Data processing in pollen analysis^{*}

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ABSTRACT. The main steps and ideas of pollen data processing are outlined, as resulted from the experience of POLPAL system exploitation on the regional scale. This system entails the following sequence: computer assisted pollen counting, through storing pollen tables, diagram plotting, numerical analysis, dating spectra and plotting isopollen lines on the map of Poland. We would like to emphasize the real possibilities of wide application of more or less advanced computer/numerical methods. The benefit of this approach of data acclamation and manipulation is that it encourages the interpersonal exchangeability of data and ideas. The system POLPAL is described as a "case study" of implementation of computer in pollen analysis. This system will only be reviewed in part, because such systems are never in their final state and are also subject to future trends.

KEY WORDS: pollen counting, pollen diagrams, numerical methods, age-depth curve, isopollen lines

INTRODUCTION

The computer is a valuable tool recognized early by palynologists. Shortly after electronic devices such as pocket computers and microcomputers came into practical use, some applications for data handling in pollen analysis were produced. They were designed for counting pollen, data collecting and storing (Melief & Wijmstra 1984, Eisner & Sprague 1987, Konert et al. 1987, Stefan & Dupont 1988, Nalepka & Walanus 1989, Ralska-Jasiewiczowa & Walanus 1991, Walanus & Nalepka 1996, 1997, 1999, Bennett 1990). Relatively early, numerical and statistical methods application motivated further development of computer applications (Birks 1979, 1986, Birks & Gordon 1985, Maher 1990). However, the widest application of the computer is in drawing the pollen diagram. The last step is to organize data bases and to use them for performing analysis on regional or continental scale (de Beaulieu & Cheddadi 1992, Walanus 1995) and a world – wide project as well (World Data Center 1992).

Unfortunately hopes for an image processing application for automatic recognition of pollen grains, are still far from practical implementation. Pollen grain classification is still based upon subjective opinion. It may be that some well-organized database of images of pollen grains would make the process more objective. Email has also enabled palynologists to easily and expeditiously exchange images of pollen grains. Anyway, questions concerning pollen images (Joynt & Wolfe 2000) will not be addressed in this text.

COUNTING POLLEN – THE FIRST STEP IN DATA PROCESSING

Counting pollen grains, from the point of view of data processing, is the primary source of data. As mentioned above, since data are "produced" in the human brain, essentially the interface between the counting person and computer system is necessary. In Polish program POLPAL, for example, that interface operates in the following steps. After starting the program, one selects the proper pollen

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table, then selects the sample to be counted, and identifies the first sporomorph on the microscope slide. Each taxon (according to the predefined list of taxa, see below) possesses a unique nickname (code) that is used to record the identified sporomorph (Walanus 1994). Most taxa are coded by a three-letter code, some, more frequent taxa have a two-letter code, and some other even a four-letter code. Such codes can be customized. An experienced user may remember the most frequent codes. However, each code may be displayed to the user in an additional window at any moment. One needs only to type the first letters of the taxon name. For example, typing "al" adds one count of Alnus to the sample, while typing "Al" gives the following list of taxa with their nicknames (codes):

 $\begin{array}{l} Alchemilla \ t. \Rightarrow alg \\ Alisma \Rightarrow ai \\ Alisma plantago-aquatica \Rightarrow alb \\ Allium ursinum \ t. \Rightarrow alc \\ Allium vineale \ t. \Rightarrow ald \\ Alnus undiff. \Rightarrow al \\ Alnus viridis \Rightarrow alf \end{array}$

When the program recognizes the code, the name of the taxon is displayed. Also a loudspeaker may say its name. A wrong code results in the message "no such code" instead of the expected taxon name. More frequently used taxa or codes can be assigned to the function keys (F1-F12), giving the possibility of counting with one keystroke. Some additional operations are accessible like: adding a half of the sporomorph and adding or subtracting counts to previously counted taxon. The process of counting is recorded, count-by-count, and the current register can be recalled in case of any doubts. Besides counting there are two other ways to input data. The first is by typing the data from hand-written (historical) protocols. The system has been designed to simplify this job. Of course, data may be typed directly into the cells of the pollen table spreadsheet. And the second way is by importing pollen tables, which have been already stored in computer files.

