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RAPID COMMUNICATION / COMMUNICATION RAPIDE

Acoustic seabed classification: improved statistical method

Pierre Legendre, Kari Elsa Ellingsen, Erik Bjørnbom, and Philippe Casgrain

Abstract: Huge amounts of money will be spent by industrialized nations during the next decades to obtain detailed maps of continental shelf seabeds. These maps, which will allow a more rational exploitation of the sea floor, are needed to assess the impact of anthropic activities. The statistical method of analysis of echosounder backscatter data described in this paper presents several improvements over existing techniques. The steps are as follows. (*i*) The backscatter data are decomposed mathematically into a number of quantitative variables, which are subjected to principal component analysis (PCA). (*ii*) Principal components representing 95–99% of the variation are used in a *K*-means partitioning procedure. A statistical criterion indicates what the number of groups is that best reflects the variability of the data. (*iii*) The groups are then plotted on maps of the survey area. Insofar as the mathematical decomposition produces variables that reflect the variations of the physical nature and composition of the seabed, the classes of the partition will correspond to different seabed types. Free software (The Q Package) implementing this method is available at http://www.fas.umontreal.ca/biol/legendre/.

Résumé : Au cours des prochaines décennies, des sommes considérables seront consacrées par les nations industrialisées à la cartographie détaillée des plateaux continentaux. Ces cartes, qui permettront une exploitation plus rationnelle des fonds marins, sont nécessaires pour évaluer l'impacts des activités anthropiques sur ces mêmes fonds. La méthode statistique d'analyse de l'onde réfléchie secondaire des sonars décrite dans cet article propose plusieurs améliorations par rapport aux méthodes actuellement sur le marché. Les étapes sont les suivantes : (*i*) l'onde réfléchie secondaire du sonar est décomposée en une série de variables quantitatives qui sont soumises à l'analyse en composantes principales (ACP). (*ii*) Les composantes principales représentant de 95 à 99 % de la variance sont utilisées pour obtenir une partition des points de sondage en groupes. Un critère statistique permet de déterminer quel est le nombre optimal de groupes pour rendre compte de la variabilité des données. (*iii*) La classification est reportée sur une carte de la région à l'étude. Si la décomposition mathématique de l'onde réfléchie secondaire produit des variables qui reflètent les variations de la nature et de la composition physique du fond, les classes de la partition correspondront à différents types de fond. Un programme d'ordinateur (The Q Package) est gratuitement à la disposition des utilisateurs à l'adresse http://www.fas.umontreal.ca/biol/legendre/.

Introduction

The future of ecology as a partner for economic development lies in the ability of ecologists to develop means, tools, and methods for rapid assessment of impacts over broad expanses, such as whole embayments, gulfs, or continental shelves in aquatic ecosystems. This paper concerns remote sensing of coastal seabed using an acoustic bottom classification system for habitat mapping. Acoustic techniques allow managers to quickly map extensive seabed surfaces; they may eventually be used to map whole continental shelves. This information is urgently needed to assess the impact of coastal urban and industrial developments.

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Classification method

This paper presents a method of statistical analysis of echosounder backscatter data, which includes several improvements over existing techniques. The (free) software implementing this method is described at the end of this paper. Our test data consist in a file of first echosounder returns (Fig. 1) decomposed into 166 variables using the QTC VIEW™ acoustic bottom classification system (Prager et al. 1995). Alternative methods (and software) for decomposing backscatters into sediment-related variables have been proposed, for example, by Chivers et al. (1990) and Clarke and Hamilton (1999). Software for statistical processing of the

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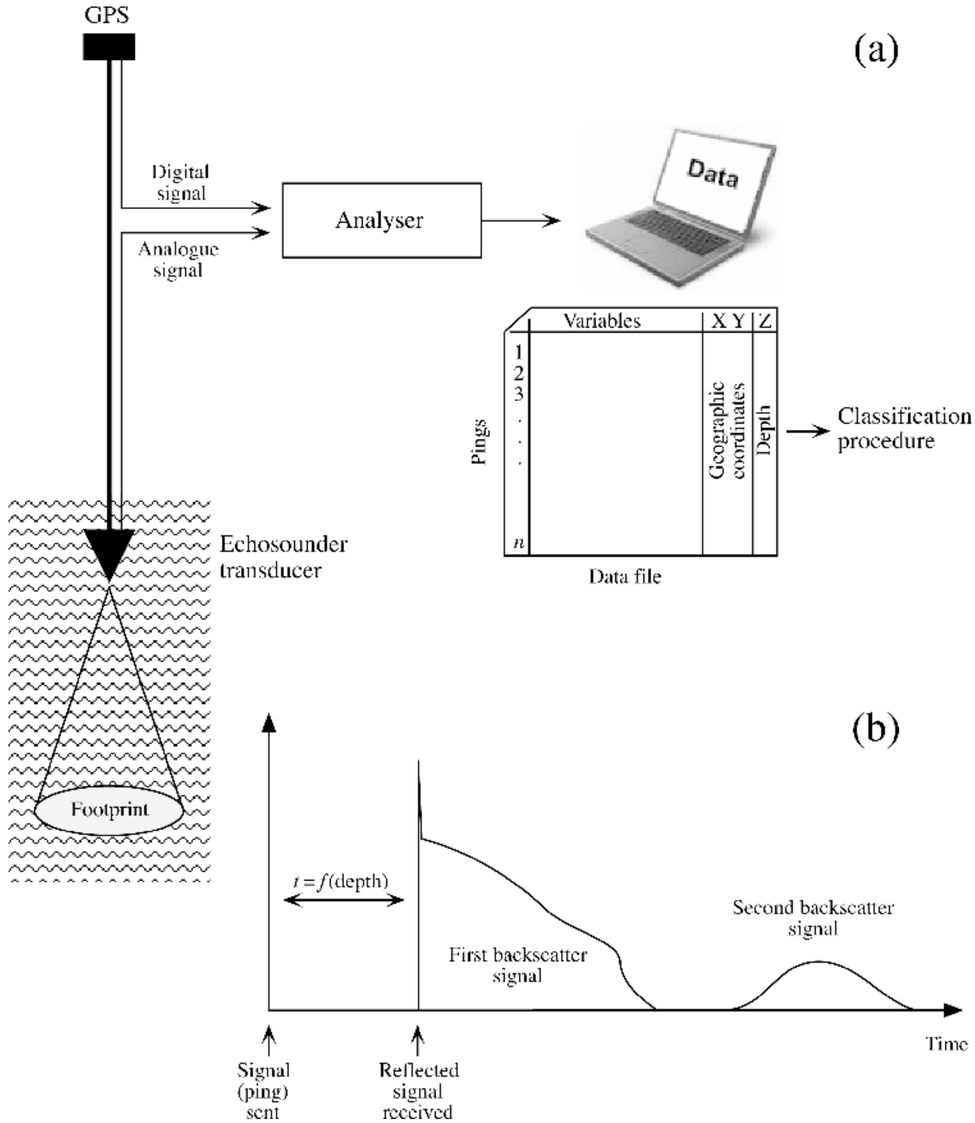
Fig. 1. (*a*) Data acquisition: the echosounder signal is decomposed mathematically into a number of variables that will be used for classification. Each acoustic record is geo-referenced for mapping. (*b*) Analogue signal from the echosounder. The first backscatter portion of each "ping" is analysed in the present paper.



