1	5	3	2	4
z	2	2	3	4	4

Factor analysis tries to find out how many different types of personality are represented by the answers to these questions. It does this by calculating the extent to which different questions are independent of each other. Each question may be treated as a “vector” of responses, in this case a 5-dimensional vector. If the vectors are normalized, their scalar product is the cosine of the angle between them. (We saw this for two dimensions in Week 2; it is true for any number of dimensions. Show this! Use the invariance of $\vec{u}^T \vec{v} = (R\vec{u})^T R\vec{v}$ for any transformation matrix R , such as a rotation, whose inverse is its own transpose, to reduce the general case to the two-dimensional case.) This cosine is close to 1 if the vectors point in nearly the same direction, and close to 0 if the vectors are nearly at right angles, which we will call “orthogonal” and can consider to be “independent”.

Before we normalize the three 5-vectors for **x**, **y** and **z**, we subtract their average values from each term. (This is not essential, but it is conventionally done in statistics, which then calls the results of the scalar products either the “variance” (product of a vector with itself) or the “co-variance” (product of a vector with another). It has the advantage of making the numbers smaller.) Here are the three vectors so reduced, with their lengths written in the first column. (The average values are 3 for each vector.)

Lengths	Question\Subject	a	b	c	d	e
$\sqrt{10}$	x	-2	2	0	-1	1
$\sqrt{10}$	y	-2	2	0	-1	1
2	z	-1	-1	0	1	1

The nine scalar products of these three vectors with each other may be written as a matrix.

$$\begin{pmatrix} -2 & 2 & 0 & -1 & 1 \\ -2 & 2 & 0 & -1 & 1 \\ -1 & -1 & 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} -2 & -2 & -1 \\ 2 & 2 & -1 \\ 0 & 0 & 0 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 10 & 10 & 0 \\ 10 & 10 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

and if all the vectors had been normalized, we get the “variance-covariance” matrix

$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

We see that \mathbf{x} and \mathbf{y} are completely correlated, which is pretty obvious from the original data. It is also obvious that there are only two dimensions in this data, which we could have seen just by plotting the original data as five points in 3-D. There are just two independent “factors” or “principle components”. The next step is to extract these, using techniques which will work even if the data is much more complex and much less obvious.

Before going on to the next step, let’s alter the original data so that the correlation between \mathbf{x} and \mathbf{y} is a little less obvious. Suppose the answers to question \mathbf{x} are 2, 4, 3, 3, 3 instead, so the (co-)variance matrix is now found from

$$\begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ -2 & 2 & 0 & -1 & 1 \\ -1 & -1 & 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} -1 & -2 & -1 \\ 1 & 2 & -1 \\ 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 4 & 0 \\ 4 & 10 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

and, when normalized, this is the (co-)variance matrix

$$\begin{pmatrix} 1 & 2/\sqrt{5} & 0 \\ 2/\sqrt{5} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Now we proceed to finding the two important dimensions. For the first case, with (co-)variance

$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

\mathbf{z} is one of the important dimensions because it is clearly independent of the others: its covariance with them is zero. But \mathbf{x} and \mathbf{y} are mixed up together, and so we must be able to find some *combination* of \mathbf{x} and \mathbf{y} which gives an independent state. (The “state” is some mixture of questions \mathbf{x} and \mathbf{y} . “Mixture of questions” is really no stranger than quantum mechanics, where states can be mixtures of other states. In factor analysis, it can be taken as a handy fiction; in quantum mechanics, we must accept it being closer to physical reality.) In fact, we want to find mixtures of \mathbf{x} and \mathbf{y} so that the (co-)variance matrix, for these mixtures and \mathbf{z} , has zeros everywhere except, maybe, on the diagonal.

Now we are on familiar ground. We want the *eigenvectors* of the (co-)variance matrix. A little trial and error gives (1,1,0), (1,-1,0) and (0,0,1) as these eigenvectors. (Normalizing them, that would be $(1/\sqrt{2}, 1/\sqrt{2}, 0)$, $(1/\sqrt{2}, -1/\sqrt{2}, 0)$ and (0,0,1).)

What is the (co-)variance matrix for these new states, $\mathbf{x} + \mathbf{y}$, $\mathbf{x} - \mathbf{y}$ and \mathbf{z} ?

$$\begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} a/\sqrt{2} & b/\sqrt{2} & 0 \\ a/\sqrt{2} & -b/\sqrt{2} & 0 \\ 0 & 0 & c \end{pmatrix},$$

where actually doing the matrix multiplication shows that $a = 2, b = 0$ and $c = 1$. These eigenvectors are orthogonal to each other, and since they are normalized,

$$\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

(The first matrix is actually the transpose of the second, but the entries in this particular matrix conceal the fact.)

Thus

$$\begin{aligned} & \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ = & \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a/\sqrt{2} & b/\sqrt{2} & 0 \\ a/\sqrt{2} & -b/\sqrt{2} & 0 \\ 0 & 0 & c \end{pmatrix} \\ = & \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{pmatrix} \\ = & \begin{pmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned}$$

The way to diagonalize a (symmetric) matrix, V , is to multiply $E^T V E$, where E is the array of (orthogonal) normalized eigenvectors of V .

