Collection VIII

The Collection VIII

Editor: Dr. Irene Sciriha

Department of Mathematics

Faculty of Science

University of Malta

Proceedings of Workshop held on the 11th November 2003

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Faculty of Science
Department of Mathematics

Date:	**11th November 2003**
Time:	**15.00 – 17.00**
Venue:	**LC 120**

A seminar/workshop is being held on Tuesday 11th November 2003 at 1500. Students and staff from the Department of Mathematics, Faculty of Science will present ideas from various fields of mathematics.

Keynote speakers:

Roberta Micallef	Isometries
Roderick Guzman	An old Japanese Theorem
Antoine Grech Ian George Walker	Couples and Handshakes
Mark Anthony Caruana	Generation of primes
Professor Anton Buhagiar	Discrimination using Eigenvectors

We shall end with a brief session for spontaneous problem posing. You are cordially invited to attend.

Abstracts of possible proofs or conjectures which you wish to share with us in this meeting, or in a future one, may be sent to Dr. I. Sciriha or Ms. A. Attard, Department of Mathematics, (marked The Collection), at any time of the year.

Dr. I. Sciriha
Organizer

Contents

Foreward

> The whole problem with the world is that fools and fanatics are always so sure of themselves, but wiser people so full of doubts.
>
> *Bertrand Russel*(1872-1970)

This workshop has once more brought together staff and students with diverse interests in mathematics. We had a taste of classical geometry from Japan, interaction between matrices and combinatorics, symmetries and inner product spaces as well as the attractive area of prime numbers. Moreover, Prof Anton Buhagiar regaled us with yet another encounter with one of the myriad powerful applications of eigenvector techniques. I leave it up to you to shuffle through the pages of this issue of *The Collection* to have a glimpse of the long and interesting journey that mathematics has travelled since the time of the Greeks.

Irene Sciriha
Editor

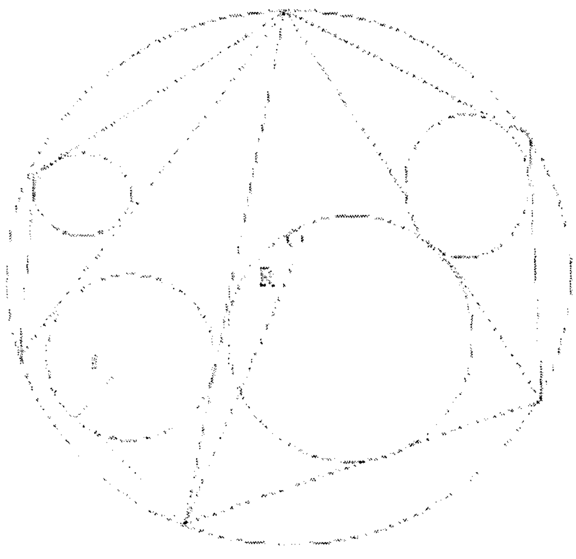
An Old Japanese Theorem

Roderick Gusman

The theorem states the following:

Theorem 1.1. *Let a convex polygon (a shape is convex if with every pair of points that belong to the shape, the shape contains the whole straight line segment connecting the two points) which is inscribed in a circle, be triangulated by drawing all the diagonals from one of the vertices and let the inscribed circle be drawn in each of the triangles. Then the sum of the radii of all these circles is a constant which is independent of which vertex is used to form the triangulation.*

As an illustration of the theorem consider the following figure.

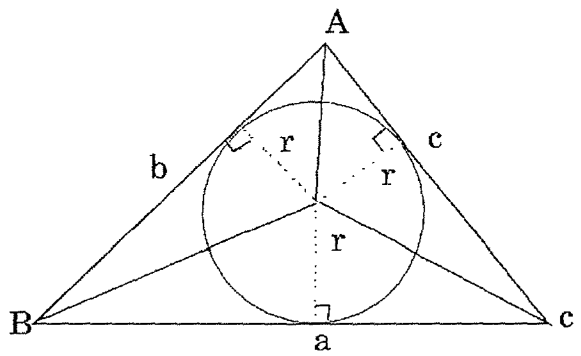


R is the radius of the outer circle while r is the radius of the inner circle inscribed in the triangle.

To prove the theorem, we must first prove the following two lemmas.

Lemma 1.2. *To show that* $r(a+b+c) = 2Area(ABC)$

Proof. Consider this diagram:



Then $\text{Area}(ABC) = \frac{1}{2}ar + \frac{1}{2}br + \frac{1}{2}cr = \frac{1}{2}(a+b+c)$
$\therefore r(a+b+c) = 2\text{Area}(ABC)$.

□

Lemma 1.3. (Carnot's Theorem) *In any triangle ABC, the sum of the distances from the circumcenter O to the sides is $R+r$, (i.e The sum of the circumradius with the inradius).*

$$OM_a + OM_b + OM_c = R + r$$

Proof. Only the case of an acute angle will be considered

Given that:

$$a = BC$$
$$b = AC$$
$$c = AB$$

and M_a, M_b and M_c are the intersecting points of the perpendicular lines from the origin O to the sides of the triangle.

For the inradius: $r(a+b+c) = 2\text{Area}(ABC)$, which was proved in lemma 1.

Also:

$$\begin{aligned}\text{Area}(ABC) &= \text{Area}(0AB) + \text{Area}(OAC) + \text{Area}(OBC)\\ &= \frac{1}{2}cOM_c + \frac{1}{2}OM_b + \frac{1}{2}OM_a\end{aligned}$$

$$\therefore r(a+b+c) = aOM_a + bOM_b + cOM_c$$

O begin the circumcenter of ABC, in the isosceles triangle AOB, $\angle A0B = 2\angle C$. Similarly, $\angle BOC = 2\angle A$ and $\angle AOC = 2\angle B$. Equipped with this knowledge, one may consider several triples of similar (right-angled) triangles:

- ABH_b, ACH_c, and BOM_a (or an equal COM_a)
- BAH_a, BCH_c and COM_b (or an equal AOM_b)
- CBH_b, CAH_a and AOM_c (or an equal BOM_c)

This is possible due to the similarity properties of the angles.
From the first triple one derives:

$$AH_b/c = AH_c/b = OM_a/R$$

which leads to: $OM_a(b+c) = R(AH_b + AH_c)$
Similarly,

$$\begin{aligned}OM_b(a+c) &= R(BH_a + BH_c)\\ OM_c(a+b) &= R(CH_a + CH_b)\end{aligned}$$

Summing these three up we get:

$$OM_a(b+c)+OM_b(a+c)+OM_c(a+b) = R(AH_b+AH_c+BH_c+CH_a+CH_b)$$

Grouping like subscript terms on the right hand side we get:

$$OM_a(b+c)+OM_b(a+c)+OM_c(a+b) = R(BH_a + CH_a+AH_b + CH_b+AH_c + BH_c)$$

Thus,

$$OM_a(b+c) + OM_b(a+c) + OM_c(a+b) = R(a+b+c)$$

Adding this to (*) and dividing by $(a+b+c)$ implies:

$$OM_a(a+b+c)+OM_b(a+b+c)+OM_c(a+b+c)=r(a+b+c)+R(a+b+c)$$

i.e. $OMa + OMb + OMc = r + R$

$\square$

We can now proceed with the original theorem:

First, observe that any triangulation of an n-gon with its diagonals consists of $(n-2)$ triangles. Next assume that the triangles in the triangulation are numbered and that the inradius of the circle in triangle i is r_i.