It is possible to export and import pollen tables from the text as well as MS Excel and Tilia (Grimm 1990) format files. In case of importing a whole table with taxa names, a new temporary list of taxa is created. The imported table may be processed further by using that list of taxa or may be translated to the main or any other list of taxa, using a dedicated application for comparison of two taxa lists.

LIST OF TAXA

In a typical pollen table, rows represent spectra or samples (identified by the depth in the profile) and columns represent taxa. The depth, in most cases, is of local importance, or even minor, however, taxa names should posses continental scale meaning. From the botanical point of view Pinus sylvestris has a well defined meaning across the northern hemisphere or even broader. For that reason, in data processing, it is necessary to create a relationship between pollen tables, which is based on taxa names. The essence of intercomparability of pollen data lies in taxa definitions. In principle only one list, as comprehensive as possible, of taxa should be used. At least, pollen analyst should use only one list of taxa for one site or region. In Poland, for example, most Quaternary pollen analysts use the same basic list of taxa, created by M. Ralska-Jasiewiczowa and M. Latałowa, additions to which are required only sporadically. To maintain the use of only one list of taxa, for example within one country, each modification of the list should be accepted by the whole community of users. Technically it would be easy, however, the community seems not to be ready yet.

Within POLPAL, each taxon is identified by a unique number; what is a typical data base construction. Each taxon name (limited to 255 characters) is accompanied with a code of up to 4 letters, used for counting pollen and for input of protocols (see above). The last attribute of taxon is in the form of one character, which identifies the so-called life form (for example ecological groups acc. to Ellenberg (1979) or division for trees, shrubs, herbs and non pollen forms, or any other division). The idea of life form, however, disputable from the botanical point of view, has been found very useful in data handling. Optionally "ecological indicators" may be added to taxa, however, that additional option depends on individual user needs and is to be developed on demand. To clarify the sense of country-wide meaning of the taxa, in fact, the meaning of unique taxa number: individual user is absolutely free in changing taxon codes used in counting. It is

also possible to change the life forms for disputable taxa (for example, if tree or shrub); it is even possible, however, not recommended to modify the taxon name (for example using t. instead of type or correcting literal errors).

Maintaining one countrywide list of taxa seems to be a daunting task today. In the POL-PAL system a dedicated application is used to recode pollen tables from a local list of taxa to a "global" list of taxa. For example to say that a person has imported a table from MS Excel. In this instance the POLPAL searches for similarities in both lists of the taxon names and then the palynologist, after reviewing the list, can introduce appropriate changes with a mouse clicks. Lists of taxa must be compared especially when many users have added any taxa to the main list independently of one another. In this instance the main list is to be compiled by a central board. In the next step, all users have to recode pollen tables according to the "central" list of taxa, what is quite easy. In some applications, like diagram plotting or numerical analysis, the idea of "sets of taxa" is very useful. The taxa set is just a specific sequence of a number of taxa (say 5 to 50), with one additional possibility to sum up taxa (for example Tilia cordata + Tilia platyphyllos). Such a set of taxa, easily prepared in the program, can be stored in a separate file for further use or modification.

The list of taxa is more or less a typical data base construction. Also the pollen table has a typical spreadsheet form and thus will not be discussed here. However, registration of individual pollen counts is a specific function of the data handling system.

