



NEWSLETTER

June 2003

Operational Research Society of New Zealand, Inc.
PO Box 6544, Wellesley St. Auckland, New Zealand, www.orsnz.org.nz

Beyond Optimal Clustering

By Hsiao-Fan Wang

Clustering is one of the most fundamental activities in pattern recognition and knowledge discovery. It aims to use certain partition techniques to reveal the characteristics of a data set such that the resultant groups meet two basic criteria: the *smallest within-group variance* and the *largest between-group variance* two basic criteria. Depending on whether the developed techniques have taken these criteria explicitly into account, three approaches have been recognized: hierarchical clustering, graph-theoretic approach of implicit approaches and objective-function method of explicit approaches [2]. In this article, we shall focus on the latter approach in which the issues raised from optimal clustering are discussed.

How to Present the Model ?

1) c-Means Model

One of the most commonly used models in the objective-function approach is the *c*-Means algorithm [1]. In a closed system, total variance (within-group variance + between-group variance) is constant, therefore, minimum within-group variance implies maximum between-group variance, which means that when modeling, only one objective function is needed. Furthermore, when partitioning *n* data points into *c* groups, each datum should belong to one and only one group and each group should contain at least one datum but not the whole data set as shown in Figure 1. Consequently, each datum belongs to a group with a degree of either 0 or 1 and such a 0/1 clustering is called 'hard'. The *c*-means Model is thus referred to as the *Hard c-Means* model (HCM).

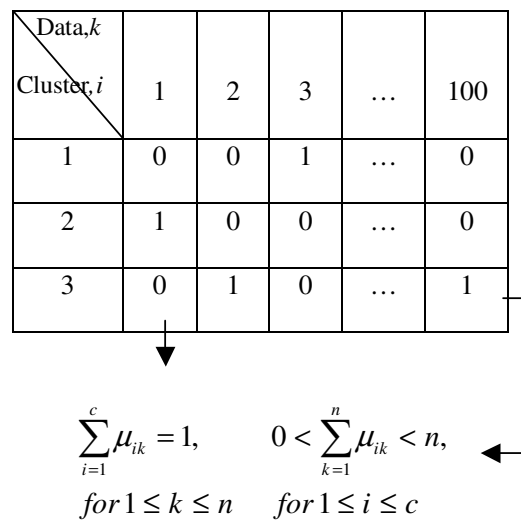


Figure 1. Hard Clustering

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By defining the variance as the Euclidean distance of each datum to the center of a group, the model can be written as

$$(HCM) \text{ Min } Z(U) = \sum_{i=1}^c \sum_{k=1}^n \|x_k - v_i\|^2$$

$$\text{subject to } \sum_{i=1}^c \mu_{ik} = 1, \text{ for } 1 \leq k \leq n$$

$$0 < \sum_{k=1}^n \mu_{ik} < n, \text{ for } 1 \leq i \leq c$$

$$\mu_{ik} \in \{0,1\}, \text{ for } 1 \leq i \leq c, 1 \leq k \leq n$$

However, if our data take the form of Figure 2, then hard clustering will result in an asymmetric butterfly as Figure 3 which is apparently not what we expect that the 'center' data point should partially belong to both clusters.

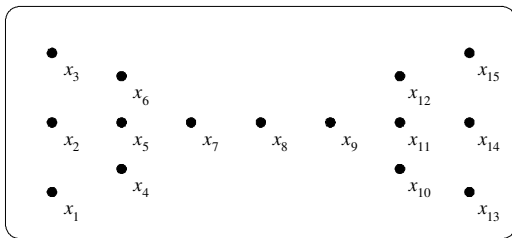
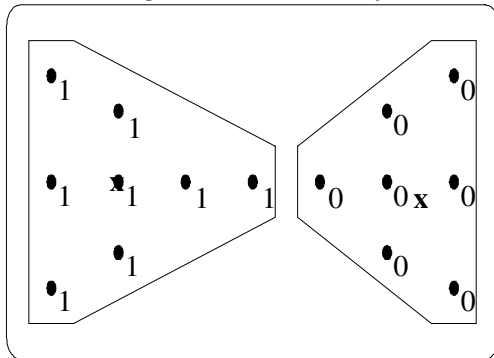


Figure 2 The Butterfly



x : center of cluster

Figure 3 Hard Clusters of the Butterfly

To resolve this problem, Bezdek [1] applied a membership value of fuzzy set theory to describe the degree of belonging to any group as follows:

2) Fuzzy c-Means Model (FCM)

The major difference between FCM and HCM is that FCM employs fuzzy partitioning such that one datum can belong to several groups with the degrees of belonging specified by

membership values between 0 and 1 as shown in Figure 4.