From Carnot's theorem, i.e lemma 2, one can prove that $R + r_i = OO_i$, where OO_i is equal to the addition of the perpendicular distance from O to each side of the triangle i.

That is:

$$\begin{aligned} OO_1 &= OO_{1a} + OO_{1b} + OO_{1c} \\ OO_2 &= OO_{2a} + OO_{2b} + OO_{2c} \\ &\vdots \\ OO_i &= OO_{ia} + OO_{ib} + OO_{ic} \\ &\vdots \\ OO_{(n-2)} &= OO_{(n-2)a} + OO_{(n-2)b} + OO_{(n-2)c} \end{aligned}$$

where

- $O_{1a} \ldots O_{(n-2)a}$ are identical to M_a in Carnot's Theorem.
- $O_{1b} \ldots O_{(n-2)b}$ are identical to M_b in Carnot's Theorem.
- $O_{1c} \ldots O_{(n-2)c}$ are identical to M_c in Carnot's Theorem.

The only difference is that in Carnot's Theorem one is considering one triangle, while in the original theorem one is considering a number of triangles that are formed by the n-gon.

$$\therefore \sum_{i=1}^{n-2} r_i + R = \sum_{i=1}^{n-2} OO_i$$

Thus $r_1 + \ldots + r_{n-2} = OO_1 + \ldots + OO_{n-2} - (n-2)R$

But $OO_1 + \ldots + OO_n - 2$ is identical to the perpendiculars of the sides of polygon counted once and the perpendiculars to the diagonals counted twice since every diagonal is the side of two adjacent triangles.

Furthermore, considering such internal perpendiculars, each is taken once as a positive value and once as a negative value and thus contributes nothing to the sum. Therefore, this sum is equal to the perpendiculars from O to the sides of the polygon. That is the right-hand side is a constant.

Thus the left-hand side i.e r_i is also a constant.

Figure 1

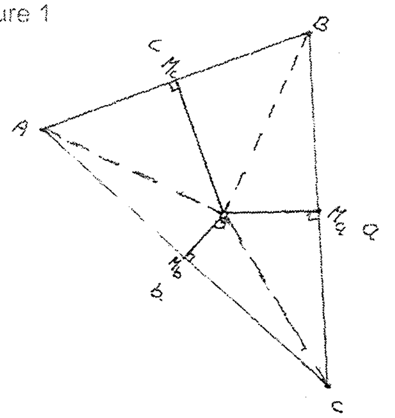
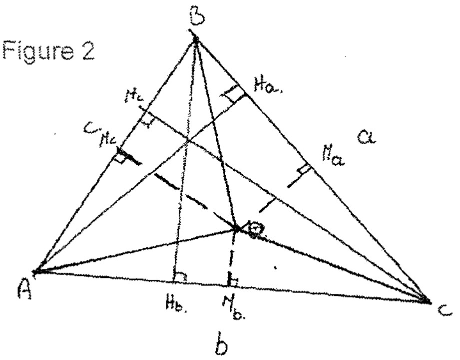


Figure 2



On Hand Shakes: A Combinatorial Problem

Antoine Grech and Ian George Walker

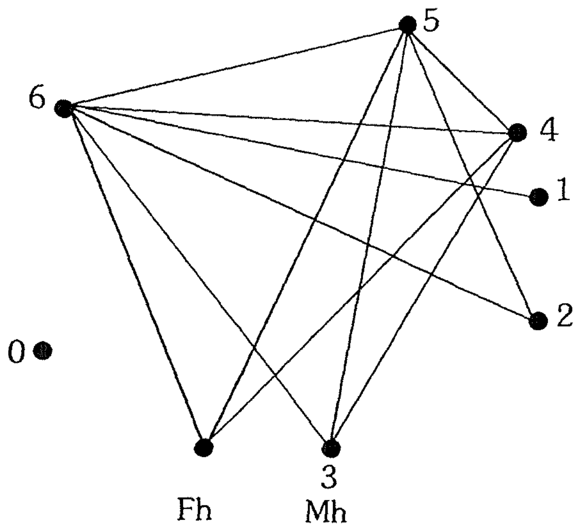
The problem is as follows:

> A number n of couples meet at one of the couples' homes. The female host (Fh) notices that no two of the people present (excluding herself) shake hands with the same number of people. No person shakes hand with the partner. With how many people does her husband (Hh) shake hands?

Solution One

The first solution will solve the problem for $n = 4$, where there are in all 8 persons. Assuming that handshaking never occurs between partners, a person can shake hands with at most 6 people. Construct a graph G having $2n = 8$ vertices each representing a single person. Two vertices are adjacent if a handshake occurs between these two people. Excluding the Fh, no two of the seven people shake the same number of hands. Therefore the possible number of handshakes are 6,5,4,3,2,1 and 0. Thus there must be some person, labelled v_6 who shakes hands with 6 people. The partner of v_6 is v_0 who does not shake hands with anyone. To see this recall that partners do not exchange handshakes; thus v_0 is not adjacent to v_6. Since all the other people shook hands with v_6 and since the number of handshakes is unique (excluding Fh), then v_0 must have shaken hands zero times (i.e v_0 is disconnected from the rest of the graph). Let v_5 be the person who shook hands five times. Then the person who shook hands once (v_1) is his/her partner, since apart from

v_1, v_0 all other persons must have shaken hands at least twice, with v_6 and v_5. Similarly, if v_4 is the person who shook hands four times, then by the same argument v_2 (the person who shook hands twice) is v_4's partner. The remaining vertex is v_3 for the person who shook hands 3 times. Who is v_3's partner? Choosing any partner from $v_0, v_1, v_2, v_3, v_4, v_5, v_6$ would contradict the premise that no two people (Fh excluded) shake hands the same number of times. Thus v_3's partner must be Fh which implies that v_3 is Mh, thus solving the problem. The following graph illustrates the solution. Note that at least two vertices in a graph must have the same degree (number of edges incident to a vertex).