DIAGRAM PLOTTING

Similarly to the individual pollen grains counting, also plotting of diagrams is the exclusive function of POLPAL (Fig. 1) and other dedicated software. In fact it is impossible to plot a conventional pollen diagram using MS Excel or other standard software. The diagram is a graphical analogue presentation of a digital pollen table. However, the mapping is not straightforward. The sequence of plotted taxa, and the pollen sum definition are to be decided. The graphical parameters, like vertical and horizontal scales are to be adjusted. Graphical details of curves, fonts of taxa



Fig. 1. POLPAL application for diagram plotting

names, sample descriptions, as well as the type of diagram (AP/NAP, histogram, pie plot, smoothed curves) may be modified. The selection of the desired taxa sequence may be a difficult task in case of a table having many taxa. There are many options for taxa arrangement in POLPAL. The most important are:

- according to the table
- set manually by typing numbers
- set manually by mouse clicks in the proper order
- stratigraphically (according to the first appearance)
- according to the 'set of taxa',

Summation of taxa is supported, for example, all trees (and all non-trees) for the AP/NAP diagram, *Hordeum* t. and cf. *Hordeum* t. for the summary barley curve, and so on.

Five basic types of diagrams can be plotted in POLPAL:

- typical silhouette diagrams (Fig. 2b)
- two types of bar diagrams (Figs 2c, d)
- summed up curves, for example used for human impact indicators (Fig. 2e) or for AP/NAP ratio (Fig. 2a)
- diagrams with Gaussian smoothing of curves (Fig. 2f, g),
- pie plots for one sample or for a sequence of samples.

There are several graphical options with respect to plotting the diagram. The assignment of colours or patterns, or colour patterns, to individual pollen curves is possible. Fonts may be modified in size and colour. The distance between curves may be modified globally or individually. Curves may be 10 times exagger-



Fig. 2. The same data presented in different forms: \mathbf{a} – silhouette of summed up curves: AP/NAP ratio, \mathbf{b} – typical silhouette, \mathbf{c} , \mathbf{d} – bar diagrams, \mathbf{e} – silhouette as human impact, \mathbf{f} , \mathbf{g} – diagrams with Gaussian smoothing of curves

ated, horizontal lines of spectra may be drawn or not. Sample numbers (depth) and pollen sums (AP, TOTAL ...) may be printed in the diagram. In case of a pollen-sterile horizon, part of the diagram (hiatus) may be plotted as an empty space. Crosses instead of curves may indicate the presence of rare taxa. Diagram may be plotted using one of the several predefined sample vertical ordinates (e.g. age BP instead of depth).

The diagram prepared for publication has to have a format readable to others (Bennett 1997). In POLPAL we have decided to use the standard MS Windows bitmap format (bmp files). That format has two main advantages and one disadvantage as compared to a vector graphic. The advantage is that it is a standard format, readable to all Windows applications (and not only Windows). It is almost impossible for bitmap to be damaged by improper file interpretation. Bitmap is fully defined by pixels, black or white or coloured points. Every computer screen is a set of pixels; every printer (laser, ink, or pin) plots pixels on the paper. Every standard graphical application is capable of handle bitmaps, even the simplest Windows accessory, namely Paint (or Paint-Brush). In fact, we strongly recommend that simplest application to POLPAL users. Any additional text description, frames or lines of zones may be added to the diagram using Paint tools. Pictures also may be joined. Some operations are not so easy with Paint, such as removing some curves or changing its position. So, two special applications are prepared in POLPAL to assist the user in creating diagrams. The mentioned disadvantage of bitmap

is that it is not as flexible as vector graphic. However, flexibility of Windows metafile graphs or other vector formats sometimes produces funny results. For example a file generated in one application is misread by another one. Generally, vector graphics is not user friendly. The same graphical precision can be obtained with either bitmap or with vector graphic.

POLPAL diagrams possess some features of vector graphic. Namely, it is possible to store almost all settings necessary to create a diagram. Thus a well organized user can store some files and reproduce the same diagrams without problem. The diagram, in the form of bitmap, is like a canvas, ready to be drawn upon with additional figures or descriptions. A good example is the "human impact" diagram (Fig. 2e).