Data,k \ Cluster,i	1	2	3	...	100
1	0	0	0.6	...	0
2	1	0.7	0.4	...	0
3	0	0.3	0	...	1

$$\sum_{i=1}^c \mu_{ik} = 1, \quad 0 < \sum_{k=1}^n \mu_{ik} < n, \\ \text{for } 1 \leq k \leq n \quad \text{for } 1 \leq i \leq c$$

Figure 4. Soft Clustering

Thus, by weighting the distances with the corresponding membership values, the HCM model becomes

$$(FCM) \text{ Min } Z(\tilde{U}) = \sum_{i=1}^c \sum_{k=1}^n \mu_{ik}^m \|x_k - v_i\|^2$$

$$\text{subject to } \sum_{i=1}^c \mu_{ik} = 1, \text{ for } 1 \leq k \leq n$$

$$0 < \sum_{k=1}^n \mu_{ik} < n, \text{ for } 1 \leq i \leq c$$

$$\mu_{ik} \in [0,1], \text{ for } 1 \leq i \leq c, 1 \leq k \leq n$$

where $m \geq 1$ is a given number.

Obviously, FCM is more flexible than HCM when determining each datum's degree of belonging. However, it was discovered that by "softening" the boundary of each group, the hard concept of variance cannot be applied. This is illustrated in Table 1 in which if the distance between each pair of data is s , by taking the distance of $d=2.5s$, two partitions in Figure 5 show that while visual representation of Figure 5(b) is more reasonable than Figure 5(c), the within-clusters variance of partition II is smaller.

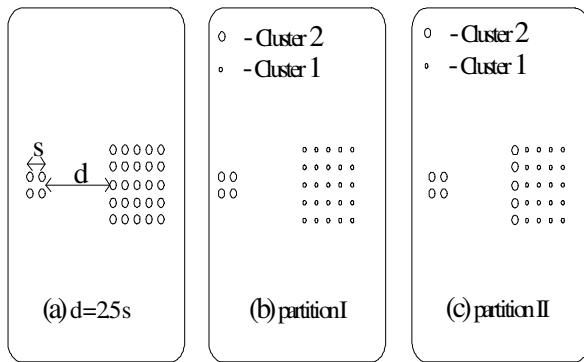


Figure 5 Visual Representation of Variance

Table 1. Variance Analysis

Partitions	Within-clusters Variance			Between-clusters	Total Variance
	Cluster 1	Cluster 2	Total	Variance	
Fig.5(b)	2.0	100.0	102.0	86.2	188.2
Fig.5(c)	32.0	65.0	97.0	91.0	188.2

This indicates that when soft clustering is performed, both criteria need to be considered.

Therefore, by including the additional criterion of maximizing the distance between two centers of groups, the model is rewritten as follows .

3). Bi-criteria Fuzzy c-means Model (BOFCM)

$$\text{Min } J = \sum_{i=1}^c \sum_{k \in K_i} \mu_{ik}^2 \|x_k - v_i\|^2$$

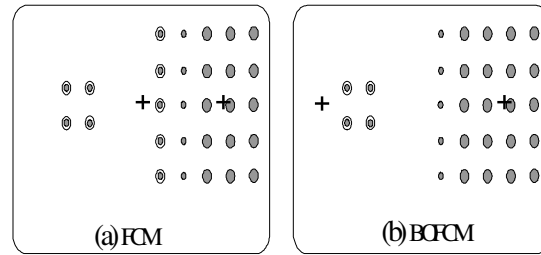
$$\text{Max } L = \sum_{i=1}^c \sum_{j < i} \|v_i - v_j\|^2$$

$$\text{s.t. } \sum_i \mu_{ik} = 1, \forall k$$

$$0 < \mu_{ik} < n, \forall i, k$$

$$\mu_{ik} \in [0,1], \forall i, k$$

with $m = 2$.



+: Cluster center @ : Cluster 1 ○ : Cluster 2

Figure 6. Example for MOFCM

As shown in Figure 6, with same data set of Figure 5(a), BOFCM provides a more reasonable partition where different sizes of dots now represent different degrees of membership values [3].

How to decide c?