Solution Two

The use of adjacency matrices provide a better model for solving the problem for a general positive integer n. As before the $2n-1$ people apart from the Fh can be labelled according to the number of handshakes $(0 \ldots 2n-2)$ which are all distinct by the above premise. Reserve the label $2n-1$ for the Fh. Construct a $2n-1 \times 2n-1$ matrix where element (i, j) is labelled if the i'th person shakes hands with the j'th person. Using a similar argument to that of solution one, $2n-2, 0$ form a couple; similarly $2n-3, 1$ form a couple. In general, $2n-k, k-2$ will form a couple for $n \geq k-1$. Thus, $n-1$ couples with $(n+1)-2=n-1$, which contradicts the uniqueness of the number of handshakes, unless this couple represents Fh, and Mh. Thus Mh shakes $n-1$ hands.

$$\begin{array}{c} 2n-2 \\ 2n-3 \\ \vdots \\ \\ \vdots \\ 0 \end{array} \begin{pmatrix} 0&1&1&1&1&0 \\ 1&0&1&1&0&0 \\ 1&1&0&0&0&0 \\ 1&1&0&0&0&0 \\ 1&0&0&0&0&0 \\ 0&0&0&0&0&0 \end{pmatrix}$$

Crystallography and Symmetry Groups

Roberta Micallef

Introduction

Crystals are assemblages of very small basic units of matter repeated periodically in 3 dimensions. The connection with group theory is that each pattern can be characterized by its symmetry group. It turns out that there are only 230 of these so-called crystallographic space groups amongst which are 22, which crystallographers prefer to regard as distinct, but which, from an abstract point of view, form 11 pairs of isomorphic groups. Thus the space groups fall into 219 isomorphism classes. The enumeration of these space groups is built upon the 14 lattices determined by Bravais. Since the enumeration is quite complicated, we here look at some of the corresponding ideas involved in the analogous 2-dimensional problem where 17 groups, no two of which are isomorphic, arise.

First recall that an isometry of the plane $\mathbb{R}^2$ is a distance- preserving mapping of R onto itself. Amongst such isometries are translations, rotations, reflections (in lines) and glide reflections. The latter being the result of an ordinary reflection in some line l followed by a translation parallel to l. Figure 1 adequately describes these movements.

Isometries of the Plane

Definition 1.4. An isometry of the plane is a distance preserving function $f : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$

Here distance preserving means that for points P and Q with position vectors $\mathbf{p}$ and $\mathbf{q}$,

$|f(P)f(Q)| = |PQ|$ i.e. $|f(\mathbf{p})f(\mathbf{q})| = |pq|$

Proposition 1.5. *Let $f : \mathbb{R}^2 \longrightarrow \mathbb{R}^2$ be an isometry which fixes the origin, then F preserves scalar products and angles between vectors.*

Proof. : Let $\mathbf{u}, \mathbf{v}$ be vectors and let U, V be the points with these as position vectors. Let $f(U)$ and $f(V)$ have position vectors $\mathbf{u}' = \overrightarrow{OF(U)}$ and $\mathbf{v}' = \overrightarrow{OF(V)}$. For every pair of points, P and Q we have:

$|f(P)f(Q)| = |PQ|$, so $|\mathbf{u}' - v'|^2 = |f(U)f(V)|^2 = |UV|^2 = |u - v|^2$. Hence $|u'|^2 + |v'|^2 - 2u'.v' = |u|^2 + |v|^2 - 2u.v$.

Since $|u'| = |Of(U)| = |f(O)f(U)| = |OU| = |\mathbf{u}|$ and $|v'| = |Of(V)| = |f(O)f(V)| = |OV| = |\mathbf{v}|$

We obtain $\mathbf{u}'.\mathbf{v}' = \mathbf{u}.\mathbf{v}$, which shows that the scalar product of two position vectors is unchanged by an isometry, which fixes the origin. Similarly, angles are preserved since the angle between the vectors $\mathbf{u}'$ and $\mathbf{v}'$ is $\arccos \frac{\mathbf{u}'.\mathbf{v}'}{|\mathbf{u}'||\mathbf{u}'|} = \arccos \frac{\mathbf{u}.\mathbf{v}}{|u||u|}$.

□

Wallpaper Patterns

The 2-dimensional repeating patterns we consider are commonly called *wallpaper patterns.* By definition these are patterns in which it is possible to find a basic pattern unit repeated periodically but not ' continuously' in each of two non-parallel directions

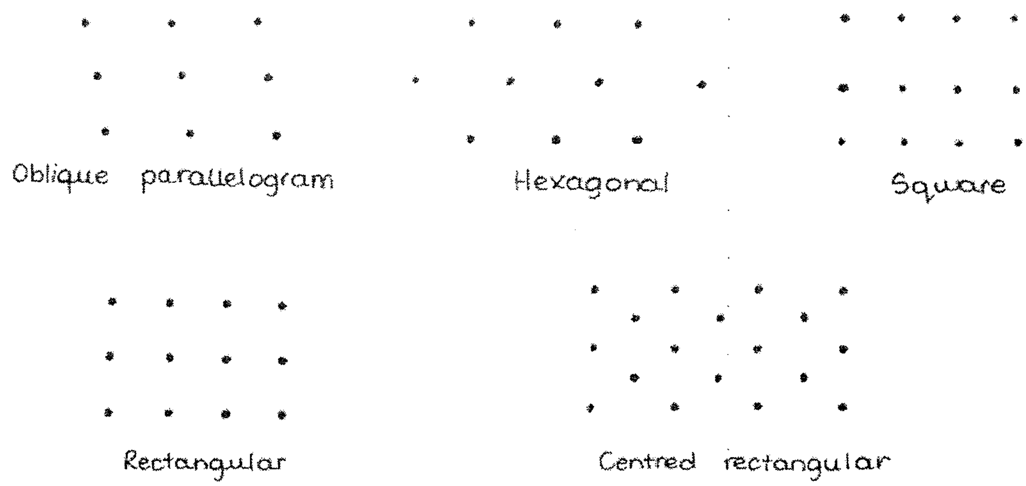
Wallpaper patterns correspond to plane symmetry groups, generated by two linearly independent translations.

The Crystallographic Restriction

Imagine you wish to tile your bathroom with only one type of tiles with the shape of a regular polygon. While this is easily possible with hexagons triangles and squares, you run into trouble with pentagons,say.

This is due to crystallographic restriction. Since the vertex angles of regular polygons are each equal to $\frac{(2n-4) \text{ right angles}}{n}$, a periodic tiling is possible only if these are integral fractions of 360° degrees. This requires that $\frac{2n}{n-2}$ is a positive integer.

Let G be a plane symmetry group. Each rotation of G necessarily has order 1, 2, 3, 4 or 6. There are only 5 basic types of lattice, which can underlie a plane symmetry group. Lattices possessing reflectional symmetry in a line must be made up of rectangles or rhombuses. Also if a lattice has glide-reflection symmetry it is necessarily of centered rectangular type. Thus there are only 5 kinds of lattices, which these are the 2-dimensional analogues of the 14 Bravais lattices.

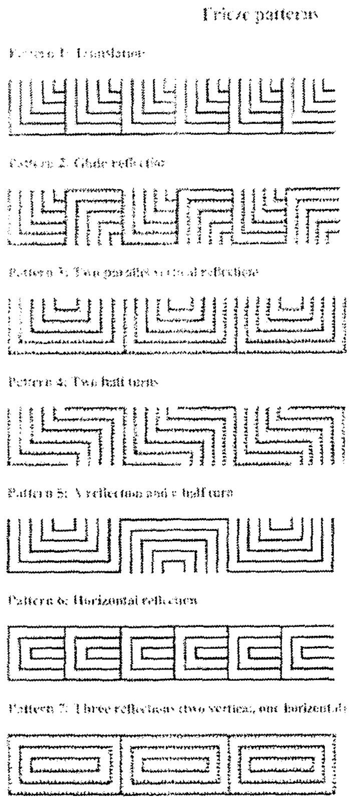


Definition 1.6. : A 2-dimensional crystallographic point group K is a group of isometries of $\mathbb{R}$, which fixes a point P and maps a 2-dimensional lattice containing P into itself.