NUMERICAL ANALYSIS

Having pollen tables in computer file should stimulate application of some other insights into the data than simple visual inspection of the diagram. The first step to explore possibilities offered by the computer may be, for example, rearrangement of taxa in the diagram. It may be really creative to analyse the succession in different versions of a taxa neighbourhood on the diagrams. Also changing the scale of depth or percentage may give new results, not only in the graphical layout, but also in its interpretation. The next step of experiments may concern pollen sums, namely the inclusion or exclusion of certain local taxon. All such possibilities are provided by the application for drawing diagrams.

Another reason to apply numerical methods related with computerized data storage is increasing amount of data to be analysed. Numerical methods are, in most cases, statistical procedures, which compress data and extract significant information against noise. Numerical methods are much less subjective than personal experience and intuition. Typical nuanalyses (Birks 1988) offer merical а substantial transformation of data. The condensed result is much simpler than the pollen diagram because it comprises of only one, two, or at most three curves (or other plots). Strictly defined (thought sometimes very complicated) mathematical transformations, instead of palynologist intuition, are responsible here for the data interpretation. Finally, the user decides, not the computer, whether the result of numerical analysis is meaningful and useful or not.

In POLPAL, the most frequently recommended numerical/statistical methods of pollen table analysis are easily available. For most of the analyses, one can easily get a result in a graphical form and then add it to the main diagram. Of course it is possible to customize some parameters of calculations as well as scales and other features of the graphs.

Standard numerical method, CONSLINK (Birks 1979,1986), gives clusters i.e. groups of similar pollen spectra under stratigraphic constraint. The resulting graph has the form of a tree diagram, easy to interpret, and gives a straightforward indication to define pollen zones. The set of taxa to be involved in the analysis may be defined as standard POLPAL set of taxa (PU file). The other option is to set a lower percentage limit. Numerical algorithm is based on the Manhattan measure of similarity of spectra. Percentages are transformed by the square root to enhance the significance of less abundant taxa.

Rarefaction analysis (Birks 1992) determines taxa richness of the samples; this "taxa richness" is calculated to the same pollen sum. In a sample with the pollen sum equal to 1000, more taxa may be expected than in the same sample counted only to 500. Such samples should be standardized prior to taxa richness comparison. Rarefaction reduces taxa richness in most samples in order to be comparable with the sample of the lowest sum. Since the resulting number of taxa is no longer an integer number, there is no loss of information here. Anyway, samples with extremely low sums may be removed from the analysis. Such samples are interpolated in the graphical result of the analysis.

Principal Component Analysis (PCA) is a multivariate analysis typical (Greenacre 1984). Most of information contained in the whole set of taxa involved in analysis is transformed by PCA into one, two or three principal components. These quasi-taxa are calculated as linear combinations of taxa. Principal components are statistically independent; which means that each component carries independent stratigraphical (also botanical) information. The first principal component carries the largest amount of information, the next components are less important. Typically the first component contains information easily seen on diagram. However, numerical precision is, in some sense, absolute. The second principal component may exhibit features, which are important but hidden in the plurality of taxa. Coefficients of linear combinations of taxa, which define principal components, are important for PCA interpretation, so they are plotted in simple form of bars in addition to the three PCA curves.

The fourth numerical method in POLPAL operates on two profiles. It compares pollen spectra from the first (horizontal) profile with those from the second (vertical) one (Fig. 3). The resulting Sample Similarity Matrix (Maher 1993a, Gardner 2000) is presented in graphical form. The more the two spectra are similar, the larger is the black square, which is plotted at crossing of the samples levels. The well correlated profiles give a diagonal band of



Fig. 3. Comparing two pollen tables by plotting sample similarity matrix

black area on such a plot. Data may be calculated as percentages, present-absence or with Equal Taxa Weight.

COMPARISON OF TWO DIAGRAMS

The last numerical methods mentioned above helps to correlate two diagrams. However, it is a numerical/statistical method that compresses the data. To compare two diagrams stratigraphically involving all botanical and background knowledge, the analyst needs to compare many pollen curves. Using standard application for plotting diagrams, one may print two diagrams on two separate transparencies, place them on the overhead, and look for similarity moving one diagram relatively to the other. The same may be performed using graphical software slightly more sophisticated than Paint. However, stretching the diagram in a vertical direction would distort the image thus prohibiting it to line up with another diagram from another software program.