Now before closing this discussion, let us raise one issue in clustering, which becomes critical when a data set is, for example, as large as a data warehouse. That is, how do we know how many clusters we are going to group? In other words, how to assign the value of c to all of above models? Many researchers have suggested trying different values of c by incrementally increasing the number of clusters, then choosing which generates a big jump in value of the objective function, which then is verified by different evaluation functions such as the Partition Function [2]. To resolve this problem, we suggest relaxing the total membership value as a fuzzy number, $\tilde{1}$, to 'soften' the boundary of the system as shown in Figure 7 [4].

Data, k \ Cluster, i	1	2	3	...	100
1	$\tilde{0}$	$\tilde{0}$	0.4	...	$\tilde{0}$
2	$\tilde{1}$	0.7	0.6	...	$\tilde{0}$
3	$\tilde{0}$	0.3	$\tilde{0}$...	$\tilde{1}$

$$\sum_{i=1}^c \tilde{\mu}_{ik} = \tilde{1}, \quad 0 < \sum_{k=1}^n \tilde{\mu}_{ik} < \tilde{n},$$

for $1 \leq k \leq n$ for $1 \leq i \leq c$

Figure 7. Soft System Clustering

By incorporating the Partition Function into the model as a measure of the distance between two groups, the model is changed to :

4). *Bi-Objective \tilde{c} -Fuzzy Means Clustering Model (BO \tilde{c} FM)*

$$\text{Min } Z_m(\tilde{U}; \tilde{V}) = \sum_{k=1}^n \sum_{i=1}^c (\tilde{\mu}_{ik})^m \|\tilde{x}_k - \tilde{v}_i\|_G^2$$

$$\text{Max } F(\tilde{U}, c) = \sum_{k=1}^n \sum_{i=1}^c \frac{(\mu_{ik})^2}{n}$$

$$\text{subject to } \sum_{i=1}^c \tilde{\mu}_{ik} = \tilde{1}_k$$

$$0 < \sum_{k=1}^n \tilde{\mu}_{ik} \lesssim n$$

$$\mu_{ik} \in [0,1], \text{ for } 1 \leq i \leq c, 1 \leq k \leq n$$

The pros and cons of this model are summarized below[4]:

Pros:

- * Relax the number of clusters
- * Facilitate linguistic data

Cons

- * Increase computational complexity

Where to Go Next ?

- 4 -We have used 600 data points to compare the clustering results of the above models via the Partition Function [4]. The result shows that BO \tilde{c} FM and FCM are better than MOFCM for this data; and while the function value of BO \tilde{c} FM is compatible with that of FCM, more clusters were found by BO \tilde{c} FM. This would imply that more specific patterns can be identified by this model.

References

- [1] Jim C. Bezdek, *Fuzzy Mathematics in Pattern Classification*, PhD Thesis, Applied Math. Center, Cornell University, Ithaca, 1973.
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- [3] H.F. Wang, C. Wang and G.Y. Wu, Multicriteria Fuzzy C-Means Analysis, *Fuzzy Sets & Systems*, vol.64, pp. 311-319, 1994.
- [4] Miao-Ling Wang, Chih-Lung Lin and Hsiao-Fan Wang, Data Clustering in Web Mining Based on \tilde{C} -Fuzzy Means Method, submitted to *IEEE Transactions on Fuzzy Systems*.

Hsiao-Fan Wang is a Professor in the Department of Industrial Engineering, National Tsing Hua University, Hsinchu, Taiwan, Republic of China. She will be on leave the Department of Management, University of Canterbury, at the beginning of 2003. She completed a Ph.D. in Operations Research at Cambridge University in 1982. Her research interests are in mathematical programming, fuzzy set theory, and multicriteria decision analysis, and she is Area Editor of the International Journal of Fuzzy Optimization and Decision Making

Professor Wang is an ORSNZ Visiting Lecturer for the first half of 2003. She is based at the University of Canterbury , in the Department of Management.



Letter from the Vice-President

From the Fould – Not Quite!

The absence of President Les Foulds, who, hopefully, should be having a wonderful and productive time in Western Australia, has given me the opportunity to say a few personal words about matters that are not earth-shattering but which are important to us in different ways.

Longevity matters! Yes, the ORSNZ is fast approaching its 40th birthday. Regardless of any doubt over the moment of conception, it is an event that we should celebrate, and which should lead to celebration throughout that year. There will be ongoing discussion and consultation about the nature of self-congratulatory indulgence that we engage in, but we should take the advantage of the opportunity to present the Society, its members, their contributions to all aspects of NZ society, in as good as light as possible. Any suggestions should be passed to Council. We celebrated our Twenty First Birthday at the Wellington conference in September 1985 with George Dantzig cutting the cake! One of my ageing colleagues, who shall remain nameless, but gave a paper on *Two Practical Methods for Determining Order Quantities and Order Cycles*, remembers it clearly and assures me that she didn't bake the cake!