In any such group there can be neither translations nor glide reflections. Consequently either all the elements of K are rotations or one half of them are rotations and the other half reflections. It follows that K is isomorphic to one of the cyclic (rotational) groups C_n or one of the dihedral groups (with two orthogonal axes of rotational symmetry), D_n where $n = 1, 2, 3, 4$ or 6. Each plane group G determines a crystallographic point group as a homomorphic image.

Frieze Patterns

These are 2-dimensional repeating patterns whose symmetry groups are discrete and infinite but also leave a line in $\mathbb{R}^2$ fixed. In such groups the subgroup of translations must be isomorphic to the infinite cyclic group. There are seven distinct frieze patterns; their symmetry groups fall into four isomorphism classes.



New Models for Quasicrystals

In 1984 a group of experimentalists has discovered diffraction patterns for electrons diffracted at the atoms of an alloy composed of an Aluminium and Manganese.

The striking features are:

1. A rotational symmetry around a 10-fold axis, called 'Forbidden Symmetry' in crystallography because it cannot occur in crystals

2. Non-translational symmetry: it is not possible to construct the whole pattern by gluing together identical copies of one shape (called the 'Unit Cell' in crystallography)

3. Long-range order: One observes a well-ordered pattern, which may be extended over the entire space according to a well-defined prescription.

These observations imply that, the new object cannot be described mathematically by the laws of usual crystallography and is called Quasicrystal.

Mathematical Models for Quasicrystals

There are new mathematical models (affine extensions of noncrystallographic Coexeter groups) for quasicrystals, which use a projection from a higher dimensional periodic lattice to construct a periodic point set of lower dimensions. The vertex of particular tilings of the plane e.g. the Penrose tiling is an example of aperiodic point sets compatible with 10-fold symmetry.

Generation of Prime Numbers

Mark Anthony Caruana

Introduction

Introduction Prime numbers are by definition numbers which are only divisible by one and by themselves. It can be proved that such numbers are infinite, as are after all, the Real Numbers, or the Natural numbers. In the following pages will be trying to shed some light over the following unanswered question:

> "Is it possible to come up with some form of equation with which one can generate such numbers?"

It is interesting to know that ever since Antiquity, mathematicians have always been haunted by this infamous question which, in virtue seems to have no straight forward answer.

History

Mathematicians like Eratosthenes (275-194 B.C., Greece) managed however to come up with interesting methods of how to find prime numbers. One of these methods is known as 'The Sieve of Eratosthenes'. The method is rather crude and time consuming but rather efficient. All one must do is to build up a chart, or a list containing the natural numbers. Then one must simply follow the set of simple instructions listed below:

- Cross out 1, (as one is not prime).

- Circle 2, because it is the smallest positive even prime. Now cross out every multiple of 2 present in the chart.
- Circle 3, the next number in the list, and again, cross out all the multiples of 3.
- Omit 4,(as four has four has been already crossed out).
- Circle 5, etc.

In later years the mathematician Euler came up with an equation which could generate 40 primes, which for the time was a break through. The equation is $y = x^2 + x + 41$ and could generate prime numbers for x between 0 and 39. In recent times, someone, whose identity is not known, came up an equation which could generate 45 prime numbers; this equation is presently the record breaker. The equation is $y = 36x^2 - 810x + 2753$, and can generate primes for x between 0 and 44.

Prime Number generation

There are various algorithms by which prime numbers can be created (one of them is the Sieve of Eratosthenes); however we are after an algebraic equation which can generate such numbers.

Approximations

These equations have not been conceived to created EXACT sequences of prime numbers but rather a sequence of numbers which are approximately prime i.e. such equations will generate numbers such as: 1.99, 2.87, 4.98 . . . These sequences when rounded off very often will give us a very good sequence of prime numbers.

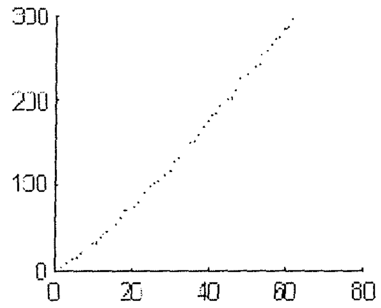
- The Linear Approximation

  In this method we will derive a linear equation which will relate the Natural Numbers to the Prime Numbers.

  Build a table like the following:

x values	1	2	3	4	5	...
y values	2	3	5	7	11	...

From the above table, the following scatter plot is constructed.



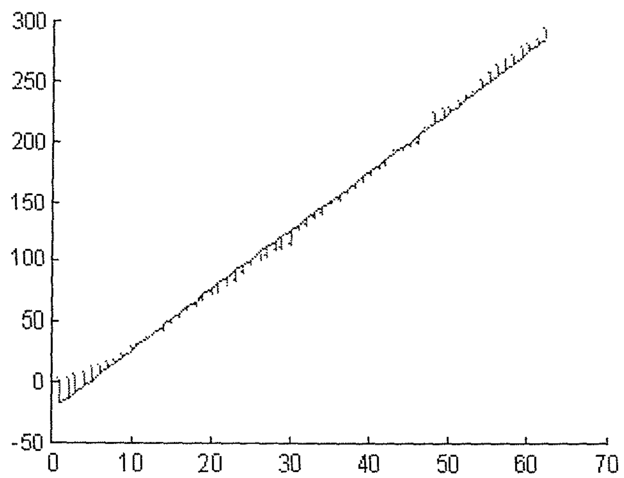
From the above figure and table we can obtain the line of best fit $Y = mx + c$, where

$$m = \frac{n\sum_{i=1}^{n} x_i y_i - (\sum_{i=1}^{n} x_i)(\sum_{i=1}^{n} y_i)}{n\sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2}$$

and

$$c = \frac{1}{n}\sum_{i=1}^{n} y_i - \frac{m}{n}\sum_{i=1}^{n} x_i$$

After having carried out the necessary computations, the following results are obtained:



The line of best fit is $Y = mX + C$, where $m = 4.97381078290650$, $C = -23.20729772607083$.

(The vertical lines represent the distance from the line of best fit to the points)

The main limitation of this approach is that in various cases the line of best fit is quite distant from the points. Thus, the approximation in these particular cases will be quite poor.

- The Second Order Approximation

  In this method we shall attempt to bend the line of best fit so as to try to accommodate all the given points.