In POLPAL there is a dedicated application (Fig. 4), which combines two diagrams and plots the pairs of curves of one taxon (*Pinus* 1,



Fig. 4. Correlating two diagrams by relative movements and adjusting the depth of scale of the selected fragments of a given profile

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Pinus 2, Betula 1, Betula 2...). The first diagram gives the reference of the depth scale. The second one should be adjusted accordingly to the first. This is done by moving the given sample of the second profile and its attachment to a new position. The other samples, between the attached samples, are moved proportionally. In general any sample may be attached to any depth, although it is not allowed to break up their stratigraphical order. The other samples (not attached, free) are moved proportionally, according to their original depth positions (close samples remain relatively close). Once attached, the sample may be made free again. Experimentation with moving up and down spectra, or with stressing or stretching profile fragments is fast and easy. To move a sample one simply needs to: (1) select a sample, (2) accept a question (e.g.: "Move sample 44?") and (3) to select a new depth, for sample 44. All of these steps can be done by clicks of the mouse. The resulting new positions of samples of the second pollen table are stored as an option for further use.

DATING SAMPLES BASED ON A FEW RADIOCARBON DATES; DEPTH-AGE CURVE

Absolute dating of pollen spectra in ¹⁴C years BP or calendar years is important element of pollen analysis. The most common is ¹⁴C dating, however, other "absolute" dates may be used, such as dendrochronological, or archaeological, if dates possess a well-defined error.

Not every sample in the profile is dated. Frequently the profile has one or two dates, and typically less than 10.

There are many mathematical models, which can be applied for interpolation (or extrapolation) of ¹⁴C dates (e.g. Maher 1992). POLPAL offers linear interpolation, polynomial of any order, and cubic spline functions. However, we recommend subjective, manual method, after "playing" with functions (Nalepka & Walanus in print). If the palynologist is not satisfied with the functional curves, we suggest to rely upon their botanical, stratigraphical, and geomorphological background knowledge and to define the depth-age relationship manually. POLPAL plots all necessary details: samples positions, lithological transitions, and radiocarbon dates with error bars (in age as well as in depth scale). The difficult and responsible task is up to the author to click a few times on the plot to define a broken line that will be the age-depth relation for the profile. After manually establishing the age-depth relationship or choosing one of the mathematical models, ages of all samples are determined. Results are saved as an option for further use.

Calibration of radiocarbon dates is also available. Also other very simple options are included such as multiplying the ^{14}C error twice. Radiocarbon date users are optimistic in the fact that true error is simply $\pm 1\sigma$. First, the $\pm 1\sigma$ error bar covers only 2/3 of the total probability. Second, the reported error (σ) is the minimum error of ^{14}C measurement; the true error of dates of samples taken from the same level is seldom so small.

ISOPOLLEN LINES

Having all spectra of some number of pollen tables dated, one is inspired to plot isopollen lines i.e. lines on the map (Fig. 5) of the same percentages of given taxon at some time slice (Szafer 1935, Ralska-Jasiewiczowa 1983). The geographical scale may be small, such that a few profiles are comprised, regional, or as big as a whole continent. In the first case the main goal of plotting isolines is to check the consistency of pollen data and dating for a few profiles.

To plot isopollen lines, all pollen tables of interest must have the same list of taxa. Geographical coordinates of sites are to be known. In POLPAL coordinates are stored in the pollen table name; for example Osłonki 949; 52°37'N, 18°48'E (Nalepka et al. 1998).

