

## An assessment of linear discriminant function analysis as a method of interpreting fossil pollen assemblages

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**Abstract** Linear discriminant function analysis (LDF) is assessed as a method of interpreting fossil pollen assemblages from Mt Hauhungatahi, Tongariro National Park, and Ohakune-Horopito, central North Island, New Zealand. Pollen types selected by stepwise discriminant analysis were used in LDF to predict the vegetation type (forest, dense scrub, open fernland, or open tussockland) and canopy type (closed or open) represented by fossil pollen assemblages from an array of sites. Chi-square Goodness-of-fit tests were used to test prediction made by LDF against the vegetation type suggested by the common “standard” method of assessment of the fossil pollen spectra, which is carried out by visual inspection of stratigraphic pollen diagrams. Some sites showed highly significant differences, with many samples obviously misclassified by LDF, especially those from montane forest vegetation. This misclassification occurred mainly because the montane forest samples were so different from the remainder that they were excluded from the prediction set, so that the pollen types most likely

to be predictors were not employed. Overall, however, more sites showed no significant differences. The LDF method is confirmatory rather than providing a clear improvement, and its validity will depend strongly on the correct choice of discriminators.

**Keywords** palynology; stepwise discriminant analysis; linear discriminant function analysis

### INTRODUCTION

Since plant species differ considerably in their pollen production, dispersal, and preservation, vegetation patterns reconstructed from fossil pollen assemblages are uncertain representations of the actual patterns at the time. In New Zealand, the first two of these biases have been addressed by studies comparing the modern pollen spectra with nearby vegetation (Moar 1970; Dodson 1976; Pocknall 1978, 1980, 1982a,b; McGlone 1982; Bussell 1988; Randall 1990, 1991; Horrocks & Ogden 1994; Elliot 1999). Several quantitative methods, such as comparison of specific tree pollen percentages with basal areas, have been used in these comparisons. However, these methods have generally not been extended to cover fossil assemblages because vegetation represented by fossil pollen assemblages obviously cannot be compared with the vegetation from which it came.

The commonly used, “standard” method of reconstructing the sequence of past vegetation types using fossil pollen spectra is based on previous knowledge of pollen production, dispersal, and preservation. Knowledge of production and dispersal of pollen is considerable (e.g., see Moore et al. 1991) and is based primarily on the difference between wind- and animal-pollinated plants. Those that are wind-pollinated generally produce abundant pollen with dispersal distances up to hundreds of kilometres and are thus often over-represented in pollen spectra. Conversely, animal-pollinated plants, which produce relatively little pollen, most of which is deposited

within a few metres of parent plants, are usually under-represented in pollen spectra. There has also been some useful research on palynomorph preservation (e.g., Havinga 1984; Holloway 1989); fern spores, for example, are more durable than pollen grains, and, consequently, are often over-represented in sediments where preservation of organic matter has been poor.

On regional scales, this body of palynological knowledge generally allows confident assessment of fossil pollen records simply by running a trained eye over stratigraphic pollen diagrams. These diagrams typically show depth or time on the vertical axis and relative (and/or absolute) pollen abundance on the horizontal axis. When vegetation patterns on smaller spatial scales are being investigated, however, such as on mountainsides or in estuaries where boundaries between vegetation types may be sharp, more precise assessment of vegetation reconstruction might be desired. This might also be required for determining the significance of subtle changes in pollen trends over time. Several statistical methods, notably principal components analysis, dissimilarity coefficients, and multiple discriminant analysis, have been found to be useful in varying degrees for reconstructing past vegetation elsewhere (e.g., Birks & Birks 1980; Birks & Peglar 1980; Birks & Gordon 1985; Liu & Lam 1985; MacDonald & Ritchie 1986; Sugden & Meadows 1989; Pearsall 2000).

Another statistical method would be to use pollen types that have been selected as having the greatest discriminatory power to "characterise" modern vegetation types to assess fossil assemblages. In an earlier study (Horrocks & Ogden 1994), we used stepwise discriminant analysis to select such discriminating pollen types on Mt Hauhungatahi in Tongariro National Park, central North Island. The aim of the present study is to use those statistically selected pollen types to reconstruct the sequence of past vegetation types from Mt Hauhungatahi and elsewhere by way of linear discriminant function analysis (LDF) of fossil pollen data. A similar type of analysis was carried out by Harris et al. (1976), who used discriminant function analysis on fossil pollen data to indicate the comparative temperatures under which Quaternary sediments accumulated in several locations in New Zealand. Our primary aim is methodological, assessing LDF as a method for reconstructing past vegetation and looking at its potential, rather than providing a detailed ecological interpretation of the fossil pollen records from the sites sampled. The fossil pollen diagrams and

detailed ecological interpretations of these sites are given in Horrocks (1994), Ogden et al. (1997), and Horrocks & Ogden (1998a,b,c, 2000).

