Appendices

A1 Acknowledgements

We wish to thank our many colleagues, whose ongoing research has supported this work by providing ideas and datasets. We trust that our citations in the text and associated with datasets provides ample evidence of the many researchers who have contributed towards the development of methods and this software. We extend special thanks to those who have organised courses and workshops with the earlier DOS and beta versions of this software, testing these methods. The software and the scope of the manual were greatly improved by these trials, especially through questions, comments and suggestions offered by participants. We offer special thanks to Antonio Terlizzi and Euan Harvey, who, by organising combined workshops at the University of Lecce and at the University of Western Australia, respectively, were largely responsible for bringing us together, leading to this joint endeavour. Thanks are also due to the University of Auckland, Plymouth Marine Laboratory and Massey University for their recognition and support of this work. KRC would like to acknowledge his Honorary Fellowships of the Plymouth Marine Laboratory and the Marine Biological Association of the UK, and his Adjunct Professorship at Murdoch University, Western Australia.

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A3 Index to mathematical notation and symbols

Matrices and vectors

A = matrix containing elements $a_{ij} = -\frac{1}{2} d_{ij}^2$
B = matrix of variables (*N* × *s*) that are linear combinations of normalised **X** variables having maximum correlation with CAP axes
C = matrix of CAP axes (*N* × *s*), standardised by the square root of their respective eigenvalues
D = matrix containing elements d_{ij} corresponding to distances or dissimilarities
G = Gower's centred matrix, consisting of elements $g_{ij} = a_{ij} - \bar{a}_{i \bullet} - \bar{a}_{\bullet j} + \bar{a}_{\bullet \bullet}$
H = 'hat' matrix = $\mathbf{X}[\mathbf{X}'\mathbf{X}]^{-1}\mathbf{X}'$, used as a projection matrix for regression models
I = identity matrix, with 1's along the diagonal and 0's elsewhere
Q = matrix of PCO axes, standardised by the square root of their respective eigenvalues
$\mathbf{Q}^0$ = matrix of PCO axes, orthonormalised to SSCP = **I** ('sphericised') **U** = matrix whose columns contain the left singular vectors from a singular value decomposition (SVD) of a matrix (e.g., **X** = **UWV**′); if **X** is (*N* × *q*) and *q* < *N*, then **U** is (*N* × *q*)
V = matrix whose columns contain the right singular vectors from a singular value decomposition (SVD) of a matrix (e.g., **X** = **UWV**′); if **X** is (*N* × *q*) and *q* < *N*, then **V** is (*q* × *N*)
W = diagonal matrix of eigenvalues from a singular value decomposition (SVD) of a matrix (e.g., **X** = **UWV**′); if **X** is (*N* × *q*) and *q* < *N*, then **W** is (*q* × *q*)
X = matrix of predictor variables (*N* × *q*) (often a set of environmental variables)
$\mathbf{X}^0$ = matrix of **X** variables, orthonormalised to SSCP = **I** ('sphericised')
Y = matrix of response variables (*N* × *p*) (often a set of species variables)
$\mathbf{Y}^0$ = matrix of **Y** variables, orthonormalised to SSCP = **I** ('sphericised')
$\hat{\mathbf{Y}}$ = **HY** = matrix of fitted values (*N* × *p*)
$\mathbf{y}_{ij}$ = vector of *p* response variables for the *j*th observation in the *i*th group
$\bar{\mathbf{y}}$ = the centroid vector of *p* response variables for group *i*
Z = matrix of dbRDA canonical axes (*N* × *s*)

Letters

a, *b*, *c*, etc… = number of levels of factor A, B, C, etc… in an ANOVA experimental design
AIC = multivariate analogue to Akaike's information criterion
AIC_c = multivariate analogue to the small-sample-size corrected version of *AIC*
B_l = the *l*th variable in the space of normalised **X** variables that has maximum correlation with the *l*th coordinate axis (C_l) from a CAP analysis
BIC = multivariate analogue to Schwarz's 'Bayesian information criterion'