QTC variables is also available from the Quester Tangent Corporation (QTC 1999, 2000). The steps of our analysis follow.

Step 1: reduction of data dimensionality

The 166 QTC variables are very highly collinear; in our example data, the mean of the absolute values of the correlation coefficients was 0.41 with values of *r* ranging from –0.9999 to +0.9999. For highly collinear data, a commonly used method to condense the variance into a small number of variables, prior to classification, is principal component analysis (PCA); this is the method also used in the QTC software. PCA computes a smaller set of new, linearly independent variables, called principal components (PCs), that account for most of the variance in the original data. The remainder of the variance is considered the error portion of the data (noise). We carried out a detailed comparison of classification results based on the whole data set, on the one hand, and on a small number (2–8) of PCs accounting for most for the variance, on the other hand. Comparable *K*-means partitioning results (see below) were obtained by using a number of PCs accounting for 95–99% of the total variance in the data. So, variance condensation into a small number of PCs is a good method if a sufficient number of PCs are used for classification. For the test data, the first three PCs accounted for 96.2% of the total variance. Using seven PCs would have accounted for 99.2% of the variance. For other QTC data sets (J.E. Hewitt, S.F. Thrush, P. Legendre, J. Ellis, and M. Morrison, National Institute of Water and Atmospheric Research (NIWA), P.O. Box 11-115, Hamilton, New Zealand, unpublished data), the first three PCs accounted for 90–97% of the variance of the 166 QTC variables; 3–5 PCs were necessary to reach 95% of the variance, and 6–10 to reach 99%.

Step 2: *K*-means partitioning

A (crisp) partition is a division of the "objects" under study into nonoverlapping subsets. Agglomerative clustering methods produce nested partitions, whereas partitioning methods produce partitions into a predetermined number of groups (K). For n objects, most agglomerative clustering algorithms require the computation of a ($n \times n$) similarity or distance matrix; this is impractical for large data sets like sonar data. Hence, we turned to partitioning methods. K-means is the most widely used numerical method for partitioning data. The K-means problem consists of dividing a set of multivariate data into nonoverlapping groups in such a way as to minimize the sum (across the groups) of the sums of squared residual distances to the group centroids; this statistic is also called the sum of within-group sums-of-squares, the error sum-of-squares, or the sum of squared errors (SSE). SSE is the global optimality criterion, or objective function, implemented in K-means algorithms. Hundreds of algorithms have been proposed in the literature to solve the K-means problem.

We implemented the following two-step iterative least-squares algorithm: (*i*) compute cluster centroids and use them as new cluster seeds; and (*ii*) assign each object to the nearest cluster seed. This algorithm is described in several books; for example, Legendre and Legendre (1998).

Since K-means is a NP-hard problem (a category of very hard problems in computer science), no algorithm can guarantee that it will find the optimum partition every time. To increase the likelihood of finding this partition, two features have been added to the basic algorithm. (*i*) The program was made to proceed in a cascade, finding first a partition into a number of groups larger than what is needed (e.g., starting at 10 groups). It is easier to find the best partition for a large number than for a smaller number of groups. When this partition has been found, the two groups whose centroids are the closest in multivariate space are fused and the algorithm iterates again to optimize the SSE function. This is repeated as far as the user wants it to go (e.g., until a partition into two groups is found). (*ii*) The whole classification process (e.g., from 10 to two groups) can be repeated a number of times (e.g., 25 or 50 times, as specified by the user) using different random starting configurations. For each number of groups (e.g., for $K = 10$, $K = 9, \ldots, K = 2$ groups), the solution where SSE_K is minimum is retained and written to the output file.

Step 3: how many acoustic classes?

How to decide on the optimal number of acoustic classes? A large number of criteria have been proposed in the statistical literature to decide on the correct number of groups in cluster analysis. A simulation study by Milligan and Cooper (1985) compared 30 of these criteria. The best one turned out to be the Calinski and Harabasz (1974) criterion, called C-H in the present paper. C-H is simply the F-statistic of multivariate analysis of variance and canonical analysis. F is the ratio of the mean square for the given partition divided by the mean square for the residuals. To help users decide on the best number of groups present in a data set, our K-means program computes the C-H criterion; the number of classes for which C-H is maximum is the best one in the least-squares sense.

One cannot assume that the best number of groups is small in acoustic sediment classification. Using the C-H criterion, J.E. Hewitt, S.F. Thrush, P. Legendre, J. Ellis, and M. Morrison (NIWA, P.O. Box 11-115, Hamilton, New Zealand, unpublished data) found cases where the best number of groups was from $K = 2$ to $K = 19$, depending on the data set.