This diagonalization effectively transforms the question-space into a space of mixed questions, so of course it transforms the questions themselves. Just as $V \rightarrow E^T V E$, so the questions $Q \rightarrow E^T Q$. Here are the new, mixed questions.

$$\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -2 & 2 & 0 & -1 & 1 \\ -2 & 2 & 0 & -1 & 1 \\ -1 & -1 & 0 & -1 & 1 \end{pmatrix} = \begin{pmatrix} -2\sqrt{2} & 2\sqrt{2} & 0 & -\sqrt{2} & \sqrt{2} \\ 0 & 0 & 0 & 0 & 0 \\ -1 & -1 & 0 & 1 & 1 \end{pmatrix}$$

One whole dimension disappears completely. This is because $b = 0$. Since the original \mathbf{x} and \mathbf{y} values lay entirely in a plane, all the variance is in that plane, giving $a = 2$, and none is orthogonal to the plane, giving $b = 0$.

Plot these results as five points in a two-dimensional space.

If the orthogonal variance is not zero, it might still be quite small. Show that the eigenvectors for the second case, with (co-)variance matrix

$$\begin{pmatrix} 1 & 2/\sqrt{5} & 0 \\ 2/\sqrt{5} & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

are also (1,1,0), (1,-1,0) and (0,0,1), but this time with “eigenvalues” $a = 1 + 2/\sqrt{5} = 1.894$, $b = 1 - 2/\sqrt{5} = 0.106$ and $c = 1$. The variance given by b , while not zero anymore, is much smaller than the other variances, and we can decide to discard it. We won’t even use this eigenvector in transforming the questions.

$$\begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ -2 & 2 & 0 & -1 & 1 \\ -1 & -1 & 0 & 1 & 1 \end{pmatrix} = \begin{pmatrix} -3/\sqrt{2} & 3/\sqrt{2} & 0 & -1/\sqrt{2} & 1/\sqrt{2} \\ -1 & -1 & 0 & 1 & 1 \end{pmatrix}$$

We again have two factors, having decided that the variance of the third is too small to count.

Plot these results as five points in a two-dimensional space. This is the factor space. Can you think of names to give the axes to suggest the kinds of personalities that would give high scores on each of the two axes?

Typically such personality measurements would consist of thousands of subjects answering tens of questions. Five dimensions of personality traits and fifty questions to assess them are in [Har05]. The long discussion in this excursion should encourage you to take it all with a pinch of salt. [Gou87, Ch. 8: “Jensen’s Last Stand”] is a cautionary tale of factor analysis in its original application to IQ testing.

11. Show that

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

is the sum of a symmetric and an antisymmetric matrix. What are they? What about any 3×3 matrix? Find the components also for the special cases of the Web matrices.

In MATLAB, run `characteristic = poly(A)`, where A is any of the Web matrices, then run `roots(characteristic)`. Discuss the results in the light of this and the last two excursions.

12. Given

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix},$$

show the effect of doing the three elementary operations on the *columns*.

13. Use Gaussian elimination to show that the inverse of the 2×2 matrix

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

is

$$\frac{1}{ad - bc} \begin{pmatrix} d & -c \\ -b & a \end{pmatrix}$$

What is the denominator? Hint: in $AX = B$ now X and $v = B$ are 2×2 matrices instead of vectors (2×1 matrices).

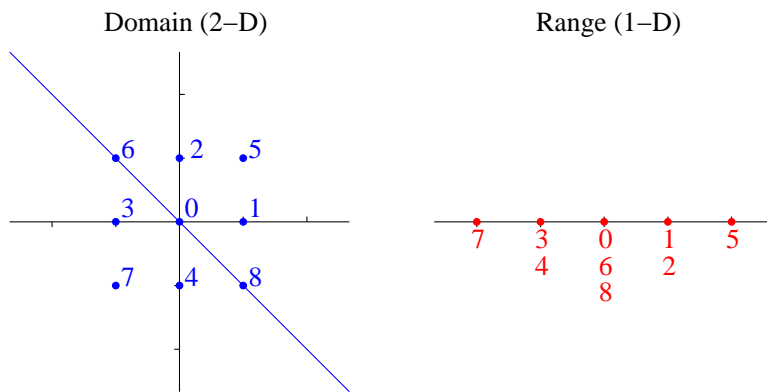
14. **Null spaces and stoichiometry.**

Note 10 discusses the equation

$$(1, 1) \begin{pmatrix} x \\ y \end{pmatrix} = 1$$

and solves it as an underdetermined equation. Let’s think about rectangular matrices as mappings of spaces. In general it is useful to think in terms of two spaces, different from each other and possibly having different dimensions.

The matrix (1,1) maps a 2-dimensional space to a 1-dimensional space as shown.



The blue points in the 2-D space on the left are mapped into the corresponding red points in the 1-D space on the right.

Notice that points 0, 6 and 8 all map into 0. These points, and the whole line connecting them, are in the *null space* of the matrix. This is a 1-dimensional subspace of the 2-dimensional space on the left.

This enables us to solve another equation, related to that of Note 10

$$(1, 1) \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

by identifying this line that is the null space: $x = -y$.