Longevity matters! and it's wonderful for us in Wellington to report that David Boland, who fast approached three score years and ten, many years ago, is still having a major impact on Branch affairs, organising our meetings and flying the flag. He has been inspiration to us, displaying the enthusiasm and readiness to promote the Society that was commonplace in its early years.

Attendance at Wellington Branch Meetings has hit levels not experienced since the early/mid eighties. Of course, the visits of Scott Armstrong, from Wharton, Mike Pidd and Mike Wright, from Lancaster, have been drawcards, but David's promotional methods – his efforts in reaching out to sister societies, to the public sector sitting on our door step in Rutherford House – have taken us past fifty attendees on several occasions. It's "Thank you, David"; and also "Thank you, Canterbury", for those Erskine Fellowships benefit all of us, as your visitors travel around the country. We also say "Thank you, ORSNZ Council" for the wisdom of providing Visiting Lecturer Scholarships.

Within the university sector, many are currently consumed with the Performance Based Research Fund (PBRF) exercise – which will see universities, schools and staff ranked on research performance, and perhaps see the high performing institutions rewarded at the margin with extra funds. The UK university sector has been subject to continually changing processes of review over the last fifteen years, yet the leading institutions and schools seem not to vary too much! Anecdotal evidence suggests, however, that the review process has had an impact on culture and collegiality within universities, as pressures build up to improve individual and institutional rankings. Some would say that the ranking system has already created a black transfer market for academics - whose moves between institutions are timed to maximise the impact the effect of recently accumulated publications on rankings! Can we look forward to an OR equivalent of David Beckham?

Nevertheless, there is much to be said for celebrating the achievements of our members in an appropriate forum. The Royal Society of New Zealand thinks so, too. The 2003 Conference, to be held in Auckland University's New Engineering Complex on November 13/14 2003, will culminate with an Awards Night in Science and Technology. The RSNZ has invited its constituent member organisations to participate in the evening so that it becomes a gala event – disrespectfully, I would suggest the S&T equivalent of the Oscars. The RSNZ will present its Rutherford Medal, the NZ Maths Society will present its Aitken Award, the NZ Association of Scientists will present its awards etc – about a dozen societies will do likewise. The ORSNZ has been invited to the Awards evening, and, if Council agrees, it will be possible for the Daellenbach Prize to be presented or re-presented on the night - alternatively, this year's recipient of the Daellenbach Prize may be showcased at next year's RSNZ Awards Night. Indeed, showcasing S&T is the RSNZ aim! Your views on whether or not the ORSNZ should be involved, and if so, how, should be conveyed to Council or any Council member.

Next time, it's back to the Fould.

John Davies Vice President

john.davies@vuw.ac.nz

ORSNZ HANS DAELLENBACH PRIZE

CALL FOR APPLICATIONS AND NOMINATIONS

To honour the considerable contributions of Emeritus Professor Hans Daellenbach to OR/Ms in New Zealand, the ORSNZ has established the ORSNZ Hans Daellenbach Prize. The purpose of this award is to elicit, recognise, and reward outstanding examples of management science and operations research in New Zealand, and to encourage their dissemination in the international literature. Candidates for the prize must be members of ORSNZ. The Prize is accompanied by a \$1000 honorarium, and winners must give a plenary address on their relevant work at the ORSNZ conference in the year of the award. The Prize is awarded every two years, at most. If the Prize is awarded in 2003, it will be presented at the 38th Annual ORSNZ Conference in Hamilton, 22 November, 2003.

**Applications and nominations are invited.
They should be sent, by 31 July, 2003 to:**

Les Foulds , President , ORSNZ
Department of Management Systems,
University of Waikato,
Private bag 3105,
Hamilton
president@orsnz.org.nz

ORSNZ VISITING LECTURER SCHOLARSHIPS

ORSNZ invites nominations for ORSNZ Visiting Lecturer Scholarships for visits to New Zealand between July 2003 and June 2004. Each Visiting Lecturer must give a talk on some topic likely to be of general interest to ORSNZ members at each of Auckland, Hamilton, Wellington, and Christchurch. A plenary address at ORSNZ'03, in Hamilton 20-22

November, 2003, is acceptable as one of these talks. However, in this case, a talk on a different topic must be given at the other three centres. Each Visiting Lecturer will be invited to write a guest editorial for the Society newsletter. The emolument of each scholarship is up to \$1000. ORSNZ will not normally consider the payment of additional costs to Visiting Lecturers.