Step 4: other computation modules

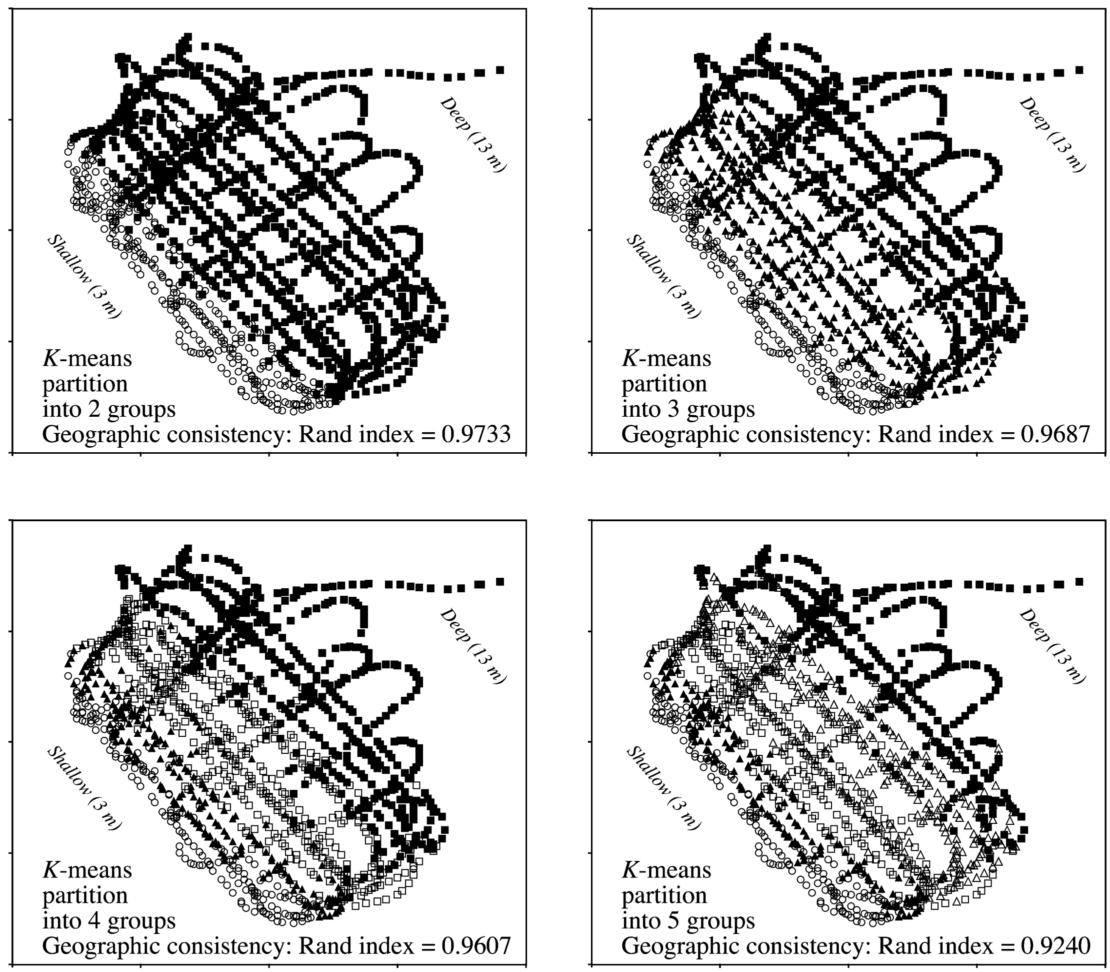
A drawing module allows users to produce simple maps from the K-means partitioning results and the geographic coordinates of the individual acoustic records. Figure 2 presents examples of these maps (printed here in black only); they may include colour, symbols, 95% confidence ellipses around groups, etc. The maps can be copied and pasted in one's favourite drawing program and saved as standard EMF (Enhanced MetaFile) format.

Another module of the package computes the "geographic consistency" of the K-means solutions. We want to know if the groups obtained by partitioning consist of geographic neighbours; if they do not, we want to know how close they are to a "geographically consistent" solution in which each group would only contain points that are contiguous in space. First, one computes a matrix of geographic contiguity among points, using one of a number of connection networks described, for instance, in Legendre and Legendre (1998). The type of connection most often used is the Delaunay triangulation. Our "Links" module, which can plot the connection network on a map of the data points, is based upon a Delaunay algorithm by Shewchuk (1996). Then, one employs the "GeoConsist" module: using the list of connections between geographic neighbours, this program subdivides each group obtained by K-means partitioning into geographically connected subsets of points, using a simplified constrained clustering algorithm (Legendre and Legendre 1998). One obtains a new partition into a larger number of groups that are nested into the groups of the K-means partition. The Rand index (Rand 1971) between the original and spatially constrained partitions is computed as an index of geographic consistency. The closer this index is to 1, the greater is the geographic consistency of the original K-means solution. Membership of the points in the geographically constrained groups is also available for mapping.

Example data

On 16 August 1999, acoustic data were collected in the Forty Baskets Beach area of Sydney Harbour, Australia (33°48′S, 151°16′E). We used a Navisound 50 echosounder at frequency 50 kHz (transducer beam width 13.5°) connected to the QTC VIEW™ acoustic seabed classification system (CAPS version 3.25, QTC IMPACT™ version 1.0 Beta of Quester Tangent Corporation), which was used to decompose the backscatter waves mathematically into 166 variables (Fourier analysis of the response wave, 64 variables; wavelet analysis, 64 variables; 38 other variables describing the shape of the first acoustic backscatter based upon the original and cumulative forms) (Fig. 1). The transducer was mounted on an over-the-side strut on the survey vessel. The positioning equipment was a differential GPS (Global Positioning System). The recorded data were corrected and validated using a "Parser" procedure, which is part of our software. The test data set consisted of 1478 data

Fig. 2. Map of the Forty Baskets Beach sampling area (Sydney Harbour, Australia: 33°48′S, 151°16′E) showing the *K*-means partition of the acoustic records into 2–5 groups (symbols) based upon the first three principal components (96.2% of the variance in the data). These partitions explain 58.4, 76.7, 81.4, and 84.1%, respectively, of the variance in the data. The partition into three groups is the one for which the Calinski-Harabasz (C-H) criterion is maximum.



lines (objects, or records) and 166 QTC variables, plus geographic positions and depths. Since three of the QTC variables did not vary at all, they were eliminated from the data set, which was thus reduced to 163 variables.