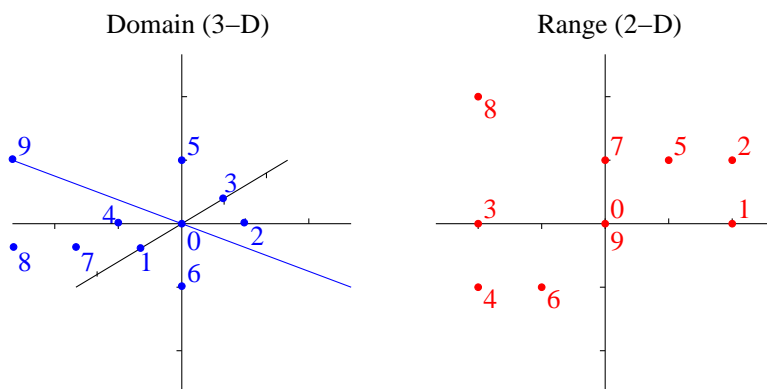
It is still underdetermined, which means that we can choose any value we like for y (the *independent* variable), but then x is determined (the *dependent* variable).

More generally, any number of dimensions, say c , may be mapped to e dimensions, with $e \leq c$. Let's try 3-D to 2-D.

The matrix

$$\begin{pmatrix} 2 & 2 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

maps as shown.



To find the null space we can use the elementary row operations of Note 4.

$$\begin{pmatrix} 2 & 2 & 1 \\ 0 & 1 & 1 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 1 & 1/2 \\ 0 & 1 & 1 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & 0 & -1/2 \\ 0 & 1 & 1 \end{pmatrix} \longrightarrow$$

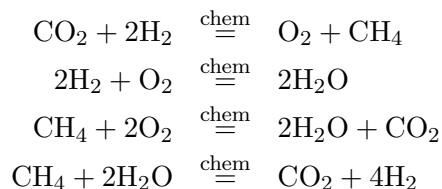
so that

$$\begin{pmatrix} 2 & 2 & 1 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \equiv \begin{pmatrix} 1 & 0 & -1/2 \\ 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

where the negative values of the stoichiometric coefficients σ_j cause the corresponding terms to be written to the left of the equal sign because these are the quantities that are supposedly decreasing as the chemical reaction proceeds from left to right.

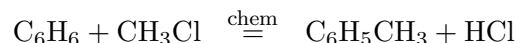
To express the reverse direction for the reaction, swap the left and right sides of the chemical equation or multiply the null-space solution by -1 . Chemical equations are not symmetrical. Nor are they algebraic: symbols such as O_2 and CO are not quantities but represent chemical compounds.

b) Given the compounds CO_2 , H_2O , O_2 , CH_4 and H_2 show that



Note that the null space is now two-dimensional and the first two equations above come from the basis that you will find for it. The second two equations come from linear combinations of this basis (find constants to multiply each vector by and sum the results to get the new vector). They describe the “dry reforming of methane” (CH_4).

c) Similarly, derive the equation for the “methylation of benzene” (C_6H_6):

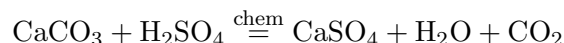


and show how “double methylation” adds the product $C_6H_4(CH_3)_2$, how “triple methylation” adds $C_6H_3(CH_3)_3$, and so on. (The MATLAB function `null(EC, 'r')` on the matrix `EC` can save you some work.)

d) In (b) above call the first equation x and the second y . Explore the combinations $x + y$, $x - y$, $2x + y$, $x + 2y$, $2x - y$, $x - 2y$, etc. How do $2x$, $2y$, $2x + 2y$, etc., relate to what you already have? What about $-x$, $-y$, $-x - y$, etc.? How many reactions are possible with these five compounds? Why are some chemically uninteresting? Where should we stop?

NB. What I have been calling “compounds” a chemist would properly call “species”: O_2 and H_2 are not considered compounds, and ultrafast spectroscopy to identify the fleeting components of the “pathways” of the reactions will find radicals such as OH , H , etc.

e) And what I have been calling “elements” can be combined if the combination is unchanged by the reaction(s). For example, in dissolving calcite by sulfuric acid



either S or SO_4 can be considered as elementary: try it both ways and show that the latter simplifies the arithmetic.

15. **Quadratic forms and stability.** a) Show that the eigenvectors of

$$\begin{pmatrix} a & \sqrt{ac} \\ \sqrt{ac} & c \end{pmatrix}$$

are $\begin{pmatrix} \sqrt{c} \\ -\sqrt{a} \end{pmatrix}$ and $\begin{pmatrix} \sqrt{a} \\ \sqrt{c} \end{pmatrix}$

with eigenvalues 0 and $a + c$ respectively. What is the null space of this matrix (Excursion “Null spaces and stoichiometry” above)? What is its determinant?

b) Show that

$$(x, y) \begin{pmatrix} a & \sqrt{ac} \\ \sqrt{ac} & c \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = (\sqrt{a}x + \sqrt{c}y)^2$$

The left hand side is an example of a *quadratic form*. Note that the matrix is symmetric. The right hand side is, in this case, a perfect square.

c) Why is

$$(x, y) \begin{pmatrix} a & \sqrt{ac} \\ \sqrt{ac} & c \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

always non-negative for any values of x and y ?