  - Build up the table and draw the scatter plot
  - Calculate the coefficients m, c for line of best fit
  - Calculate the vertical distance from each point to the line of best fit
  - If we have 90 numbers, say, in the x-values row, namely 1,2,3,,90; then sub divide this interval into three intervals, each of equal size. Say first interval contains numbers 1, 2, 3. . . 30; the second interval contains the numbers 31, 32, 34 60. Similarly for the third interval.
  - From each interval choose: 1. the point which is closest to the line, 2. the point which is most distant from the line. In so doing we would end up with three points which are closest to the line in their respective intervals, a1, a2, a3, and three points which are the most distant from the line 1, 2, 3
  - Now we want a quadratic equation of the form $y = ax^2 + bx + c$
  - Now we can insert $\alpha_1, \alpha_2, \alpha_3$ in the above equation and find the values of a, b, c which we shall be calling a_1, b_1, c_1 (recall the fact that α_i is a point which contains an x- value and a y-value).
  - The same procedure can be done with $\beta_1, \beta_2, \beta_3$ in this case the values we shall obtain are a_2, b_2, c_2. Now to find the actual values of a, b, c simply compute the following:

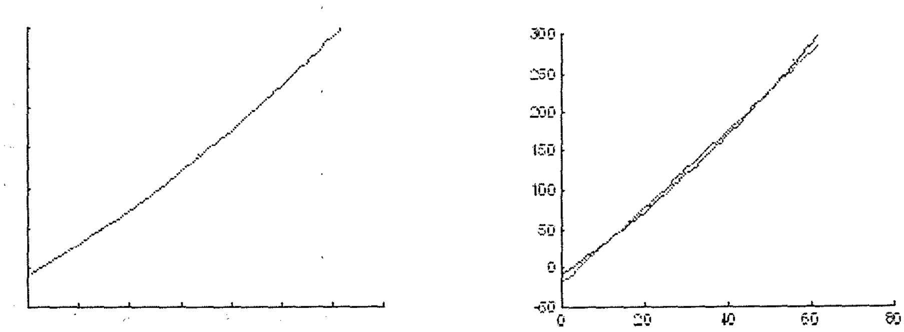
$$a = \frac{a_1 + a_2}{2}; b = \frac{b_1 + b_2}{2}; c = \frac{c_1 + c_2}{2}$$

The equation which can generate the first 300 primes is,

$$y = ax^2 + bx + c$$

where: $a = 0.02070189842422, b = 3.68979741019214, c = -10.55260457177425$

In the following figures, we can see that the curve now fits the given points much better.



Equations Which can Generate Exact sequences of Prime Numbers

These equations have been created to generate exact sequences of prime numbers. However one must say that although these equations can do this remarkable job, such equations can become very long and rather messy to work with. For example, to generate the first 6 prime numbers we would require a polynomial of order 6. Similarly, to generate the first 100 primes, a polynomial of order 100 would be required. The method used is rather easy and in fact it uses Gaussian elimination.

- Decide for the number of primes that the equation will generate.
- Let the equation be of the form:

$$y = \alpha_n x^n + \alpha_{n-1} x^{n-1} + \ldots \alpha_1 x$$

(where n is the number of primes that the equation is capable of generating)

- To find the coefficients $\alpha_1, \alpha_2, \ldots, \alpha_n$ Gaussian elimination can be used.

As an illustration, the equation required to derive the first six prime numbers is:

$$Y = ax^6 + bx^5 + cx^4 + dx^3 + ex^2 + fx$$

where

$$\begin{aligned} a &= -0.020833333 \\ b &= 0.3625 \\ c &= -2.39583 \\ d &= 7.520833333 \\ e &= -11.083 \\ f &= 7.616666667 \end{aligned}$$

Discriminating between two groups using eigenvectors

Anton Buhagiar
Department of Mathematics.

Introduction

Consider g populations or groups, $g \geq 2$. The object of discriminant analysis is to allocate an individual to one of these g groups on the basis of his/her measurements on the p variables $x_1, x_2, \ldots, x_p$. It is desirable to make as few 'mistakes' as possible in classifying these individuals to the various groups.

For example, the populations might consist of different diseases and the p variables $x_1, x_2, \ldots, x_p$ might measure the symptoms of a patient, eg. blood pressure, body temperature, etc. Thus one is trying to diagnose a patient's disease on the basis of his/her symptoms. As another example, one can consider samples from three species of iris. The object is then to allocate a new iris to one of these species on the basis of its measurements eg. sepal length, sepal width, etc.

In the case of two groups, $g = 2$, in the univariate case, when $p = 1$ and x_1 is the only variable measured, it is quite easy to see when the two groups are well separated from each other. For this purpose, one can perform a t-test on $x_1$to see whether the two groups have significantly different means. Equivalently, one can define the ratio:

$$\frac{\text{the difference } \textit{between} \text{ the means of the two samples}}{\text{deviations } \textit{within} \text{ the samples}}.$$

A large value for this ratio, which is proportional to the $t-$statistic, would indicate that the means of the samples are well separated from each other;

conversely, a small value for this ratio would imply that within sample variations are relatively large, and that readings from the two samples would tend to overlap. This would in turn lead to poor discrimination between the two groups in terms of x_1, and to a non-significant difference between the sample means for x_1.

In the case when $g \geq 2$, that is for two or more groups, and when $p = 1$, one-way analysis of variance, the F-test, can be performed to examine whether the mean of x_1 differs significantly over the groups. Equivalently, one can define the ratio:

$$\frac{\text{Variation } \textit{between} \text{ the means of the samples}}{\text{Variation } \textit{within} \text{ the samples}}. \tag{1.0.0.1}$$

Again in this case, a large value for this ratio, which is closely related to the F-statistic, signifies good separation between the groups and a significant difference for $x_1$between the groups. In fact, in the case of two groups ($g = 2$), the F-test and the t-test are equivalent to each other, with $F = t^2$ for a given problem.

In the case when the number of variables is larger than one, $p >1$, one can perform separate univariate tests on each of the p variables $x_1, x_2, \ldots, x_p$. For purposes of discrimination, however, it is often preferable to define a linear combination y of the x_k's, namely $y = \sum_{k=1}^{p} a_k x_k$, with the object of maximising the ratio defined in equation (1). Finding the best linear combination which maximizes this ratio is equivalent to maximizing the statistical distance between the groups. This in turn would guarantee greater success in discriminating between the different groups. As shown below, the problem of finding the optimum choice of the coefficients a_i can be reduced to a suitable eigenvalue problem.

Partitioning the total variation of y

We will now discuss briefly a very important identity in the context of discrimination and analysis of variance. We will assume that there are g different groups in all, and that there are n_i cases in the i'th group, where $i = 1, 2, \ldots, g$. For each case, the p variables $x_1, x_2, \ldots, x_p$ are measured. We then denote by x_{ijk} the value of the k^{th} variable (x_k) for the j'th case in the

i'th group. Note here that the suffixes have the following bounds:

$$x_{ijk}: \quad 1 \leqslant k \leqslant p, 1 \leqslant j \leqslant n_i, 1 \leqslant i \leqslant g.$$

value of variable x_k for case j in sample i.