K-means divided the acoustic data into a series of bands that follow the depth gradient (Fig. 2). Unfortunately, we do not have geographically localized visual observations to validate the classification results, but divers reported that the sediment changed along this gradient and that seagrass formed a bed parallel to the coast. The C-H criterion indicated that the partition into three groups was the best one in the least-squares sense. As a statistical model, this partition explained 79.8% of the variance in the first three PCs, or 76.7% of the variance in the 163 original QTC variables. Acoustic classification results should be subjected to ground truthing, which consists of relating the acoustic classes to visually observed data describing the seabed. J.E. Hewitt, S.F. Thrush, P. Legendre, J. Ellis, and M. Morrison (NIWA, P.O. Box 11-115, Hamilton, New Zealand, unpublished data) have done such a validation study, using underwater video data, of an acoustic seabed classification obtained from QTC variables analysed by our software.

Program and report

A computer package (The Q Package) has been developed, with the financial help of NIWA of New Zealand, to implement the seabed classification method described in this paper and analyze large data sets. In its present state of development, it can handle 10 000 data points in real time and 100 000 points with a small delay, using a recent Windows-based operating system. Any computer capable of running Microsoft Windows 95 or later versions (including Windows NT and Windows 2000) can be used to run the Q Package. A low-end Pentium with 32 Mb of RAM and Windows 95 is powerful enough to run the program, and is perfectly adequate in most cases. The package, which comes complete with a user's manual, is available free of charge at http://www.fas.umontreal.ca/biol/legendre/.

A report, available from the first author, presents a user's comparison of the method described in this paper with that of the QTC VIEW™ CAPS and QTC IMPACT™ software of Quester Tangent Corporation. The report shows that PCA followed by *K*-means partitioning produces statistically better results than the classification method implemented in the QTC software with which we experimented during the SCALE EX-

PERT workshop (Spatial Comparisons Across Large Estuaries: EXPerimental Evaluation of Recent Technologies) organized and hosted by Professor A.J. Underwood at the University of Sydney, Australia, 2–22 August 1999.

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DISCUSSION / DISCUSSION

Comment on “Acoustic seabed classification: improved statistical method”[1]

J.M. Preston and R.L. Kirlin

In a discussion of methods for acoustic seabed classification, Legendre et al. (2002) claim to offer improvements over existing techniques and assert that their method “produces statistically better results than the classification method implemented in the QTC [Quester Tangent Corporation] software”. Reasons for this assertion are not given in that paper but are given in an unpublished document. In this paper, we examine the basis for the assertion and discuss whether it should be accepted.

The method of Legendre et al. (2002) implements a *K*-means partitioning by an iterative process. They claim this as an advantage over QTC; however, QTC also implements a *K*-means partitioning with an iterative process (see, e.g., Preston et al. 2001), so this cannot be the explanation. Choosing the optimal number of clusters can be problematic, but Legendre et al. report differences between their methods and QTC even when both are computing with the same number of clusters, so the explanation cannot lie entirely here. What is left?

The answer, it appears, is that Legendre et al. (2002) wish to minimize the within-group sums of squares using a homogeneous measure of distance to the centre of a cluster (squared Euclidean distances), whereas QTC uses a likelihood-based measure in which the distance to the centre of any cluster is scaled by the variance of that cluster. A one-dimensional example illustrates the point at issue. Suppose we have a population that is an equal mixture of two Gaussian distributions: A, which is distributed as $N(0,(0.5)^2)$, and B ~ $N(2,(0.1)^2)$. How do we assign an observation at 1.5? Legendre et al. would say that it is a distance of 0.5 from the centre of B and 1.5 from the centre of A and therefore should be assigned to B. QTC would say that is it 5 standard deviations from the centre of B and 3 standard deviations from the centre of A and therefore should be assigned to A. In the example that we have sketched, the statement “x is from A and $x = 1.5$” has a higher probability density than “x is from B and $x = 1.5$”; that is, our method has a higher probability of making a correct assignment to a component of the mixture. Therefore, one cannot unambiguously identify Legendre et al.’s “best in the [homogeneous] least-squares sense” with best in the statistical sense. Attempts to prove the latter fail because any statistical test is also based on either homogeneous or variance-based measures; if the clustering method and the test use the same measure, the test scores will often be higher for that reason alone.

The paragraphs above summarize our comment. Legendre et al.’s (2002) claim to “statistically better results” is without support, arising as it did from applying a test that used squared Euclidean distances to two clustering methods, one using squared Euclidean distances and one using a likelihood-based measure. What remains is to provide a justification for using non-Euclidean measures for clustering and to extend this example to more dimensions.

A reasonable principle for choosing the class assignment is the maximum a posteriori probability (MAP). In other words, a vector $\mathbf{x}$ is observed and is to be assigned to one of q classes $\{\omega_1,\omega_2,\ldots,\omega_q\}$. MAP selects the class of maximum a posteriori probability from the candidates as

$$(1) \qquad \omega_k = \arg \max_{k=1,2,\cdots,q} P(\omega_k|\mathbf{x})$$

where $P(\omega_k|\mathbf{x})$ is the a posteriori probability for class ω_k. From Bayes’ theorem, the a posteriori probability can be written as

$$(2) \qquad P(\omega_k|\mathbf{x}) = \frac{p(\mathbf{x}|\omega_k)P(w_k)}{p(\mathbf{x})}$$

where $p(\mathbf{x}|\omega_k)$ is the density of the data given that they are drawn from ω_k, $P(\omega_k)$ is the a priori probability for ω_k, and $p(\mathbf{x})$ is the marginal density of observed data $\mathbf{x}$. If the a priori probability $P(\omega_k)$ is uniform, the MAP rule becomes

$$(3) \qquad \omega_k = \arg \max_{k=1,2,\cdots,q} p(\mathbf{x}|\omega_k)$$

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which is the maximum likelihood (ML) selection. Because $p(\mathbf{x})$ does not depend on class assignments, it drops out of the selection computations and each vector is assigned to cluster ω_i if (Cover and Hart 1967)

$$(4)\qquad P(\omega_i)p(\mathbf{x}|\omega_i) > P(\omega_j)p(\mathbf{x}|\omega_j),\ \forall j \neq i$$

It is usual to assume a multivariate normal density (Fraley and Raftery 1998):

$$(5)\qquad p(\mathbf{x}|\omega_i) = \frac{1}{(2\pi)^{M/2}|\mathbf{C}_i|^{1/2}} \exp[-1/2(\mathbf{x}-\mathbf{m}_i)^T\mathbf{C}_i^{-1}(\mathbf{x}-\mathbf{m}_i)]$$

where M is the dimensionality, and $\mathbf{m}_i$ and $\mathbf{C}_i$ are the estimated mean and covariance of cluster w_i. Legendre et al. (2002) and QTC both cluster in three-dimensional space called Q space, thus $M = 3$.