## METHODS

In the previous study where the pollen types most discriminatory of vegetation types were selected (Horrocks & Ogden 1994), surface samples of pollen were collected from moss cushions at 36 sites on Mt Hauhungatahi. Sites were chosen to represent the main vegetation communities ascending the altitudinal gradient: montane forest, sub-alpine forest, dense scrub, open fernland, and open tussockland (Atkinson 1981; Druitt et al. 1990), covering an altitude of 730–1520 m. In addition, samples were taken laterally along the tree-line from within the forest edge and adjacent non-forest communities. By convention, the pollen sum for each sample was at least 250 grains, excluding swamp plants and ferns, except *Pteridium*, which may form a dominant cover of vegetation (McGlone 1989). A stepwise discriminant analysis (SAS Institute 1988) of these modern pollen assemblages was used to select pollen types with the most discriminatory power in relation to local vegetation types (Horrocks & Ogden 1994). These selected pollen types constitute the "training data set". The montane forest sites, recognised as outliers on the basis of cluster analysis and DECORANA ordination, were excluded from the analyses discussed here (LDF).

In linear discriminant function analysis (LDF), a set of data points (i.e., pollen counts) is allocated to predefined classes (i.e., vegetation types). In the current study we use this method to allocate the fossil pollen assemblages (the "allocation data sets") at each depth in the pollen profiles from 11 sites on Mt Hauhungatahi (Horrocks 1994; Ogden et al. 1997; Horrocks & Ogden 1998a,c, 2000) into one of the four vegetation types (sub-alpine forest, scrub, fernland, and tussockland) previously determined from the analysis of the modern pollen assemblages. The site names are their altitude above sea level. The pollen profile from a site 15 km to the south between Ohakune and Horopito (Gibsons' Swamp) (Horrocks & Ogden 1998b) is also included. The fossil pollen sum was the same as that of the modern pollen sum. The software package SAS (SAS Institute 1988) was used for LDF.

To assist in the interpretation of the LDF analysis, the 12 pollen profiles were sub-divided into zones

(42 in total), within which samples (506 in total) are similar in their essential characteristics. Zones are commonly assigned to pollen profiles to make presentation of results easier. In our case, zones were defined by a TILIA classification (E. Grimm, Illinois State Museum, Springfield, Illinois) into groups using the agglomerative cluster analysis method of incremental sum of squares (CONISS) with a square root transformation (Grimm 1987). We recognised zones at the second, third, and, occasionally, fourth levels of division by CONISS, generally aiming to divide each profile into 3–5 zones. To reduce the effects of “noise” in the analysis, pollen types with values < 1% were excluded from CONISS (Norton et al. 1986).

Based on the standard method of interpretation of the fossil pollen diagrams, each zone was assigned to one or two of the four vegetation types determined by the stepwise discriminant analysis: forest, dense scrub, fernland, or tussockland. Zones assigned two vegetation types had pollen assemblages that appeared to have been produced by more than one vegetation type. This applies to assemblages produced by forest and dense scrub, which may be difficult to differentiate because these two vegetation types are comprised of some of the same taxa and often grade into one another near the treeline. Standard assessment of the fossil pollen data was based on local modern pollen/vegetation relationships (Horrocks & Ogden 1994), and on previous knowledge and experience of pollen production and dispersal generally in the New Zealand flora (e.g., McGlone 1988). High values for tall tree/other forest types or for small tree/shrub

pollen coupled with lower values for taxa found in open environments indicate that the site is in forest or dense scrub, respectively; high values for the local spore disperser *Gleichenia* indicate open fernland; and the presence of Poaceae and Restionaceae (*Empodisma minus*) pollen identifies an open tussockland site.

Linear discriminant function analysis was then used to analyse the fossil pollen data for each site. In comparing the LDF (observed) vegetation categories with those assigned by the standard method (the expected values), comparisons were made for each zone within which observed and expected categories occurred. For any vegetation category (e.g., tussockland) it was considered invalid to include observed values for zones in which the vegetation type was not predicted. For example, two samples were predicted as tussock in Zone 2 at Site 1140a (Table 1) but these were not included in the “tussock” comparisons at this site, which was restricted to Zone 1, where both observed and expected values were present (Table 2). The LDF “observations” for each zone were compared with the standard predictions using a Chi-square Goodness-of-fit test for each vegetation type (i.e., sub-alpine forest, scrub, fernland, or tussockland). The method of calculation of the Chi-square value is given in Table 1. This was carried out for all sites and the Chi-square values summed across all sites. In addition, agreement of LDF predictions with standard predictions for canopy type, i.e., “closed” (forest and/or scrub) or “open” (fernland and/or tussockland) was assessed, also using Chi-square Goodness-of-fit tests.