C_l = the *l*th coordinate axis scores from a CAP analysis
d_{ij} = distance or dissimilarity between sample *i* and sample *j* *df* = degrees of freedom
F = pseudo-*F* statistic for testing hypotheses in PERMANOVA or DISTLM
i = index used for samples (i.e., *i* = 1, …, *N*) or index used for groups (*i* = 1, …, *a*)
j = second index used for samples (i.e., *j* = 1, …, *N*) or index used for replicates within a group (*j* = 1,…, *n*)
k = index used for variables (i.e., *k* = 1, …, *p* or else *k* = 1, …, *q*)
l = index used for canonical axes or eigenvalues for either dbRDA or CAP (i.e., *l* = 1, …, *s*) or either the abbreviation for ‘log-likelihood’ or the ‘length’ of a vector (depending on context).
m = number of PCO axes chosen as a subset for analysis by CAP *MC* = Monte Carlo
MS = mean square
N = total number of samples
n = number of samples (replicates) within a group or cell in an experimental design
P = *P*-value associated with the test of a null hypothesis *p* = number of multivariate response variables in matrix **Y** *q* = total number of predictor variables in matrix **X**
r = Pearson correlation coefficient
R = the ANOSIM *R* statistic (see Clarke 1993)
R^2 = proportion of explained variation from a model
s = number of canonical eigenvalues and associated canonical axes obtained from either a dbRDA *or* a CAP analysis *SS* = sum of squares
SSCP = sum of squares and cross products
SVD = singular value decomposition
t = pseudo-*t* statistic = $\sqrt{\text{pseudo-}F}$
tr = ‘trace’ of a matrix = the sum of the diagonal elements
X_k = the *k*th predictor variable
Y_k = the *k*th response variable
z_{ij} = distance to group centroid for the *j*th replicate within the *i*th group.

Greek symbols and matrices

α = significance level chosen for a test (usually α = 0.05).
δ_l^2 = the *l*th eigenvalue from a CAP analysis, a squared canonical correlation
Δ = diagonal matrix containing the square roots of the eigenvalues from a CAP analysis (a capital delta)
γ_l^2 = the *l*th eigenvalue from a dbRDA analysis, a portion of the explained (regression) sum of squares from a dbRDA model.
Γ = diagonal matrix containing the square roots of the eigenvalues from a dbRDA analysis (a capital gamma)
λ_i = the *i*th eigenvalue from a PCO analysis
Λ = diagonal matrix of eigenvalues from a PCO analysis (a capital lambda)
ν = number of parameters in a particular model during model selection
ρ= Spearman rank correlation (rho)
$\sum$ = sum over the relevant index

A4 Index to data sets used in examples

Below is an index to the data sets used in examples, listed in order of appearance in the text. With each dataset are given the name and location of the data file, the original reference, a description of its use as an example in the manual and the page number where this can be found (italicised and in parentheses).

1. Ekofisk oil-field macrofauna (ekma.pri in Examples v6\Ekofisk), Gray, Clarke, Warwick *et al.* (1990) - demonstrate one-way PERMANOVA (*1.8*), model selection procedures, diagnostics and building models in DISTLM (*4.10*) and visualising models using dbRDA (*4.11*).
2. Victorian avifauna (vic.pri in Examples add-on\VictAvi), Mac Nally & Timewell (2005) – demonstrate Monte Carlo *P* values (*1.12*). Also used at the level of individual surveys (vicsurv.pri) to demonstrate a repeated measures design (*1.32*) and also PCO (*3.4*), negative eigenvalues (*3.5*), scree plots (*3.5*) and vector overlays (*3.6*).
3. Subtidal epibiota (sub.pri in Examples add-on\SubEpi), Glasby (1999) – demonstrate a two-way crossed design (*1.14*) and contrasts (*1.19*) in PERMANOVA.
4. Tasmanian meiofauna (tas.pri in Examples add-on\TasMei), Warwick, Clarke & Gee (1990) – demonstrate fixed versus random factors (*1.20*), components of variation (*1.21*), expected mean squares (*1.22*), constructing F from EMS (*1.23*), exchangeable units (*1.24*), inference space and power (*1.25*), and testing the design (*1.26*).
5. Holdfast invertebrates (hold.pri, holdenv.pri and Mollusca.agg in Examples add-on\HoldNZ), Anderson, Diebel, Blom *et al.* (2005) – demonstrate a nested design (*1.27*), estimating components of variation (*1.28*), and pooling or excluding terms (*1.29*). Also used later to demonstrate analyses with covariates in PERMANOVA (*1.35*) and marginal and conditional tests with DISTLM (*4.6*).
6. Plankton net study (plank.pri in Examples add-on\Plankton), Winsor & Clarke (1940) – demonstrate designs that lack replication (*1.30*) and increased power as a result of blocking (*1.30*).
7. Woodstock plants (wsk.pri in Examples add-on\Woodstock), Prober, Thiele & Hunt (2007) – demonstrate a split-plot design (*1.31*).
8. Birds from Borneo (born.pri in Examples add-on\BorneoBirds), Cleary, Genner, Boyle *et al.* (2005) – demonstrate an unbalanced design (*1.34*).
9. New Zealand fish (fishNZ.pri in Examples add-on\FishNZ), Anderson & Millar (2004) – demonstrate analyses involving linear combinations of mean squares (*1.36*).
10. Mediterranean molluscs (medmoll.pri in Examples add-on\MedMoll), Terlizzi, Scuderi, Fraschetti *et al.* (2005) – demonstrate an asymmetrical design (*1.37*).