It is then easy to write down the mean of the k'th variable over the i'th sample, and the grand mean of the k'th variable over all groups:

$$x_{i.k} = \frac{1}{n_i}\sum_{j=1}^{n_i} x_{ijk} \quad ; \quad x_{..k} = \frac{1}{\sum_{i=1}^{g} n_i}\sum_{i=1}^{g}\sum_{j=1}^{n_i} x_{ijk} \quad .$$

In an analogous fashion, the linear combination y for the i'th case in the j'th sample can be written as $y_{ij} = \sum_{k=1}^{p} a_k x_{ijk}$. Its mean over the i'th sample and its overall (grand) mean are then given as:

$$y_{i.} = \frac{1}{n_i}\sum_{j=1}^{n_i}\sum_{k=1}^{p} a_k x_{ijk} = \sum_{k=1}^{p} a_k x_{i.k} \quad ; \quad y_{..} = \frac{1}{\sum_{i=1}^{g} n_i}\sum_{i=1}^{g}\sum_{j=1}^{n_i}\sum_{k=1}^{p} a_k x_{ijk} = \sum_{k=1}^{p} a_k x_{..k} \quad .$$

The sum of the square of the deviations of the values of y_{ij} for each case from their overall (grand) mean $y_{..}$ is then given by
$\sum_{i=1}^{g}\sum_{j=1}^{n_i}(y_{ij} - y_{..})^2$ or $\sum_{i=1}^{g}\sum_{j=1}^{n_i}\left[\sum_{k=1}^{p} a_k(x_{ijk} - x_{..k})\right]^2$.

This quantity is often referred to as the *total variation* of y, or equivalently as the *total sum of squares*, often abbreviated as *SST*. Algebraic manipulation of the SST will result in a very important partitioning of this variation into two separate parts as follows:

$SST \equiv$ Total sum of squares

$$= \sum_{i=1}^{g}\sum_{j=1}^{n_i}\left[\sum_{k=1}^{p} a_k(x_{ijk} - x_{..k})\right]^2$$

interchange order of summation:

$$= \sum_{1 \leqslant l,m \leqslant p}^{a_l a_m} \sum_{i=1}^{g}\sum_{j=1}^{n_i}(x_{ijl} - x_{..l})(x_{ijm} - x_{..m})$$

add and subtract mean of sample from which reading is taken, leaving sum unchanged:

$$= \sum_{1\leqslant l,m\leqslant p}^{a_l a_m} \sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{ijl} - x_{i.l} + x_{i.l} - x_{..l})(x_{ijm} - x_{i.m} + x_{i.m} - x_{..m})$$

multiply out the terms in pairs:

$$= \sum_{1\leqslant l,m\leqslant p}^{a_l a_m} \sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{ijl} - x_{i.l})(x_{ijm} - x_{i.m}) + \sum_{1\leqslant l,m\leqslant p}^{a_l a_m} \sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{i.l} - x_{..l})(x_{i.m} - x_{..m})$$

+ the other two cross terms which each equal zero using the definition of the sample means

simplify second term since brackets are independent of suffix j:

$$= \sum_{1\leqslant l,m\leqslant p}^{a_l a_m} \sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{ijl} - x_{i.l})(x_{ijm} - x_{i.m}) + \sum_{1\leqslant l,m\leqslant p}^{a_l a_m} \sum_{i=1}^{g} n_i (x_{i.l} - x_{..l})(x_{i.m} - x_{..m})$$

$$\equiv SSW \ + SSB$$

The first term in the penultimate line, often abbreviated as SSW, estimates the size of deviations of the readings from *their own* sample mean, and is often called the *within-variation* or *within sum of squares.* The second term, often abbreviated as SSB, estimates the size of the deviations of the sample means from the overall mean and is referred to as the *between-variation*, or the *between sums of squares.* The above identity can be therefore written as

$$\text{SST} = \text{SSW} + \text{SSB} \tag{1.0.0.2}$$

or *total variation = variation within samples + variation between samples*

This important identity is often referred to as *partitioning the sums of squares.* It is important to note that the terms SSB and SSW are, respectively, the numerator and denominator in the ratio defined by equation (1). The groups are more easily separated if the ratio in equation (1), $\frac{SSB}{SSW}$, is large or equivalently $\frac{SST}{SSB}$ is small. Statistical tests have been devised using these ratios to determine whether the sample means are significantly different from each other.

Matrix formulation

The sums of squares, SST, SSW and SSB are all quadratic forms in the coefficients a_k

and can be elegantly represented in matrix form. Rearranging the p coefficients a_k as the$p \times 1$ column vector a, one can rewrite the partitioning identity (2) as

$$a^tTa \quad = \quad a^tWa \quad + \quad a^tBa$$

$$\text{SST} = \text{SSW} + \text{SSB}$$

where T, W and B are symmetric $p \times p$ matrices, the l, m'th entry of which are given by the terms multiplying $a_l a_m$ in the corresponding sum of squares. Thus,

the l, m'th entry of T is $\sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{ijl} - x_{..l})(x_{ijm} - x_{..m})$;

the l, m'th entry of W is $\sum_{i=1}^{g} \sum_{j=1}^{n_i} (x_{ijl} - x_{i.l})(x_{ijm} - x_{i.m})$; (3)

the l, m'th entry of B is $\sum_{i=1}^{g} n_i(x_{i.l} - x_{..l})(x_{i.m} - x_{..m})$.

The matrices T, W and B are called *sums of squares and cross-product matrices.* Since the partitioning holds for any arbitrary vector a, these three matrices satisfy the identity

$$T = W + B \tag{1.0.0.4}$$

In fact, B is usually calculated from $B = T - W$ in practise.

Maximising the ratio of between to within variation

For optimum separation of the groups, we would therefore seek to maximise the ratio $\frac{SSB}{SSW}$. In matrix form, we would like to find a suitable column vector a with entries $a_1, a_2, \ldots, a_p$, such that $\frac{a^tBa}{a^tWa}$ is a maximum. Equivalently, since multiplying a by a scalar would not change the ratio, we can maximise the numerator, subject to the constraint that the denominator is one. Using

Lagrangian multipliers, we maximise the function $\varphi(a)$defined by

$$\varphi(a) = \quad a^t Ba + \lambda(1 - a^t Wa).$$

This function $\varphi(a)$ can then be differentiated with respect to each of the a_k's, $k = 1, 2, \ldots, p$, and the derivatives $\frac{\partial\varphi(a)}{\partial a_k}$ are each set to zero. When the resulting set of p equations are rearranged in matrix form, one obtains the homogeneous linear system

$$\frac{\partial\varphi(a)}{\partial a} \quad = \quad 2Ba - 2\lambda Wa \quad = \quad 0,$$

where 0 is the $p \times 1$ column vector of zeros. Dividing by 2 and factorising, we then obtain the condition:

$$(B - \lambda W)a = 0, \text{ or equivalently} \tag{1.0.0.5}$$
$$(W^{-1}B - \lambda I)a = 0. \tag{1.0.0.6}$$

Therefore a is an eigenvector of $W^{-1}B$ and λ is its corresponding eigenvalue. Further, pre-multiplying equation (5) by a^t, we get

$$\begin{aligned} a^t(B - \lambda W)a &= 0, \text{ that is} \\ a^t Ba &= \lambda a^t Wa \text{ or} \\ \lambda &= \frac{a^t Ba}{a^t Wa}. \end{aligned} \tag{1.0.0.7}$$

From equations 6 and 7, one can therefore conclude that the maximum possible value of the ratio $\frac{a^t Ba}{a^t Wa}$ ($\equiv \frac{SSB}{SSW}$) is the largest eigenvalue λ of $W^{-1}B$ and the optimum choice of a is the eigenvector of λ. The linear combination $y = \sum_{k=1}^{p} a_k x_k$ can be written in matrix form as $a^t x$. For this particular choice of the vector a, this linear combination is the one which best separates the groups. It is called *Fisher's discriminant function* (Fisher, 1936) after its inventor.