A matrix with this property is called *positive definite* (although it should be called non-negative definite).

d) Show that a positive definite matrix must have non-negative eigenvalues.

e) Show that the condition that the quadratic form

$$(x, y) \begin{pmatrix} a & b \\ b & c \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

is never negative, no matter what values x and y have is

$$a \geq 0 \quad \text{and} \quad ac - b^2 \geq 0$$

Hint. The condition is met when $a \geq 0$ and $ac - b^2 = 0$; which part of $ax^2 + 2bxy + cy^2$ might go negative otherwise?

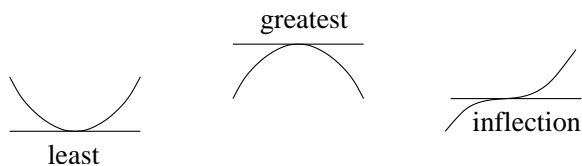
f) Repeat the above discussion for

$$(x, y, z) \begin{pmatrix} a & b & c \\ b & d & e \\ c & e & f \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

considering in particular the special case $b = \sqrt{ad}$, $c = \sqrt{fa}$ and $e = \sqrt{df}$. (Eigenvectors, say, $(\sqrt{f}, 0, -\sqrt{a})^T$, $(0, \sqrt{f}, -\sqrt{d})^T$, $(\sqrt{a}, \sqrt{d}, \sqrt{f})^T$: how can you find these?)

Stability. In Note 10 we discussed “minimizing” a function by setting its slope to zero.

In fact all this does is establish that the function is *stationary* at that point: zero slopes also yield maxima, points of inflection, saddle points, etc. Of all these, only a minimum is *stable* in that a ball rolling around on top of the curve will necessarily settle at the stationary point. Here for a function of 1 variable (“1 dimension”) are the three types of stationary point.



Of all the stationary points in n dimensions, only minima are stable. We find stationary points by setting slope to zero but if we want to know that they are stable we must show that the matrix in the quadratic form that approximates the curve at that point is positive definite.

In 1 dimension there are three types of stationary point, shown above. Only one of these is stable.

g) For functions of 2 variables, show that there are $\Delta_3 = 6$, the 3rd triangular number (Week i, Notes 1,2) stationary points, and classify them as minima, maxima, saddle points, and extensions of the 1-D points of inflection.

You can do this

i) by combining the three 1-D stationary points into a 3-by-3 matrix and then eliminating entries that do not describe new types, e.g., x goes up in both directions while y goes down is a saddle point just as is y goes up in both directions while x goes down; or

$$\begin{array}{ccc} 0 & 1 & x \\ 0 & 1 & y \\ 1 & 1 & 1 \end{array} \quad \text{and} \quad \begin{array}{ccc} 1 & 0 & x \\ 0 & 1 & y \\ 1 & 1 & 1 \end{array}$$

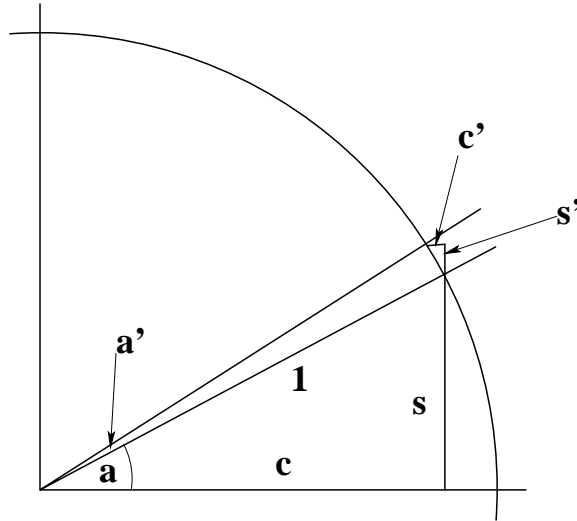
and compare with the diagonals method of finding these 3×3 determinants.

19. We defined the determinant of a $d \times d$ matrix to be the d -dimensional hypervolume of the hyperparallelogram whose edges are the target vectors of $(1,0,\dots,0)^T$, $(0,1,0,\dots,0)^T$, etc., i.e., the columns of the transforming matrix; and we said that swapping any two of these vectors changes the sign of the volume and of the determinant. How should we interpret the *rows* of the matrix as a volume, and should there be a similar rule for sign change on swapping rows?
20. What is the determinant of the projection transformation,

$$\begin{array}{cc} c^2 & cs \\ cs & s^2 \end{array}$$

(from Week 1 on polarized light)? Why?