Each candidate must be nominated by a current member of ORSNZ, "the Champion". The nomination must include the c.v. of the nominated Visiting Lecturer, the dates and location in New Zealand of the hosts of the visit, the name of the Champion, and an undertaking by the Champion to coordinate a visit by the nominee to the four above named centres.

Enquiries concerning, or nominations for, scholarships should be sent to:

Les Foulds,
Department of Management Systems,
University of Waikato,
Private bag 3105,
Hamilton.

THE YOUNG PRACTITIONERS' PRIZE, TO BE AWARDED AT THE ANNUAL CONFERENCE OF ORSNZ, HAMILTON, NOVEMBER, 2003

Full-time students who: will be under 25 years of age on 21 November, 2003, are members of ORSNZ, and plan to present a single-authored paper at the above conference, are invited to compete for the ORSNZ Young Practitioners' Prize. When registering for the conference, competitors should request that their paper should be scheduled in the Young Practitioner's Prize Session and must provide evidence of their eligibility.

The level of emolument of the prize, or prizes, awarded will be decided by a Prize Panel at the time of the conference.

Les Foulds, President

The 38th Annual Conference of the ORSNZ in 2003

ORSNZ'03: "OR Making a Difference in Industry"

The Department of Management Systems at the University of Waikato, in Hamilton, is pleased to host the 38th Annual Conference of the Operational Research Society of New Zealand, ORSNZ'03, on Friday 21 and Saturday 22 November, 2003 (with a pre-conference social on the evening of 20 November).

Call for Papers

We welcome papers on any aspect of operational research, especially practical applications. Please submit your abstract, in 200 words or less, in plain text, to the conference organiser, Stuart Dillon (conference@orsnz.org.nz). We prefer submission by email, but you may post a hard copy of your abstract instead to:

ORSNZ'03

Department of Management Systems

University of Waikato

Private Bag 3105

Hamilton 2020

NEW ZEALAND

Submission deadline for abstracts: 30 September, 2003.

Following acceptance of your abstract, we shall invite you to submit a full-length paper for publication in the conference proceedings. A copy of the proceedings will be given to every attendee at the conference. Full papers must be submitted by email in Postscript (.ps) or Adobe Acrobat (.pdf) format to the proceedings editor, Les Foulds (conference@orsnz.org.nz). Guidelines for the preparation of full papers, and further information about the conference, will be available on the conference website www.orsnz.org.nz/conf

Submission deadline for full papers: 31 October, 2003.

ORSNZ STUDENT GRANTS-IN- AID FOR THE ANNUAL CONFERENCE OF ORSNZ, HAMILTON, NOVEMBER, 2003

ORSNZ invites applications for Student Grants-in-Aid to assist with travel to ORSNZ'03, Hamilton, 20-22, November, 2003. Each candidate must be:

- A full-time university student,
- A current member of ORSNZ,
- Prepared to present a single-authored paper of their own work at ORSNZ'03.

When registering for the conference, candidates must have their application, countersigned by their supervisor or Department Chair, and provide evidence of their eligibility. The level of emolument of the Grants-in-Aid will be decided by a Council meeting prior to the conference.

Enquiries concerning, or applications for, the Grants-in-Aid should be sent to Les Foulds

(Cajoling didn't work – the only news for this Newsletter comes from Hamilton! Ed.)

HAMILTON NEWS

Following a relatively short period of bribery and blackmail (including a spot of physical and mental torture) John Scott has kindly agreed take over the reins as Chair of Management Systems while Eric and Jim are on leave during B semester. We have all signed a declaration stating that we will endeavour to be nice to John, especially when he puts large amounts of money into our research accounts. We are all grateful to have John's experience with which to draw on.

After identifying the best locations for tramping (trekking) and snow skiing, Jim Corner has decided to accept visiting positions at Kent State and Case Western Reserve Universities. He will also visit some of his co-authors in Ohio (AFIT), and Arizona, as well as attending conferences in Seattle and Italy. We hope that the time away will provide Jim respite from his OOS which he has developed from playing too many games of darts.