We can straightforwardly estimate the mean, covariance, and prior probability of the ith class if the marginal density of x,

$$(6)\qquad p(\mathbf{x}) = \sum_{i=1}^{q} P(\omega_i)\frac{1}{(2\pi)^{M/2}|\mathbf{C}_i|^{1/2}} \exp[-1/2(\mathbf{x}-\mathbf{m}_i)^T\mathbf{C}_i^{-1}(\mathbf{x}-\mathbf{m}_i)]$$

can be appropriately simplified. The required simplification results when the clusters or modes of the Gaussian mixture are well separated. In that case $p(\mathbf{x})$ is well approximated in the region of the ith cluster by

$$(7)\qquad p(\mathbf{x}) = \frac{P(\omega_i)}{(2\pi)^{M/2}|\mathbf{C}_i|^{1/2}} \exp[-1/2(\mathbf{x}-\mathbf{m}_i)^T\mathbf{C}_i^{-1}(\mathbf{x}-\mathbf{m}_i)],\quad \mathbf{x} \in \omega_i$$

and we can assume that all samples of $\mathbf{x}$ assigned to cluster i have been drawn only from the approximate distribution in eq. 7. In this case, we can obtain ML estimates of the required parameters using only samples of $\mathbf{x}$ assigned to cluster i.

When selecting the maximum under eq. 4, it is convenient to minimize the logarithm of the reciprocal of the left-hand side, log being a monotonic function. This gives what may be called a Bayesian metric:

$$(8)\qquad d_i(\mathbf{x}) = -\log P(\omega_i) - \log(p(\mathbf{x}|\omega_i)) = -\log P(\omega_i) + ½\log|\mathbf{C}_i| + ½(\mathbf{x}-\mathbf{m}_i)^T\,\mathbf{C}_i^{-1}(\mathbf{x}-\mathbf{m}_i)$$

Two simplifications of eq. 8 deserve mention. The Euclidean metric, as used by Legendre et al. (2002), is the simplification of eq. 8 that assumes equal $P(\omega_i)$ and that the covariance matrices are equal, constant, and diagonal. Because assignments are based on minimization across classes, class-independent terms and constant factors are dropped, giving

$$(9)\qquad d_i(\mathbf{x}) = (\mathbf{x}-\mathbf{m}_i)^T(\mathbf{x}-\mathbf{m}_i)\quad \text{(Euclidean)}$$

Secondly, if we continue to use equal priors $P(\omega_i)$, but now allow the covariance matrices to differ but with approximately equal determinants, we have the weighted sum of squares metric

$$(10)\qquad d_i(\mathbf{x}) = (\mathbf{x}-\mathbf{m}_i)^T\,\mathbf{C}_i^{-1}(\mathbf{x}-\mathbf{m}_i)\quad \text{(Mahalanobis)}$$

The general case, using all terms of the Bayesian metric (eq. 8), requires estimates of the a priori probabilities, as well as the means and covariances of each cluster. QTC has implemented these estimates iteratively, with an outer loop for estimating priors and covariances and an inner K-means loop that adjusts assignments and cluster means. This is an optimal process under the MAP criterion, the only approximation being that in eq. 7 which approximates the whole density of $\mathbf{x}$ by its component due to class i alone, which is valid under the assumption of well-separated classes or mixture components.

For classifying regions of acoustic similarity, as part of acoustic sediment classification, we have described three metrics: the general case and two simplifications. Which gives optimal results? This will likely remain an open question. We have found very few statistical tests or clustering processes that work well with both simulated and real data sets and thus have come to believe that comparison with ground truth is the most meaningful basis for comparisons. However, it is unusual to have ground truth that is adequate in quantity and scope. For example, surface roughness can affect acoustic character but is destroyed when sampling with a grab. Over the years, the QTC implementation described above has repeatedly been found to give practical, useful, and accurate classes. Some recent examples are described by Morrison et al. (2001), Anderson (2001, 2002), and Ellingsen et al. (2002).

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DISCUSSION / DISCUSSION

Reply to the comment by Preston and Kirlin on "Acoustic seabed classification: improved statistical method"[1]

Pierre Legendre

Legendre et al. (2002) described a statistical method for analysing echosounder backscatter data, which consisted of the following steps: the backscatter data were decomposed mathematically into a number of quantitative variables, which were subjected to principal component analysis (PCA). Principal components representing 95–99% of the variation were then used in a K-means partitioning procedure. A least-squares statistical criterion indicated the number of groups that best reflected the variability of the data. The groups were then plotted on maps of the survey area. Insofar as the mathematical decomposition of the backscatter echo produced variables that reflected the variation of the physical nature and composition of the seabed, the classes of the partition were likely to correspond to seabed types. This procedure presented several improvements over the Quester Tangent Corporation's QTC VIEW™ acoustic bottom classification method (Prager et al. 1995), and it was described in easy-to-understand terms. Free software implementing this method — *The Q Package* for Windows and *The R Package* for Macintosh — is available on the Web site http://www.fas.umontreal.ca/biol/legendre/.

J.M. Preston, from the Quester Tangent Corporation (QTC), and R.L. Kirlin wrote a comment on that paper, to which I was invited to reply. I will first address some statistical points in Preston and Kirlin's note and then go to more fundamental issues.