21. Use MATLAB's `det()` function to explore the determinants of some 2×2 and 3×3 matrices. Try deliberately to create some sign changes and some zeros, and look carefully at the matrices that give those results.
22. Representing $x^2 - 3/4$ as $\mathbf{ex} = [1, 0, -3/4]$ and $y^2 - 2y + 1/4$ as $\mathbf{ey} = [1, -2, 1/4]$, use MATLAB's `polyval(ex,x)` and `polyval(ey,y)` to evaluate these polynomials at different values of x (such as 0, 0.5, 1) and y (such as 0, 0.5, 1), respectively. Use one of MATLAB's plotting routines to plot each of these curves.
23. How many additions and how many multiplications are needed to calculate $ax^2 + bx + c = axx + bx + c$? How many are needed for $c + x(b + x(a))$? How about a polynomial of degree d , with $d + 1$ coefficients?
24. Plot $(x - 1)^2 + (y - 1/2)^2$ using MATLAB's `mesh()`, and use the plot window controls to move the plot around until you are convinced that slope_x and slope_y are both 0 at the minimum. For some other function (for instance, the negative of the function you just plotted), 0 values for slope_x and slope_y have another meaning: what is it?
25. Given a polynomial (in MATLAB representation) `[a,b,c]`, what is its slope in the same representation?
26. What does the binomial theorem tell you about the slope of x^n for any positive integer n ?
27. What function is its own slope everywhere, $f(x) = \text{slope}_x f(x)$?
Two things to try:
1. Draw curves until you get a feel for the shape of such a function.
 2. Find coefficients a_i in the series $f(x) = a_0 + a_1x^1 + a_2x^2 + \dots$
- Note that $\text{slope}_x f(x)$ is conventionally written $d f(x)/dx$, and that this excursion is exploring the differential equation that gives the fixed point of the derivative operator, d/dx .
28. **Slopes of cos and sin.** Use the figure

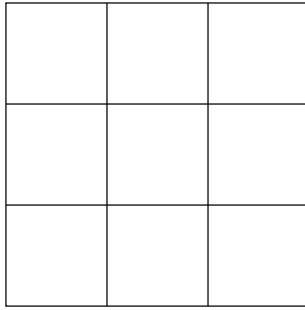


to find the slopes of $\sin()$ and $\cos()$ everywhere: s is $\sin(a)$, s' is the difference between $\sin(a+a')$ and $\sin(a)$, and similarly for c , c' and $\cos()$. Hint: in the c' - s' triangle, which angle is the same as a ?

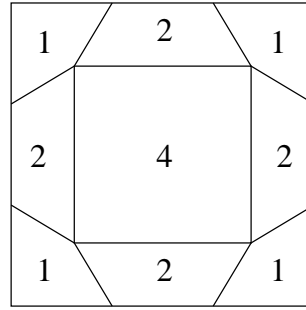
What is the slope everywhere of $\cos() + i \times \sin()$? How does this relate to the function that is its own slope everywhere of the previous excursion?

What series, $a_0 + a_1x^1 + a_2x^2 + \dots$, might apply to $\sin()$? To $\cos()$? How might you then write a MATLAB program to calculate $\sin()$ and $\cos()$, pretending that MATLAB does not have these as builtin functions?

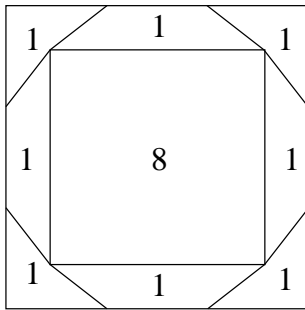
29. For the underdetermined equation, $x + y = 1$, what does MATLAB's `pinv(A)*b` give? ($A = [1, 1]$, $b = [1]$) What distinguishes this solution from any other of the infinite number of solutions? Why is it not satisfactory as a Sketchpad solution?
30. Why do we minimize the square of the error, $AX - B$, giving least square error, rather than minimizing the error, giving, "least error"?
31. For ordinary variables, a, b and x , show that $\text{slope}_x((ax - b)^2) = 2a(ax - b)$.
For matrices, A, B, X , why does $A^TAX = A^TB$ not imply $AX = B$?
For A, B and X from the overdetermined equation of the lecture, show that $A^TAX = A^TB$ does result from minimizing on all variables.
32. Solve the overdetermined equation of the lecture, $AX = B$, using $A \setminus B$ in MATLAB.
33. What are the constraints to make Sketchpad turn six points, approximately located by the user, into the vertices of a hexagon? Work through an example, taking the first two points drawn as immovable.
34. Look up Ivan Sutherland, 1938–, and his 1963 MIT Ph.D. thesis, *Sketchpad: A Man-machine Graphical Communications System* [Sut80]. (See also `sketchpad.ps` in the notes for this course.) How does Sketchpad simulate linkages such as the Peaucellier linkage for drawing straight lines?
35. We can apply the techniques of Sketchpad to warp maps so as to visualize quantities displayed on the maps. For example, suppose the quantity is population and we want to distort the regular grid of (a) in the figure to show that there is a city in the middle holding in the central square alone a quarter of the population of the whole 3×3 grid. That is, we want to stretch the central square of the grid so that it looks something like (b) of the figure. In (b), the population is distributed more or less uniformly across the whole map.