Following six years of teaching without a break, Eric Deakins has been rewarded with 12 months of study leave and he has a varied programme lined up. During the first 6 months Eric plans to complete a backlog of research projects and articles before embarking on a round the world trip which, subject to travel restrictions, will enable him to personally check on post-war/post-SARS progress being made in the Middle East/Hong Kong respectively. In England he intends to revisit old haunts and esteemed colleagues at the University of Plymouth and to spend some time at a large-scale ecological tourism facility in Cornwall, -to see first-hand what lessons might be applied to the Maungatautari Ecological Island project here in the Waikato. In the United Arab Emirates Eric plans to conduct e-government research at the American University of Sharjah, and will observe their teaching methods. Jim Grant, who last year spent time in the Marketing Department at UW, will host Eric. From the end of 2003 following his return to NZ, he will be working on a major project in the area of information and decision visualisation, in collaboration with the Computer Science department and Mighty River Power. Les has been busy working on some research into freeway lane direction specification in rush hour use. He found time for some R & R

south of Perth and has now visited every vineyard open to the public in Western Australia. He has also been tramping in the SE of WA, in "The Valley of the Giant Trees", The Porongarrups, and the Stirling Ranges. He will be back for the start of B semester, and we are anticipating some seminars on Western Australian wine appreciation, Portuguese, and how to avoid tiger snakes.

Contributed by Stu Dillon

PUZZLE CORNER

Hyacinth and Henry are two staff members of a university department. They not only share a passion for their joint research, but also for each other. Their first six children, in order of age, are: Linda, Beryl, Boris, Carl, Nicholas, and Oscar. To which department do they belong and what will be the first two letters of the given name of their forthcoming baby?

(Source: Ms Nicola Petty, Department of Management, University of Canterbury.)

(From the OR Society Newsletter (UK) June 18 2003 <http://www.orsoc.org.uk>

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Of honeycombs, cannonballs and oranges – Kepler made the connection

By Nigel Cummings

The 17th century mathematician and astronomer Johannes Kepler is well known for his work on a 'model' which explained the relative distances of the planets from the Sun. He is perhaps less well known for his work in problem solving of a more mundane nature.

Johannes Kepler was very interested in the mathematics of packing, indeed in an age where military might was judged on the number of cannon balls one's armoury contained, he decided to find a more efficient cannonball stacking system. Kepler's decision to undertake a series of experiments with cannonballs was probably prompted by the poet and adventurer Sir Walter Raleigh, who wanted to know, if there was a quick way of estimating the number of cannonballs in a pile.

Raleigh was no mathematician, but Kepler was, and when the problem was presented to Kepler in 1606 he immediately began experimenting with different ways of stacking spheres. He soon concluded that the "face-centred cubic lattice" was best. Using this method, Kepler calculated that the packing efficiency rose to 74%, constituting the highest efficiency one could ever get.

Kepler's conclusion that the "face-centred cubic lattice" was the most efficient can be demonstrated thus. If you arrange 100 oranges (cannonballs are replaced by oranges for convenience's sake) in a flat layer of 10x10 and then place a similar layer directly on top, you have created a "simple cubic lattice". As long as your oranges have not rolled apart, your pile has a packing efficiency of only 52% - you're effectively stacking as much air as oranges.

BUT... with Kepler's "face-centred cubic lattice" approach the first layer of oranges is formed in the same way you would spread coins on a desk to cover it leaving the least amount of gaps. Nature seems to dictate that a coin, surrounded by 6 others in a honeycomb arrangement, is best. If you build a single layer of oranges whereby every orange is surrounded by six other oranges, then for the second layer, place your fruit in the "dimples" created by the honeycomb beneath. Each successive layer is then built in the same way so the pile forms a pyramid. Using this method, Kepler calculated that the packing efficiency rose to 74%, constituting the highest efficiency you could ever get.



Unfortunately Kepler did not explain how he arrived at his conclusion – the conjecture dogged mathematicians for centuries. Was Kepler right, was 74% the most optimal packing percentage? Over 390 years later, in 1998, Thomas Hales (photo above), a Professor from the University of Michigan, aided by his research student Samuel P. Ferguson confirmed Kepler's conjecture

Hales devised an equation based on a cluster of 50 spheres. The equation and its 150 variables expressed every conceivable arrangement of these spheres. They then used computers to confirm that no combination of variables led to a packing efficiency higher than 74%. Remarkably the proof Kepler's conjecture generated over 250 pages of argument and 3 gigabytes of computer files.

Space does not permit us to provide a more detailed article on this topic, but more information can be found at the following web addresses:

- <http://es.rice.edu/ES/humsoc/Galileo/People/kepler.html>
- <http://www.math.pitt.edu/fall2001.html>

http://www.maa.org/features/mathchat/mathchat_6_17_99.html





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