**Table 1** Example of method of calculation of expected (subjectively assigned) (E) and observed (LDF categorisation) (O) vegetation assemblages (Site 1140a). FO, sub-alpine forest; S, scrub; FE, fernland; T, tussockland. FO/S implies that the zone was subjectively classified as representing a mixture of forest and sub-alpine scrub. In such cases the two components were given equal weighting.

Zone	No. of samples	Subjective veg. type (E)	LDF prediction (O)
1	5	T	4T, 1S
2	7	FO/S	5S, 2T
3	13	FO/S	6S, 4T, 3FO
4	4	FO	3T, 1FE
Total	29	5T, 14FO, 10S	4T, 3FO, 11S

**Table 2** Goodness-of-fit tests for vegetation types across sites. E, expected frequency; O, observed frequency; D, difference between E and O; GS, Gibsons' Swamp. The  $\chi^2$  values of interest are not those indicating significant differences, but rather those (highlighted) which indicate no significant difference (i.e.,  $\chi^2$  values totalling less than the  $P < 0.05$   $\chi^2$  value given in the second to right column). Significant agreement would be indicated by very small  $\chi^2$  values equivalent to  $P > 0.95$ , but none of the totals meet that more stringent criterion, although selected "open canopy" comes quite close (sum of  $\chi^2 = 1.731$ ;  $\chi^2$  with  $P > 0.95 = 0.711$  with 4 d.f.).

Site	730	800	1020	1140a	1140b	1160	1170	1190	1285	1410	1470	GS	$\chi^2$ for all sites ( $P < 0.05$ )	$\chi^2$ for selected sites ( $P < 0.05$ )	Prop. of sites with no signif. difference
Forest	E	40	24	14	20.5	18.5	21	24		18		91			
	O	4	18	3	12	4	22	20		18		93			
	D	36	6	11	8.5	14.5	1	4		0		2			
	$\chi^2$	32.4	<b>1.5</b>		8.643	<b>3.524</b>	11.365	<b>0.048</b>	<b>0.667</b>	<b>0</b>	<b>0</b>	<b>0.043</b>	58.19 (15.507)	<b>5.782</b> (11.07)	6/9
Scrub	E			10	10.5	14.5	18	11							
	O			11	13	29	12	10							
	D			1	2.5	14.5	6	1							
	$\chi^2$			<b>0.1</b>	<b>0.595</b>	14.5	<b>2</b>	<b>0.091</b>					17.286 (9.488)	<b>2.786</b> (7.815)	4/5
Fernland	E	41.5					5.5		7.5			7			
	O	11					2		3			7			
	D	30.5					3.5		4.5			0			
	$\chi^2$	22.416					<b>2.227</b>		<b>2.7</b>			<b>0</b>	27.343 (7.815)	<b>4.927</b> (5.991)	3/4
Tussock-land	E	16.5		5			5.5		24.5	26	30				
	O	27		4			9		22	7	13				
	D	10.5		1			3.5		2.5	19	17				
	$\chi^2$	6.682		<b>0.2</b>			<b>2.227</b>		<b>0.255</b>	13.885	9.633		32.882 (11.070)	<b>2.682</b> (5.991)	3/6
Closed canopy	E	40	24	24	31	33	39	35		18		93			
	O	16	24	14	29	33	36	30		18		92			
	D	24	0	0	2	0	3	5		0		1			
	$\chi^2$	14.4	<b>0</b>		4.167	<b>0.129</b>	<b>0</b>	<b>0.73</b>	<b>0.714</b>	<b>0</b>	<b>0</b>	<b>0.011</b>	19.659 (15.507)	<b>5.251</b> (14.067)	7/9
Open canopy	E	58		5			11		32	26	30	7			
	O	58		4			11		25	7	13	7			
	D	0		1			0		7	19	17	0			
	$\chi^2$	<b>0</b>		<b>0.2</b>			<b>0</b>		<b>1.531</b>	13.885	9.633	<b>0</b>	25.249 (12.592)	<b>1.731</b> (7.815)	5/7

## RESULTS

In the previous study (Horrocks & Ogden 1994), pollen types selected by stepwise discriminant analysis as having the most discriminatory power in relation to the four selected local modern vegetation types were *Libocedrus* (sub-alpine forest), *Myrsine* (dense scrub), *Gleichenia* (fernland), and *Restionaceae* (tussockland). Together they explained 68% of the variance. All have local pollen dispersal. Although *Myrsine* explained more of the variance (23%) than the others, it was not necessarily the most important discriminator since this method does not necessarily select variables in order of importance. Relatively little variance is explained by pollen types selected after the fourth step. Lachenbruch (1975) stated that the first three to five variables are usually all that can be safely selected by stepwise discriminant analysis.