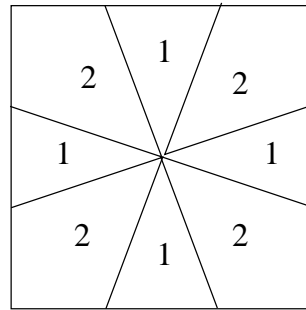
a) Regular 3*3 grid



b) Warped to fit population



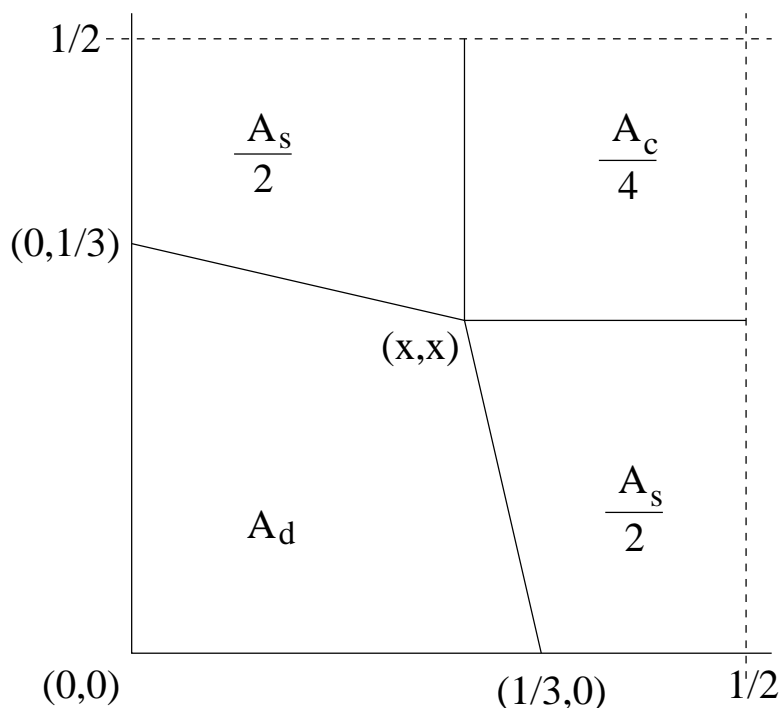
c) Population more concentrated



d) Empty downtown core

Parts (c) and (d) of the figure show more extreme population distributions. In (c) the city core is even more concentrated. In (d) the core has been deserted: everybody lives in the suburbs, so the central square has dwindled to a point.

Note that the three populations shown are *symmetric*: any rotation or reflection that does not change our view of a blank square will also not change our view of the four maps shown. Such symmetry is not required, but it does simplify the calculations. We can look only at the lower left corner of each map, and we can further consider that $x = y$. Thus we have only one variable, x , to solve for.



Note that we can suppose that the whole map has side 1 and hence overall area

$$A_c + 4(A_s + A_d) = 1$$

a) We need the three areas in order to adjust the vertex (x, x) common to each region in this corner so that the areas equal the specified areas. A_c is easy, the region being square: $A_c/4 = (1/2 - x)^2$. For the other regions we can work with a general formula for the area of any simple polygon in terms of its vertices.

$$\frac{1}{2} \sum_{i=1}^n x_i y_{i+1} - x_{i+1} y_i$$

with the index, i , increasing modulo n so that $n + 1$ is just 1.

(This can be shown by induction—find the excursion in Week 12 that does it—given that it works for triangles. A *simple polygon* is one that does not cross over itself the way a bow-tie does if drawn with only four vertices.)

Here is how we can show $A_s = (2/3 - x)x$ and $A_d = x/3$.

$2(A_s/2)$				$2A_d$			
x_i	y_i	$x_i y_{i+1}$	$x_{i+1} y_i$	x_i	y_i	$x_i y_{i+1}$	$x_{i+1} y_i$
1/3	0	0	0	0	0	0	0
1/2	0	$x/2$	0	1/3	0	$x/3$	0
1/2	x	$x/2$	x^2	x	x	$x/3$	0
x	x	0	$x/3$	0	1/3	0	0

Check that the third and fourth columns arise from the first and second for each of these areas, and that each area is the sum of the third column minus the sum of the fourth column.

b) For the first two areas, A_c and A_s , these expressions are nonlinear in x , so we must approximate them by linear functions if we are to get a set of linear equations to solve (repeatedly until the solution converges).

So that it can work with any nonlinear functions whatsoever, Sketchpad would move x around a little, evaluate the functions at these different points, and average the resulting slopes. Since our areas are simple nonlinear functions—quadratics, actually—in x , we shorten this by finding the slopes analytically.

$$\begin{aligned}\text{slope } A_c/4 &= 2x - 1 \\ \text{slope } A_s &= 2/3 - 2x\end{aligned}$$

The linear approximations are

$$\begin{aligned}A_c/4 &\simeq A_c^0/4 + \text{slope } A_c/4|_0 (x - x_0) \\ &= (1/2 - x_0)^2 + (2x_0 - 1)(x - x_0) \\ A_s &\simeq A_s^0 + \text{slope } A_s|_0 (x - x_0) \\ &= (2/3 - x_0)x_0 + (2/3 - 2x_0)(x - x_0)\end{aligned}$$