Statistical issues

(1) The K-means problem was defined by MacQueen (1967) as that of partitioning a data set in Euclidean space into K nonoverlapping groups in such a way as to minimize the sum (across the groups) of the within-group sums of squared Euclidean distances to the respective group centroids. The statistical problem had first been stated by Fisher (1958). What QTC seems to be doing, if I understand their description correctly, is implementing a partitioning method based on Mahalanobis distances for solving the mixture problem, like the one described by Demers et al. (1992), for instance. So they are implementing a modified form of K-means partitioning. This does not mean that the results produced by such an algorithm are more meaningful that those of a standard K-means algorithm.

The description of the classification algorithm implemented by the QTC software, provided by Preston and Kirlin, is wrapped in Bayesian language. A true Bayesian approach would require that prior probabilities be known beforehand; that is not the case in acoustic seabed classification. What is being described is simply a two-step iterative algorithm, preserving Mahalanobis distances, in which objects are assigned to the clusters and the statistical parameters of the clusters are recomputed.

(2) Preston and Kirlin (2003) criticize the closing statement of our 2002 paper, which read: "The report [Legendre, unpublished report, available at http://www.fas.umontreal.ca/biol/legendre/] shows that PCA followed by K-means partitioning produces statistically better results than the classification method implemented in the QTC software…". The sentence should have read: "… statistically better results *in the least-squares sense*…". The statement was based on results presented in the unpublished report and summarized in the following paragraphs.

On 16 August 1999, acoustic data were collected in the Forty Baskets Beach area of Sydney Harbour, Australia (33°48′S, 151°16′E). We used a Navisound 50 echo sounder (Navitronic Systems AS, Hasselager, Denmark) at frequency 50 kHz (transducer beam width 13.5°) connected to the QTC VIEW™ acoustic seabed classification system (CAPS version 3.25, QTC IMPACT™ ver-

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[1]Reply to J.M. Preston and T.L. Kirlin. 2003. Can. J. Fish. Aquat. Sci. **60**: 1299-1300.

sion 1.0 Beta). The transducer was mounted on an over-the-side strut on the survey vessel. The positioning equipment was a differential GPS (global positioning system). After validation, the data set consisted of 1478 data lines (objects or records) and 166 QTC variables, plus geographic positions and depths. Because three of the QTC variables did not vary at all, they were eliminated from the data set, which was thus reduced to 163 variables. These data were used to illustrate the acoustic seabed classification method described in Legendre et al. (2002).

The first three principal components accounted for 96.2% of the variance in the QTC variables. Using seven principal components would have accounted for 99.2% of the variance. For fairness of comparison, I only used the first three principal components in the comparison of partitions, because this is what the QTC software uses. The data were subdivided into groups using the procedure outlined in the QTC manuals (QTC 1999, 2000). The score value was used to determine which class should be split next. As the classes were subdivided, the total score decreased; however, at split level seven (i.e., eight groups), the total score increased again. Results of the partitions into three to seven groups are reported in Table 1*a*. In an a posteriori calculation, the Calinski–Harabasz statistic (described below) selected the partition into five groups as the best one in the least-squares sense.

The same data were partitioned by *K*-means, using the first three principal components (PC1–PC3), as in the QTC procedure. The *K*-means program was asked to produce from ten to two groups; the partitioning was restarted 10 times. The best partitions into $K = 2$ to $K = 7$ groups were retained; some of these results are shown in Table 1*b*. The Calinski–Harabasz statistic (see below) selected the partition into three groups as the best one. We also computed *K*-means partitioning for all 163 QTC variables, without prior filtering by PCA. The Calinski–Harabasz statistic selected again the partition into three groups as the best one (Table 1*c*). This partition is very similar to that obtained by *K*-means on PC1–PC3.

The partitioning procedure described in the QTC manuals (QTC 1999, 2000), which we used in 1999, is not the one described by Preston and Kirlin in their Comment (see Seabed classification issues, subsection 1, below). The partitioning results of QTC IMPACT™ and *K*-means are compared in Table 1 using common measures based on least squares: the sum of within-group sums-of-squares, also called the "sum of squared errors" (SSE), and the Calinski–Harabasz statistic (C–H) (see Legendre et al. 2002 (Classification method, step 3), as well as Seabed classification issues, subsection 4, below). SSE is the global optimality criterion implemented in *K*-means algorithms. C–H is a statistical criterion indicating the best number of groups in the least-squares sense. Least-squares is a widely accepted criterion and has a long history in statistics (Legendre 1805).

By the SSE criterion, Table 1 shows that the QTC partition into three groups is not as good as the *K*-means partitions into three groups based on either the first three principal components or all 163 variables, with respect to either the first three principal components (32% larger SSE) or the 163 QTC variables (27% larger SSE). Likewise for the partitions into five groups: according to SSE, the QTC solution into five groups is much worse than the *K*-means solutions based on either PC1–PC3 or all 163 QTC variables, with respect to either the first three principal components (15% larger SSE) or the 163 variables (10% larger SSE). This shows that the QTC partitions (even the "best one" into five groups) were far from being as good, for this example and in the least-squares sense, as those obtained by *K*-means.

(3) Preston and Kirlin (2003, their paragraph 3) talk about performing an (undescribed) test of statistical significance in their partitioning method. It is not clear to what they are referring. In any case, there is nothing that can be tested for significance in *K*-means or Mahalanobis distance partitioning without invoking an external, independently obtained data set. In particular, the results of a partitioning procedure should not be tested for significance using the same data that were used to produce the partition. This would be a logical mistake, as explained by Milligan (1996, p. 366) and Legendre and Legendre (1998, p. 379).

(4) Preston and Kirlin (2003) state that "Legendre et al. (2002) and QTC both cluster in three-dimensional space". This is not what we wrote; see Legendre et al. (2002, abstract and step 1 of the Classification method). What we recommended was to use as many principal components as were necessary to explain at least 95%, and preferably 99%, of the variance of the data. In the example presented in that paper, three principal components accounted for 96.2% of the variance, so we used three for *K*-means partitioning. We also reported that in the analysis of other acoustic seabed data sets, 3–5 PCs were necessary to reach 95% of the variance and 6–10 to reach 99%. In subsection 2 above, I only used three principal components in the tables to present a fair comparison with the QTC IMPACT™ results, which are limited to three principal components by design of the program. Preston et al. (2001) present that as a feature of the QTC software, but I think it is an objectionable limitation. This point will be revisited below.

