

ISOPLOT for MS-DOS
A PLOTTING AND REGRESSION PROGRAM FOR
RADIOGENIC-ISOTOPE DATA, FOR
IBM-PC COMPATIBLE COMPUTERS
Version 1.00

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This report is preliminary and has not been reviewed for conformity with U.S. Geological Survey editorial standards and nomenclature. Any use of trade names is for descriptive purposes only, and does not imply endorsement by the U.S. Geological Survey.

Although this program has been extensively tested, the U.S. Geological Survey cannot guarantee that it will give accurate results for all applications, nor that it will work on all computer systems.

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K.R. Ludwig, U.S. Geological Survey

INTRODUCTION

ISOPLOT is a program designed primarily for radiogenic-isotope geochemists, may be useful for plotting or regressing any X-Y data in a simple, flexible manner. Data can be entered either from the keyboard or from ASCII files produced by spreadsheet or word-processing programs, and can be plotted as a variety of symbols, including various error-symbols and polygons. ISOPLOT can regress data using a modification of the most-widely used two-error regression algorithm, and will calculate isochron ages directly from the regression lines.

In addition to the basic X-Y plotting and isochron calculation functions, the program can also:

- * construct concordia ($^{206}\text{Pb}/^{238}\text{U}$ - $^{207}\text{Pb}/^{235}\text{U}$) plots and calculate concordia-intercept ages and errors;
- * construct single-stage growth-curves for plots of common-Pb data;
- * calculate and construct plots for weighted averages of a single variable;
- * calculate useful isotopic functions such as radiogenic $^{207}\text{Pb}/^{206}\text{Pb}$ ages, common-Pb model ages, Nd and Sr model ages, and ages from the secular global-marine Sr-isotope trend;
- * do curvilinear (polynomial) regressions for X-Y data (weighted or unweighted);
- * fit a smooth curve (either precisely or in a least-squares sense) to data of arbitrary complexity using spline curves;

The pedigree of ISOPLOT extends back several years, starting with programs written in the mid 70's for HP-9830/9831 computers, in the early 80's for HP-86/87 computers (Ludwig, 1983), and most recently for

HP Series 200/300 computers (ISOPLOT VERSION 2; Ludwig, 1987). This version of ISOPLOT is largely a translation, into the QuickBasic 4.0 language, of a subset of ISOPLOT VERSION 2. Compared to the version for Hewlett-Packard computers, ISOPLOT for MS-DOS lacks several capabilities, including:

- 1) Support for a plotter,
- 2) Extensive HELP screens,
- 3) Logarithmic, histogram, and REE-plots, and
- 4) Simplex curve-fitting.

On the other hand, ISOPLOT for MS-DOS offers high-quality color graphics on the CRT (if an EGA or VGA screen is used), significantly faster execution times (for 80286- or 80386-based computers with a numeric coprocessor), simpler and more rapid datafile access, and compatibility with files generated by PBDAT for MS-DOS (Ludwig, 1988). Support for HP plotters and/or Laser printers are planned for future revisions.

To obtain a disk containing ISOPLOT for MS-DOS, write directly to me (K.R. Ludwig, U.S. Geological Survey, Denver CO, 80228) and enclose a disk formatted on your system. You may also request the source-code (as an ASCII file on your formatted disk); the code is lengthy, however, and in a less-common dialect of BASIC.

HARDWARE REQUIRED BY ISOPLOT for MS-DOS

ISOPLOT for MS-DOS was written for IBM-PC compatible computers, and supports CGA, EGA, and Hercules graphics modes, and a numeric coprocessor (all optional). You should have at least 512 kilobytes of RAM. The program assumes the presence of a printer at parallel port LPT1, though only Epson-compatible dot-matrix printers will produce graphics dumps.

GETTING STARTED

LOADING THE PROGRAM

If you have a hard disk, transfer the program together with its sample datafiles to a subdirectory on the hard disk. First, set the default disk and directory to be that of ISOPLOT. Type ISOPLOT, then press the ENTER (or RETURN) key to start. As sent to users, this will

First, select whether you want the output sent to the screen or the printer with the F9 key. Look at the lower-right of the screen to see what the current status is. Notice that the function-key labels will always be the opposite of the status display, because the function key labels indicate what the key will do when pressed, not what the current status is.

For color screens, select whether you want your display in color or monochrome. For some CGA-graphics screens, and for all monochrome Compaq computers, you'll get better results specifying monochrome output.