Show that the linear equations we must now solve are

$$\begin{pmatrix} 2x_0 - 1 \\ 2/3 - 2x_0 \\ 1/3 \end{pmatrix} x = \begin{pmatrix} x_0^2 - 1/4 + A_c/4 \\ -x_0^2 + A_s \\ A_d \end{pmatrix}$$

c) Three equations in one unknown are overdetermined and unlikely to agree with each other. So we minimize the sum of the squares of the differences between the specified areas and the areas we get. Note 13 above says this is the same as solving $A^T A X = A^T B$. Show that this gives

$$\frac{1}{9}((72x_0 - 60)x_0 + 14)x = (4x_0 - \frac{5}{3})x_0^2 - \frac{1}{2}x_0 + \frac{1}{4} + (2x_0 - 1)\frac{A_c}{4} + (\frac{2}{3} - 2x_0)A_s + \frac{A_d}{3}$$

and program a function to evaluate this starting at A_c0 , A_s0 , A_d0 and $x0$ to give the next A_c , A_s , A_d and x . Run the function for the population values above, repeatedly until the results converge (e.g., do not change to four decimal places) in each case. (Test it first with examples you know the answer to, e.g., $A_c = A_s = A_d$.) Check the population maps shown above with the values of x you get. Check how close the areas you calculate are to the specified populations.

For this example, show that $A^T A X = A^T B$ is the least-squares solution by writing down the sum of the squares, then setting its slope to 0. Can you show it in general?

d) Now break the symmetry a little, by no longer supposing that $x = y$. How many unknowns will there be? How many different areas? Work through everything as above and run *that* on your computer.

Be sure to test your program with the full-symmetry examples you ran in (c).

e) If you break the symmetry completely, how many equations and how many unknowns will there be?

f) For an $m \times n$ grid to have the same number of equations as unknowns, what must m and n be? (Note that we are freezing the locations of the intersections of the grid lines with the boundary. Only the strictly internal grid intersections are allowed to move.) Add cells on the outside of this grid in a spiral fashion until there are more unknowns than equations. How must the solution technique now change?

g) How many equations and how many unknowns arise from a 4×4 grid with full symmetry? With full symmetry but not $x = y$? With no symmetry?

How about a $2n \times 2n$ grid or a $(2n + 1) \times (2n + 1)$ grid, where $n > 2$?

h) Go back to the 3×3 grid and change the problem by allowing the grid lines to move rigidly

instead of bending at internal points and having their boundary intersections frozen. What is the solution, x , to $A_c = 4, A_s = 2, A_d = 1$ in this formulation? Is there any $m \times n$ grid of this sort which gives underdetermined equations?

i) Starting from a single hexagon, add hexagons in a spiral around it until: first, there is an internal vertex, (x_1, y_1) , which would give an overdetermined linear system of equations; second, the number of equations equals the number of unknowns; and finally, the unknowns are underdetermined. This is a honeycomb grid, which is an alternative to the rectangular grid. You can use the area formula in (a) to find the area of each hexagon. Note that this formula does not notice if the hexagon has been translated any distance or direction from the origin.

After how many hexagons do the equations become nonlinear?

j) Explore triangular grids along the same lines.

k) How big a calculation is needed for a 1000×1000 grid? Remember that Gaussian elimination for an $n \times n$ matrix costs $\mathcal{O}(n^3)$ (Note 5. Actually it's $n^3/3 +$ constant multiples of lower powers of n , but “big- \mathcal{O} ” notation allows us to ignore the smaller powers and any constant multiples.) So we must find something faster to deal with large maps or with high-resolution.

Since we already must iterate in general, maybe we can find a direct way of iterating, ideally with each iteration costing only $\mathcal{O}(n)$ operations. Here's an idea. In a rectangular lattice, each internal vertex connects with four regions. At any stage, each of these regions is, presumably, the wrong size: say it is A when it should be A_0 . The coordinates of the vertex, in general, contribute quadratically to the area, in products with coordinates of other vertices. So let's change the distance between the vertex and the centroid of the region by the factor $\sqrt{A_0/A}$. This gives a vector at the vertex along which it could move to correct the area of that region: at least if all four vertices of the region moved similarly, the area would come out right.

But each vertex has four regions to contend with and so four vectors. So we add up the vectors and let the vertex move along the average. Then we do it again, then again, until all the areas, if not satisfied, at least stop changing between iterations up to some appropriate number of decimal places.

The only regions that must not be treated this way are the corner regions, which vary only linearly with the coordinates of their one free vertex. The new vector from the centroid should increase by the factor A_0/A .

Try this. You can use `meshgrid()` to generate the initial regular grid, `X0`, `Y0`, and `mesh()` to plot the resulting grid, `X`, `Y`, provided you are careful to observe `meshgrid()`'s and `mesh()`'s convention that y is the first coordinate and x the second. How quickly does it converge, say to four decimal places? What happens if the $\sqrt{A_0/A}$ scaling is replaced by A_0/A ?

You will need to know that the centroid of a simple polygon is

$$(C_x, C_y) = \frac{1}{6A} \sum_{i=1}^n x_i y_{i+1} - x_{i+1} y_i (x_i + x_{i+1}, y_i + y_{i+1})$$

where A is the area.