11. Bumpus' sparrows (spar.pri in Examples add-on\BumpSpar), Bumpus (1898) – demonstrate test of dispersion in Euclidean space (*2.3*).
12. Tikus Island corals (tick.pri in Examples v6\Corals), Warwick, Clarke & Suharsono (1990) – demonstrate test of dispersion for ecological data (*2.7*) and how choice of dissimilarity measure matters (*2.8*). Also used later to demonstrate how CAP tells you nothing about relative within-group dispersions (*5.9*).
13. Norwegian macrofauna (norbio.pri and norenv.pri in Examples add-on\NorMac), Ellingsen & Gray (2002) – demonstrate use of the test of dispersion to investigate beta diversity (*2.9*).
14. Okura macrofauna (okura.pri, in Examples add-on\Okura), Anderson, Ford, Feary *et al.* (2004) – demonstrate tests of dispersion in nested designs (*2.11*). Also used to demonstrate PCO of distances among centroids (*3.8*) and PCO versus MDS when samples are split into groups (*3.9*).
15. Cryptic fish assemblages (cryptic.pri in Examples add-on\Cryptic), Willis & Anderson (2003) – demonstrate PERMDISP for a two-factor crossed design, in conjunction with PERMANOVA (*2.12*).
16. Clyde macrofauna and environmental data (clma.pri and clev.pri, in Examples v6\Clydemac), Pearson & Blackstock (1984) – demonstrate PCO versus PCA for environmental data (*3.7*) and simple linear regression using DISTLM (*4.4*).
17. Thau lagoon bacteria (thbac.pri and thevsp.pri in Examples add-on\Thau), Amanieu, Legendre, Troussellier *et al.* (1989) – demonstrate analysing variables in sets using DISTLM (*4.14*).
18. Oribatid mites (ormites.pri and orenvgeo.pri in Examples add-on\OrbMit), Borcard, Legendre & Drapeau (1992) – demonstrate analysing categorical predictor variables using DISTLM (*4.15*).
19. Flea-beetles (flea.pri in Examples add-on\FleaBeet), Lubischew (1962) – demonstrate the rationale for CAP by comparing unconstrained vs constrained ordination (*5.2*).
20. Poor Knights Islands fish (pkfish.pri in Examples add-on\PKFish), Willis & Denny (2000) – demonstrate discriminant analysis based on Bray-Curtis using CAP (*5.4*).
21. Iris data (iris.pri in Examples add-on\Irises), Anderson (1935) – demonstrate classical discriminant analysis and MANOVA test statistics using CAP (*5.6*). Also used later to show how the positions of new samples are added into a discriminant-type analysis, with prediction of group membership (*5.10*).
22. Fal estuary biota (Fa.xls in Examples v6\Fal; falbio.pri and falenv.pri in Examples add-on\FalEst), Somerfield, Gee & Warwick (1994) – demonstrate canonical correlation analysis with CAP based on the Bray-Curtis measure relating biota to a single environmental gradient (*5.11*).
23. Hunting spiders (hspi.pri and hspienv.pri in Examples add-on\Spiders), van der Aart & Smeek-Enserink (1975) – demonstrate a canonical correlation-type analysis using CAP on the basis of chi-squared distances (*5.16*).