(5) Preston and Kirlin (2003, last paragraph) concluded by citing a number of papers that allegedly showed that the QTC classification method "has repeatedly been found to give practical, useful, and accurate classes". It is worth noting that the paper by Morrison et al. (2001), cited by Preston and Kirlin, was directed at developing a technique to identify habitat boundaries. Their analysis compared the accuracy of the transitions predicted by the QTC VIEW™ confidence values with those predicted by the class-dominance Berge–Parker statistic. Morrison et al. (2001) concluded that the Berge–Parker index provided a more consistent transition indicator than the QTC software confidence values.

Seabed classification issues

(1) People have long wondered what was the classification

Table 1. Comparison of partitions (least-squares statistics SSE and C–H) using two different bases: PC1–PC3 (middle) and 163 QTC variables (right).

	No. groups	Base: PC1–PC3		Base: 163 QTC variables	
Software and variables	K	SSE	C–H	SSE	C–H
(*a*)					
QTC (PC1–PC3)	3	55.16	2026	62.94	1781*
QTC (PC1–PC3)	4		1969		1678
QTC (PC1–PC3)	5*	29.85	2182*	37.00	1771*
QTC (PC1–PC3)	6		2053		1620
QTC (PC1–PC3)	7		1921		1484
(*b*)					
K-means (PC1–PC3)	3*	41.86	2904*	49.67	2453*
K-means (PC1–PC3)	5	25.97	2561	33.53	1992
(*c*)					
K-means (163 QTC var.)	3*	41.87	2903*	49.67	2453*
K-means (163 QTC var.)	5	25.97	2563	33.51	1993

Note: SSE, sum of within-group sums-of-squares (small is best, for a given number of groups); C–H, Calinski–Harabasz statistic (high is best among partitions obtained using the same data). Asterisk (*) indicates the best number of groups for that classification, according to C–H.

method used by QTC. We asked questions to that effect to the Quester Tangent Corporation in 1999 but received no answer. When they use a method, scientists need to know, and be able to describe in scientific papers, how the data are processed. However, there seems to be greater openness and QTC is now providing more details of their statistical procedure.

The Comment by Preston and Kirlin (2003) is, to my knowledge, the first published paper describing the fact that the QTC software now uses a two-step iterative algorithm preserving Mahalanobis distances. Only now are we learning from Preston and Kirlin (2003) that the QTC software is using Mahalanobis distances instead of Euclidean distances. It is not clear from Preston and Kirlin's Comment whether they state that this approach has been implemented all along the development of the QTC proprietary software, or not. In any case, the procedure used in the 1999 CLUSTER™ and the 2000 QTC IMPACT™ programs and described in the software manuals (QTC 1999, 2000) was one-dimensional (the clusters were split along the first principal component in earlier versions of the software and along a single principal component chosen by the user in the 2000 version). An evolution of the software is summarized in Preston et al. (2001), who simply described it as "an automated variant of the k-means clustering method. Clustering is done in the space of the three principal components and is iterative and stable." What is now described in the Preston and Kirlin (2003) Comment seems to be a new evolution of the QTC software, recently released or perhaps still in the testing phase. In earlier manuals provided by QTC with their statistical software (QTC 1999, 2000), there was no indication about the nature of the calculations leading to partitioning, except for the description of how to use it, which implied a lot of fiddling and left room for personal, unreplicable decisions on the part of the user.

I also applaud the fact that QTC has recently (Preston et al. 2001) released some information about the mathematical nature of the 166 variables produced by the QTC VIEW™ software. The information found in Preston et al. (2001) provides a general qualitative overview of the variables generated by QTC VIEW™ from the backscatter, but the methods by which they are derived and the quantitative nature of the information remain unexplained.

(2) In the summer of 1999, Hewitt et al. (J.E. Hewitt, National Institute of Water and Atmospheric Research, P.O. Box 11-115, Hamilton, New Zealand, unpublished data) carried out a multiresolution nested survey in Kawau Bay, located on the northeast coast of North Island, New Zealand. The spatial distribution of epibenthic communities was studied using side-scan sonar, single-beam sonar, and video. The objective was to find relationships between assemblages visible from the video and the single-beam and (or) side-scan data that would enable the researchers to use these devices to both interpolate between and extrapolate from the restricted video survey. The substrate was soft sediment in all eight 1-km^2 sites investigated. There were reasonably dense but patchy epibenthic communities. At each site, six pairs of 1-km-long transects were sampled with single-beam sonar. The transects ran down the depth gradients. Three of the eight sites could not be videoed because of the presence of shoals and subsea cables. However at the other five sites, three 1-km-long video transects were run in approximately the same positions as three of the single-beam transects. The sonar was a Simrad EA501P hydrographic sounder (Simrad AS, Horten, Norway), attached to the boat, and operated at 200 kHz, 250 W transmit power, with a ping rate of 5 s^{-1}, and a fixed beam width of 7°. This was connected to a QTC VIEW™ series 4 (Collins et al. 1996) data acquisition system. Settings for the QTC VIEW™ system were a reference depth of 14 m and a base gain of 15 dB. Sampling resolution varied from 0.37 to 3.0 m^2, depending on depth, although more generally the range was from 1.22 to 2.44 m^2. As QTC

VIEW™ uses a stack of five consecutive pings for each record, at our speed of about 5 knots (2.6 $m \cdot s^{-1}$), a ping stack (generally covering 6–12 m) was processed approximately every 8 m.