36. Use the slope of $x^2 - a$ to make a linear approximation to it near $x = \sqrt{a}$ and hence discover a procedure for finding square roots. How fast does it converge? How does it relate to the long-division-like procedure for extracting square roots you may have learned in school? Will a similar procedure work for finding cube roots?

Find out how `sqrt()` is implemented in MATLAB or on your calculator or in any programming language, such as FORTRAN, the original high-level language. How is your new method used?

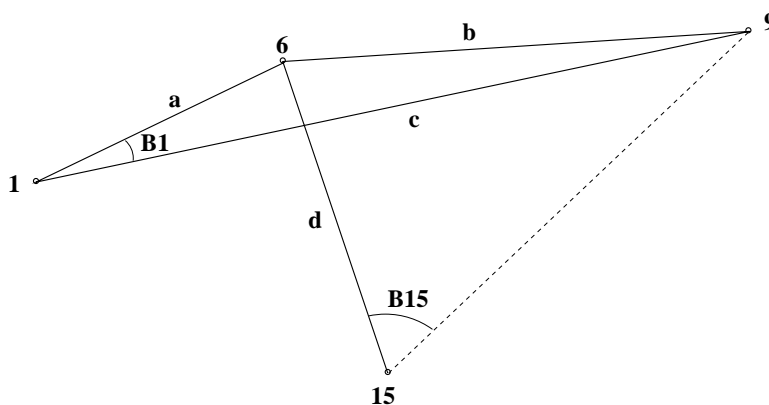
37. If nonlinearity and iteration are closely connected, why does iteration give an eigenvector, v , of matrix, M , as defined by the linear equation $Mv = \lambda v$?

38. Least squares solutions to overdetermined equations are used in surveying to find the coordinates of a location after taking redundant measurements. This is used by GPS (global positioning systems) to locate a receiver given its distances from the several NAVSTAR satellites that may be visible at any one time.

Here is a two-dimensional, ground-based surveying problem which is simpler to treat than 3-D satellite positioning with all the complexities of doing orbit calculations (taking account orbit changes due to solar radiation), spherical trigonometry (adjusting for the imperfect ellipsoidal shape of the “geoid”), and very precise clocking needed to convert radio transmission times through space and the atmosphere into distances (dealing with the irregularities in the Earth’s rotation, the movement of the north pole, and continental drift). This example is taken from chapter 5 of [Lei95], an informative (especially chapters 2 and 3) book but sadly inaccessible to beginners.

There are four locations, two with known coordinates

$$x_1 = 603.11, y_1 = 3102.44, x_{15} = 833.52, y_{15} = 2975.50.$$



The coordinates of the other two are only guesses

$$x_6 = 900, y_6 = 3600, x_9 = 900, y_9 = 3600.$$

But four distances and two angles have been measured

$$a = 179.7, b = 309.7, c = 480.4, d = 218.3, \cos B_1 = 0.9683, \cos B_{15} = 0.4203.$$

If we specify five distances (all nonlinear)

$$\begin{aligned} \alpha(x_6, y_6) &= (x_6 - x_1)^2 + (y_6 - y_1)^2 \\ \beta(x_6, y_6, x_9, y_9) &= (x_6 - x_9)^2 + (y_6 - y_9)^2 \\ \gamma(x_9, y_9) &= (x_9 - x_1)^2 + (y_9 - y_1)^2 \\ \delta(x_6, y_6) &= (x_6 - x_{15})^2 + (y_6 - y_{15})^2 \\ \epsilon(x_9, y_9) &= (x_9 - x_{15})^2 + (y_9 - y_{15})^2 \end{aligned}$$

we can write six equations in the four unknowns, x_6, y_6, x_9, y_9

$$\begin{aligned} \alpha(x_6, y_6) &= a^2 \\ \beta(x_6, y_6, x_9, y_9) &= b^2 \\ \gamma(x_9, y_9) &= c^2 \\ \delta(x_6, y_6) &= d^2 \\ \alpha(x_6, y_6) + \gamma(x_9, y_9) - \beta(x_6, y_6, x_9, y_9) &= 2 \times \sqrt{\alpha(x_6, y_6)\gamma(x_9, y_9)} \times \cos B_1 \\ \delta(x_6, y_6) + \epsilon(x_9, y_9) - \beta(x_6, y_6, x_9, y_9) &= 2 \times \sqrt{\delta(x_6, y_6)\epsilon(x_9, y_9)} \times \cos B_{15} \end{aligned}$$

The rest of this excursion is for you: linearize these equations about the guessed values $x_6 = 900, y_6 = 3600, x_9 = 900, y_9 = 3600$; set up the linear equations $\vec{B} = A\vec{X}$ with A a 6×4 matrix and \vec{X} the four unknown coordinates; solve the least-squares version, $A^T A\vec{X} = A^T \vec{B}$ for the next approximation to the coordinates in X ; repeat this until the values for the unknown coordinates converge to the same kind of precision that the known coordinates started out with; compare your answers with the locations given in Table F.3 of [Lei95, page 532] (those data are in degrees, minutes and seconds of longitude and latitude; yours will come out in seconds to be added to $(291^\circ, 44^\circ)$, a location in Maine).

39. Any part of the lecture that needs working through.

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