For the current study, Chi-square Goodness-of-fit tests for the vegetation types across sites are shown in Table 2. Expected values (standard assignments) tend to be greater than the observed (LDF) values. This is because each zone as a whole was categorised, so that all samples within it were generally given the same class, or else split between two classes. The LDF method categorised each sample separately, so samples within a zone could have different categorisation.

With all relevant sites included, the Chi-square Goodness-of-fit tests show that LDF predictions and standard predictions for vegetation type and for canopy type were significantly different ( $P < 0.05$ ). However, some sites showed a much greater difference than other sites. When these were excluded from the tests (on the basis of  $\chi^2 > 3.841$ , 1 d.f.), differences were not significant ( $P < 0.05$ ) for vegetation type: 6 out of the 9 relevant sites for forest, 4 out of 5 for scrub, 3 out of 4 for fernland, and 3 out of 6 for tussockland (16 out of 24 total); for canopy type: 8 out of 9 for closed canopy, and 4 out of 6 for open canopy (12 out of 15 total). Although some sites show highly significant differences, overall more sites show no significant differences between the zone categories defined by LDF and by the standard method.

## DISCUSSION AND CONCLUSIONS

The high degree of disagreement between LDF predictions and standard predictions for vegetation type and for canopy type at some sites is due to obvious misclassification of samples. This occurred

mainly because the allocation data sets (fossil pollen assemblages) contained significant amounts of pollen of taxa belonging to none of the groups within the training data set (selected from the modern pollen assemblages). In particular, the exclusion of montane forest moss polsters from the training set selection process (because they were outliers) meant that LDF predictions were biased towards sub-alpine vegetation types. Thus, it was impossible for montane forest to be accurately identified, although sub-alpine forest could be. Consequently, we did not expect as good a fit between observed (LDF predicted) and expected (standard allocations) forest types as between the other vegetation types. However, the agreement with forest prediction (6/9) is just the same as that for the other vegetation types (10/15).

Examples of bias towards sub-alpine vegetation are apparent with *Libocedrus* and *Myrsine*. Where *Libocedrus* (characteristic of sub-alpine forest) pollen values were very low, LDF tended to predict sub-alpine scrub or tussockland, despite the fact that some taxa (excluded from the training set because they were in outlier sites, e.g., *Weinmannia*) clearly indicated that they were representative of forest. Likewise, although *Myrsine* was used to discriminate sub-alpine scrub, high *Myrsine* values can also occur in forest. *Myrsine divaricata* is found in sub-alpine scrub and forest while *M. salicina* occurs in the montane forest. *Myrsine* is therefore not a good discriminant of vegetation sequences containing both species.

Because data from outlier sites were excluded, *Weinmannia* and *Cyathea smithii*-type could not be recognised as discriminators for the montane forest. However, their high pollen values (Horrocks & Ogden 1994) clearly show that they are.

In our earlier study only four sites were sampled in the dense scrub category (Horrocks & Ogden 1994). These were the least clearly discriminated of any of the sites, and were classified by cluster analysis into a group that also contained a forest, tussockland, and fernland site. Also, these sites were widely scattered on the second axis of the ordination (Horrocks & Ogden 1994, fig. 4).

As some sites showed highly significant differences, and as overall more sites show no significant differences between the zone categories defined by the standard method and by LDF, our conclusion is that the LDF method is confirmatory rather than providing a clear improvement, and its validity will depend strongly on the correct choice of discriminators. Presumably this is at least in part

because the standard assessment takes into account the whole suite of taxa within any grouping. We also conclude that, while LDF may be of limited use in the interpretation of fossil pollen assemblages, the stepwise discriminant analysis is useful, because it draws attention to the most important taxa on which divisions should be based. Emphasis on these taxa will improve the standard assignment of zones to categories, but little additional improvement is gained by the application of LDF. However, the interpretation of sites showing a strong disagreement in several categories (e.g., Sites 730 and 800 in the current case) should be re-evaluated.

A further problem (although not restricted to LDF) is that the LDF approach assumes that existing vegetation types (as reflected in present-day surface pollen assemblages) are analogues of the past. Assuming individualistic plant responses to environmental change, we must conclude that, in detail, "species composition analogues" are unlikely, although "broad vegetation analogues" may have occurred. Thus, LDF based on prior stepwise discriminant analysis will simply pick out "vegetation types" based on the abundance of the key discriminatory taxa, which can probably be done equally well by the eye of a knowledgeable observer.

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