The single-beam sonar data were processed as follows: on the one hand, using the first three principal components computed by the proprietary principal component analysis procedures available in the program QTC IMPACT™ (QTC 2000), cluster splits were made in the principal component data scatter until further splits failed to reduce the overall variance in an important way. Splitting decisions were made as detailed in Morrison et al. (2001) using inflexion points of the total scores and the QTC cluster performance index. On the other hand, principal component analysis was applied to the 166 variables produced by the QTC VIEW™ system using the data from all five sites; the number of principal components required to explain 95% of the variance was five. Ping scores along those five axes were used in the *K*-means partitioning procedure of *The Q Package* freeware. The Calinski–Harabasz statistic was used as a stopping criterion to determine the best number of groups for each data set, in the least-squares sense.

The QTC IMPACT™ classification into seven groups was more related to depth than was the six-group *K*-means classification. Discriminant analysis identified that 53% of the points could be allocated correctly to the QTC IMPACT™ groups based on depth alone, compared with 34% for the *K*-means classification. As a consequence, the rest of the analyses reported by Hewitt et al. (J.E. Hewitt, National Institute of Water and Atmospheric Research, P.O. Box 11-115, Hamilton, New Zealand, unpublished data) were based on the *K*-means classification, on which depth had less of an influence.

The first principal component of the 166 QTC variables was highly correlated with depth (Spearman's $r = -0.91$). The relationship found between depth and partition was not totally avoidable in that study because the transects ran down depth gradients and the size of the sonar footprint is a function of depth. Obviously, the fact that QTC IMPACT™ only uses three axes in determining its partition makes it especially sensitive to depth. By opposition, Legendre et al.'s (2002) *K*-means partitioning uses the number of axes necessary to explain 95% (or 99% in other studies) of the variability in the data; that explains the differences between the results of the two methods. There is certainly an advantage in using more than three principal components as the basis for classification.

(3) Preston and Kirlin (2003) argue that elongated (hyperellipsoidal) clusters, produced by their Mahalanobis-based clustering method, are more natural than, and thus preferable to, the hyperspherical clusters produced by *K*-means. There is no particular reason why the data points (sonar backscatters, decomposed into QTC-generated variables) should be structured in any particular way in multivariate space, or in a reduced space of principal components. Within the range of variation of the 166 QTC variables, any intermediate value is possible, so that observations may be found anywhere within the convex envelope surrounding the data points in multivariate space. Natural separation of clusters is predicted, for instance, by the theory of biological evolution, which was the starting point for the development of many of the methods of numerical classification (Sokal and Sneath 1963), but I do not think any theory predicts the existence of regions occupied by points, in the space of acoustic variables, separated by regions where no observations are possible. Nor do we have a theory that predicts that the clusters should have any particular shape. We only want to empirically divide the sonar backscatters into groups, to simplify their multivariate description. These groups will be useful if they are found to correspond to characteristics of the seabed. A division of the space into multivariate boxes of equal sizes would produce a perfectly good classification of the seabed. This can easily be done, for example, in the two-dimensional space of RoxAnn™ variables E1 and E2 developed by Marine Micro Systems Ltd. (Chivers et al. 1990; E1 and E2 are often referred to as "hardness" and "roughness"), but it would be impractical to attempt doing it in a space with 166 dimensions. The reason that we resort to partitioning methods in that space is because we only need to define boxes that are occupied by a sufficient number of points; in particular, we do not want boxes (or classes) containing no point at all. So it is perfectly reasonable to look for spherical or hyperspherical *K*-means clusters in that space. Because they have borders forming flat interfaces, their shape is actually hyperpolyhedric rather than hyperspherical. On these grounds, any other cluster shape is also perfectly acceptable, including those produced by the Mahalanobis-based QTC algorithm. In summary, I believe that the particular metric used for partitioning is not a key point to insure a useful partition of the data points. The choice of the variables derived from the sonar backscatter, and the number of principal components retained for partitioning (see above), are much more important.

(4) There are computational and statistical reasons to prefer a solution implementing a least-squares criterion. The first one is that it runs faster than a Mahalanobis-based algorithm. So, the available computing time can be used to try more random starts of the algorithm; this, in turn, increases the chances of finding an optimal partition (in the least-squares sense). The second reason is that least squares go well with least squares: because *K*-means is a partitioning method optimizing the least-squares criterion, as in multiple regression, it allows the application of a criterion based on least squares to determine the "best" number of clusters. In the *K*-means algorithm incorporated in *The Q Package* and *The R Package*, we are using the Calinski–Harabasz (1974) criterion (C–H), which is a least-squares criterion. This criterion is simply an *F* statistic of multivariate analysis of variance; the partition displaying the highest value of this criterion is the best one in the least-squares sense. Actually, the partitions corresponding to the various maxima of the graph of the C–H statistics against the number of

groups may be worth examining and mapping. There is no direct equivalent of this criterion in Mahalanobis space, at least none that I know of. I encourage the Quester Tangent Corporation to offer our procedure as an option in their computer package. We published our procedure in the scientific literature (Legendre et al. 2002), so it is not proprietary.

(5) The relative usefulness of the partitions produced by QTC VIEW™ and our software should be judged by ground truthing. Because our *K*-means software is freely available, users in governmental and private research institutions, as well as universities, should be encouraged to analyse QTC data using the QTC VIEW™ classification software (based on three PCA axes) and our *K*-means software (using a sufficient number of PCA axes to account for 95% or 99% of the variation in the QTC data) and to compare the results to ground-truthing data, as was done by Hewitt et al. (unpublished data; see subsection 2 above). Comparisons of this kind are part of the scientific process needed to determine the usefulness of acoustics for mapping features of the seabed and, in particular, the horizontal distribution of ecological communities.

Conclusion

This debate does point to a more general dilemma, where technological innovation leads to proprietary products that are used and should be scrutinized by the scientific community. Although science is supposed to be based on free and open communication and debate, companies may choose to act differently in commercial activities. There is clearly a need for new and cost-effective surveying devices that enable us to image and map large areas of the seafloor in a routine and timely fashion. Every surveying device has its limitation and it is important that we recognize them so that technologies can continue to be developed and improved. This note is meant to contribute to that process. I also hope that our paper (Legendre et al. 2002) and freeware (*The Q Package* for Windows and *The R Package* for Macintosh) will be used for seafloor management, especially by researchers in underdeveloped countries, who can benefit from freely available software implementing sound statistical procedures.

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