Extraction of data for isopollen plotting is a typical data base operation and is in fact a query. For all pollen tables one needs to select a given taxon (or group of taxa – e.g. trees) and a given time slice. The result is one number (percentage) per one table (geographical position). Definition of "time slice" is a slightly delicate question. For the data base (POLPAL) it is easy to take the exact time slice by interpolation of two spectra. For example, from two samples dated to 4789 yr BP and 5123 yr BP, one can easily obtain the "exact" pollen percentages for 5000 yr BP. However, a reasonable calculation of the resulting precision im-



Fig. 5. Presentation of pollen data on the map

plies the use of more than one or two spectra. The precision of dating samples is, as a rule, lower than expected. Taking into account the real dating precision, or error bars, one obtains interval instead of "time slice'. If such an interval covers a few spectra, all of them should be averaged (weighted average is the best way) in order to increase the reliability of pollen percentage (by increasing pollen sum).

In the POLPAL system, query to database is performed by a separate application. The result is a spreadsheet in standard text format CSV with sites in columns and taxa and time slices in rows. For the given row, i.e. given taxon and given age, the isolines may be produced by any standard software. However, application for drawing isolines is also prepared in POLPAL.

The advantage of having a dedicated application for drawing isopollen lines on the map lies not only in good communication between all POLPAL applications but also in having some special features. Unlike typical commercial applications POLPAL cancels plotting isolines for areas with no data (with no sites nearby). Another special option, which seems to be very useful, is the possibility to display two numbers on a map for every site: pollen percentage from that site and pollen percentage expected for that site (place) from other sites (with that site excluded). Comparison of both percentages makes it possible to exclude or, at least to review sites (pollen tables) that do not agree with neighbouring sites. Thus it may indicate that the depth-age relationship needs to be corrected, or some local properties of the site are to be realized, e.g. with the aid of the application for comparing two diagrams (see above).

TECHNICAL REMARKS

POLPAL today operates in a 32-bit format for Windows (up to XP), however, a 16-bit version for Windows 3.1 is also available but no longer technically supported. Also the DOS version is in use for diagram plotting (for the conservative user) and for counting (for the user with an outdated 286 machine standing near the microscope). All main data are exchangeable between all three versions of POL-PAL. For example the counting results from an older system i.e. DOS may be plotted on Windows 2000. Moreover it is possible to copy pollen tables created under Windows to DOS.

POLPAL, and other such types of applications are versatile. Not only can pollen grains be counted and pollen diagrams plotted, but also other microfossils (e.g. spores, other palynomorphs, diatoms, Cladocera, charcoal particles (see Ralska-Jasiewiczowa et al. 1998) or macrofossils (see Latałowa 1999) may be handled as well.

The palynological niche of computer users is not readily affected by the fast development of new techniques of data handling. Ideas like data mining, techniques like OLE DB, data bases like Oracle or DB2 are of minor interest to palynologists. As the amount of data which pollen analysts produce is small, modern databases are not suited to the specific needs of pollen analysts. For example, using the compressed format in POLPAL (Walanus 1989), the bulk of all Polish pollen data comprises only 0.01% of a typical (15GB) hard drive. Consequently such a small file may easily be sent anywhere by e-mail. Of course the influence of the internet upon the work of palynologists can hardly be overlooked (Maher 1993b). It may be that the development of the XML language (Harold 1999) and its graphical possibilities will improve the exchange of data and ideas, which is very important in science.

CLOSING REMARKS

An idea of computer assistance in pollen counting, pollen data storage, diagrams plotting, numerical analysis, and geographical presentation of pollen data is not new. However, some particular concepts applied when embedding general ideas into practice (into computer codes) were given here. (1) The users and producers of data handling system are usually two groups which, however, should overlap. (2) The data handling system must be internally consistent and, at the same time should be open for import and export of data in almost every step. Basic standards of computer operational systems (we use MS Windows) are to be applied. (3) Some statistical (numerical) methods are not easy in their background, it is disputable to which extent such methods may be used "mechanically" by clicking buttons. (4) Reliability of obtained results has to undergo to some criticism. The statistical and other errors of the data analysed are to be realized. The danger is that rule seems to appear: the easier is to obtain an analysis result the less critical is the author. Computer has very limited responsibility.

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