An example on discrimination between two groups

To illustrate the above, we now give an example of discrimination between two groups ($g = 2$) on the basis of two variables ($p = 2$). The following 'botanical' example is inspired by Fisher's classic paper on discrimination (Fisher, 1936), which is described in Mardia *et al.* (1979), whilst the numerical data are derived from Tacq (1997).

The datafile in our example contains measurements on two types of iris. The variables Y, X_1 and X_2 are defined as follows:

$$Y = \text{ type of iris } = \begin{cases} 0, \text{ if iris is of the } \textit{setosa} \text{ type (group 1);} \\ 1, \text{ if iris is of the } \textit{versicolor} \text{ type (group 2).} \end{cases}$$

$$X_1 = \text{ sepal length and } X_2 = \text{ sepal width.}$$

X_1 and X_2 are assumed to be normally distributed with similar covariance structure in the two groups (Tacq, 1997).

The data-file contains 15 cases in all, 6 in the first group (*setosa*), and 9 in the second group (*versicolor*). For each individual case (flower), we give its group membership (Y), its sepal length and sepal width (X_1 and X_2). The data-file is listed in **Table I**.

Table 1: The datafile and its statistical description.

Calculation of the matrices W, T and B, using equations (3) and equation (4).

	Y	X_1	X_2
Setosa	0	1	1
	0	1	4
	0	2	1
	0	4	5
	0	5	5
	0	5	9
Versicolor	1	4	2
	1	4	4
	1	5	6
	1	6	3
	1	6	6
	1	7	6
	1	8	7
	1	9	7
	1	9	8

Group 1: *Setosa*

Cases in sample: $n_1 = 6$

Mean: $\overline{X_1} = 3.000$ $\overline{X_2} = 4.166$

Variation: $\sum(X_1 - \overline{X_1})^2 = 18.000$ $\sum(X_2 - \overline{X_2})^2 = 44.833$

Covariation: $\sum(X_1 - \overline{X_1})(X_2 - \overline{X_2}) = 22$

$\therefore W_1 = \begin{pmatrix} 18 & 22 \\ 22 & 44.833 \end{pmatrix}$; *within variation in group* 1.

Group 2: *Versicolor*

Cases in sample: $n_2 = 9$

Mean: $\overline{X_1} = 6.444$ $\overline{X_2} = 5.444$

Variation: $\sum(X_1 - \overline{X_1})^2 = 30.222$ $\sum(X_2 - \overline{X_2})^2 = 32.222$

Covariation: $\sum(X_1 - \overline{X_1})(X_2 - \overline{X_2}) = 25.222$

$\therefore W_2 = \begin{pmatrix} 30.222 & 25.222 \\ 25.222 & 32.222 \end{pmatrix}$; *within variation in group* 2.

$\therefore W = W_1 + W_2 = \begin{pmatrix} 48.222 & 47.222 \\ 47.222 & 77.056 \end{pmatrix}$. $\therefore W^{-1} = \begin{pmatrix} 0.052 & -0.032 \\ -0.032 & 0.032 \end{pmatrix}$.

variation within samples; *inverse of W.*

Groups 1 and 2 together:

Total number of cases: $n = n_1 + n_2 = 15$

Overall mean: $\overline{X_1} = 5.067$ $\overline{X_2} = 4.933$

Total Variation: $\sum(X_1 - \overline{X_1})^2 = 90.933$ $\sum(X_2 - \overline{X_2})^2 = 82.933$

Total Covariation: $\sum(X_1 - \overline{X_1})(X_2 - \overline{X_2}) = 63.067$

$\therefore T = \begin{pmatrix} 90.933 & 63.067 \\ 63.067 & 82.933 \end{pmatrix}$. $\therefore B = T - W = \begin{pmatrix} 42.711 & 15.844 \\ 15.844 & 5.858 \end{pmatrix}$.

total variation *variation between samples*

In **Table I**, we also give the statistical description of each group separately, and of both groups pooled together. In particular, we give the means of the two variables X_1 and X_2, namely $\overline{X}_1$ and $\overline{X}_2$, for each sample separately, and the within sums of squares for each sample, W_1 and W_2, from which the within sum of squares matrix W for both groups could be simply calculated using $W = W_1 + W_2$. The groups are then pooled together, to obtain the grand means of X_1 and X_2, and hence the total sum of squares matrix T. The between sum of squares matrix B is then calculated as $B = T - W$. The reader is referred to **Table I** for the calculation of the 2x2 matrices W, B, T and W^{-1}.

One can then calculate $W^{-1}B$ as follows:

$$W^{-1}B = \begin{pmatrix} 0.052 & -0.032 \\ -0.032 & 0.032 \end{pmatrix} \begin{pmatrix} 42.711 & 15.844 \\ 15.844 & 5.858 \end{pmatrix} = \begin{pmatrix} 1.711 & 0.635 \\ -0.843 & -0.313 \end{pmatrix}.$$

This matrix has non-zero eigenvalue λ =1.399, with unit eigenvector $a = \begin{pmatrix} 0.897 \\ -0.442 \end{pmatrix}$.

Fisher's discriminant function is therefore given by $a^t x = 0.897X_1 - 0.442X_2$. This is the linear combination which gives the largest value (=λ) of the ratio $\frac{SSB}{SSW}$ in equation (2), namely, the ratio of the variation *between* samples to the variation *within* samples.

Test of significance on the eigenvalue.

One normally performs Hotelling's T^2 test to see whether the mean of the discriminant function $a^t x$ differs significantly between the two groups.

The T^2 statistic is defined as

$$T^2 = (n-2)\lambda,$$

where $n = n_1 + n_2$ is the total number of cases in the two samples.

T^2 should be 'large' if the means of the two groups are well separated.

Conversely, T^2 is 'small' if there is no significant difference between the two sample means. In this case, Hotelling showed that the quantity $\frac{(n-p-1)}{p(n-2)}T^2$ should be distributed according to the F-distribution with p, $n-p-1$ degrees of freedom, where p is the number of variables featuring in the discriminant function and n is the total number of cases in the two groups.

In this application, $p = 2$, $n = n_1 + n_2 = 6 + 9 = 15$,

$$T^2 = (n-2)\lambda = (15-2)(1.399) = 18.182,$$

$$F = \frac{(n-p-1)}{p(n-2)}T^2 = \frac{(15-2-1)}{2(15-2)}(18.182) = 8.392.$$

Degrees of freedom for F-test $= p,\ n-p-1 = 2,\ 15-2-1$
$= 2,\ 12$.

In our case therefore, if there is no significant difference between the groups, the F-statistic should be distributed according to the F-distribution with 2, 12 degrees of freedom.

From the tables, the critical F-value for 2, 12 degrees of freedom with $\alpha = 0.05$ is 3.89. Since $8.392 > 3.89$, we can conclude that the means of the two groups are significantly different. For this reason, discriminant analysis could be done profitably on this dataset.

A typical statistical package would also include the following items in the output of a discriminant analysis:

1. a classification rule to determine the group to which a given case is assigned;

2. application of this classification rule to the cases whose group membership is known *a priori*, so as to obtain an estimate of the misclassification rate;

3. application of this classification to classify cases of unknown type.

We now describe briefly the classification rule and its application.

The Classification Rule

The discriminant function is often used to establish a classification rule whereby group membership of a given case can be determined. This could be done both for cases whose group membership is known *a priori*, and also for cases with unknown group membership.

One classification rule can be set up in the following way.

The value of the discriminant function $a^t x$ is first calculated at the centroid of each group:

Group 1: 0.897(3.000)-0.442(4.167) = 0.849,
Group 2: 0.897(6.444)-0.442(5.444) = 3.374.
The cut-off is then taken to be the average of these two values:

$$t_c = \frac{0.849 + 3.374}{2} = 2.112.$$

Then any case $(X_1, X_2)$is assigned to Group 1 if $0.897X_1 - 0.442X_2 < 2.112$, and to Group 2 otherwise.

Using this rule, one can classify the original cases to find how good the discriminant analysis is. Prior group membership could be compared to the posterior grouping predicted by the classification rule. This comparison is summarized in a classification table. One can also use this rule to classify new cases for which group membership is not known. The use of the classification rule is illustrated in **Table II**.

Table II: Use of the classification rule:

i) to classify original cases and hence
ii) to obtain a prior versus post classification table; and
iii) to classify new cases with unknown group membership.

i) Classification of original cases:

	Y	X_1	X_2	$0.897X_1 - 0.442X_2$	Posterior Classification
Setosa	0	1	1	0.455	0
	0	1	4	-0.871	0
	0	2	1	1.352	0
	0	4	5	1.378	0
	0	5	5	2.275	1
	0	5	9	0.507	0
Versi-	1	4	2	2.704	1
Color	1	4	4	1.820	0
	1	5	6	1.833	0
	1	6	3	4.056	1
	1	6	6	2.730	1
	1	7	6	3.627	1
	1	8	7	4.082	1
	1	9	7	4.979	1
	1	9	8	4.537	1

ii) Classification Table:

		Posterior Classification:	
		Group 1	Group 2
Prior Classification :	Group 1	5	1
	Group 2	2	7

80% of the cases are classified correctly.

iii) Classification of new cases with unknown group membership:

Y	X_1	X_2	$0.897X_1 - 0.442X_2$	Posterior Classification
?	6	5	3.172	1
?	5	6	1.833	0
?	3	7	-0.403	0
?	4	3	2.262	1
?	6	4	3.614	1

Conclusion and suggestions for further reading

Discriminant analysis is a very popular multivariate technique. Like many other techniques in multivariate statistics, the method is based on the algebraic eigenvalue problem. In this respect it is very similar to principal component analysis, factor analysis, correspondence analysis and multivariate analysis of variance (Manova), in all of which one has to find the eigenvalues and eigenvectors of a suitable matrix (Lebart, Morineau and Warwick, 1984). The eigenvalue problem defined by equation (5) is also important in the solution of vibrational problems of mechanics (Lunn, 1990 and Segerlind, 1983) and in the buckling of structures (Dawe, 1983).

Discriminant analysis is also related to linear regression and logistic regression, where group membership, y, is regressed on the measured variables x_i, (Flury and Riedwyl, 1993).

Most books on multivariate statistics have a chapter on discriminant analysis. The books by Tacq (1997), Manly (1986), and Flury and Riedwyl (1993) are very readable and should be reasonably easy to an undergraduate in mathematics or statistics.

For students who wish to read further on discriminant analysis, one can suggest more mathematical texts such as Morrison (1990), Everett and Dunn (1991), Johnson and Wichern (1992) and Mardia, Kent and Bibby (1979). In addition to the statistical theory, these books also give many practical examples of this technique.

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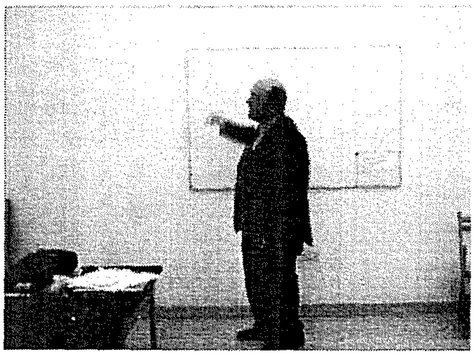
Photographs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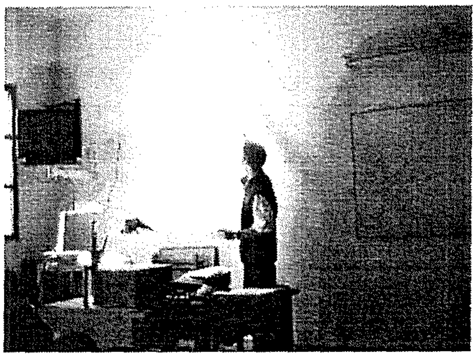
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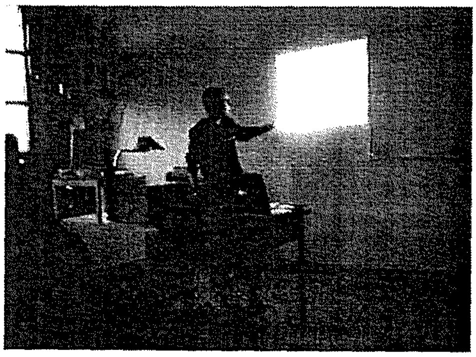
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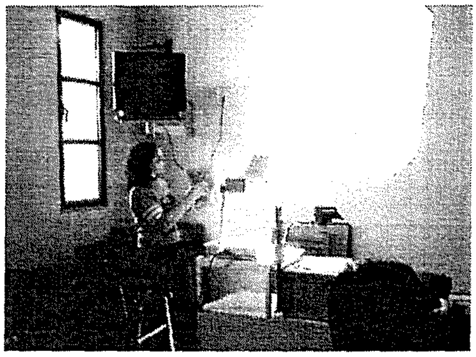
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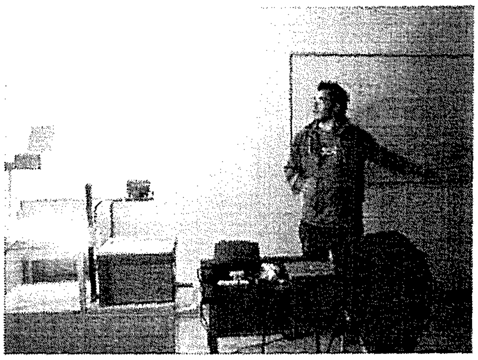

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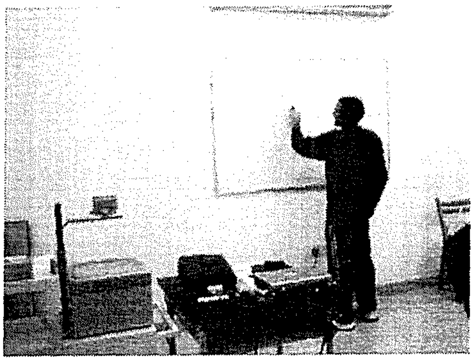

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