If you're using a Texas Instruments computer running under Romberg's EMULATE program, turn off the sound (F2) before you do anything else. Attempts to use the computer's speaker will crash the TI. Even better, invoke ISOPLOT with ISOPLOT TI rather than just ISOPLOT. This will eliminate even accidental use of the speaker.

If you don't need graphical output of your data, press F3 to cancel the graphics. The output will be more rapid and, for CGA screens, more legible if no graphics are used.

At the lower left of the starting screen, ISOPLOT indicates the error-format that will be assumed. The default format is for errors to be entered in percent, and at the 2-sigma (or 95%-confidence) level. You can toggle between percent and absolute errors with the F5 key.

CHOOSING THE AXIS NAMES

When you've finished selecting the physical parameters of the plot with the function keys, as described above, press either X or the ENTER key. The screen will then be:

X-Y PLOT

X-Axis Label ==> X
Y-Axis Label ... Y

Lower-Limit of X ... 0
Upper-Limit of X ... 10

Lower-Limit of Y ... 0
Upper-Limit of Y ... 10

F1 Beta/Alpha F2 Gamma/Alpha F3 Rb/Sr F4 Sm/Nd

F9 Recall Esc Exit Form ENTER Enter Response CTRL-ENTER Done

To fill out this "form", move the cursor with the arrow-keys, enter your responses, and press **ENTER** (or **RETURN**). When you've entered all the values, press **CTRL-ENTER** (or **CTRL-RETURN**) to "submit" the "form".

The X- and Y-axis labels are the labels that will appear below the X-axis and to the left of the Y-axis; the X- and Y- limits define the minimum and maximum limits of the plot's X- and Y-dimensions.

You can specify some of the more-common axis names with the **F1-F4** keys, giving you the axis names for, respectively, a $^{207}\text{Pb}/^{204}\text{Pb}$ versus $^{206}\text{Pb}/^{204}\text{Pb}$ plot, a $^{208}\text{Pb}/^{204}\text{Pb}$ versus $^{206}\text{Pb}/^{204}\text{Pb}$ plot, an Rb-Sr isochron plot, or an Sm-Nd isochron plot.

If data from a datafile were already loaded into memory when the "form" appeared, the default axis names will be the column-headings for the datafile, and the axis limits will be the extreme values from the datafile. In this case, you might not need to enter anything into the form yourself -- just press **CTRL-ENTER**.

When you've entered the above form, **ISOPLOT** will draw the plot-box with labelled axis-ticks and labelled axes, and wait for you to specify data to be plotted.

PLOTTING DATA-POINTS

THE SELECT PLOTTING-SYMBOL SCREEN

After ISOPLOT has constructed the plot box, tick labels, and axis names, you're ready to start plotting your data. First, though, you must specify a plotting symbol. The screen will show:

PRESS A KEY TO SPECIFY A PLOTTING-SYMBOL...

<u>E</u> Error Ellipse	<u>C</u> Error Cross
<u>B</u> Error Box	<u>P</u> Polygon
<u>S</u> Square Box	<u>X + * .</u>

Symbol Color#14 ** (change with U/D arrows)

<u>F4</u> Label		
<u>F5</u> Dump Graphics	<u>F8</u> Datafile	<u>F10</u> Alpha/Graphics

I'll refer to this as the SELECT PLOTTING SYMBOL screen. You can do several things from this part of the program besides just selecting a plotting symbol, but for now we'll ignore them. As soon as you specify a symbol (by pressing E, C, B, P, S, X, +, *, or a period), ISOPLOT will ask you for the data to be plotted. If you have an EGA or VGA color screen, you can change the color of the plotting-symbols (with the Up/Down arrow keys, and the background color of the plot with the PgUp/PgDn keys¹.

¹Use ALT Up/Dn arrows for TI computers to change the background color.

POLYGON PLOTTING--SYMBOL

You can use a polygon for a plotting symbol, with any number of sides, size, and rotational orientation by pressing the P key. The screen will then query:

POLYGON SYMBOL:
 ENTER #SIDES, [,SIZE (mm) [,ROTATION (0-360)]...

The parameters in brackets represent optional input, so you can enter either 1, 2, or 3 values (or press ENTER to specify the values that were used last). The number of sides can vary from 3 (a triangle) to a large number. The SIZE parameter refers to the diameter of the polygon in millimeters; default is 2.5. The ROTATION parameter refers to the angular orientation (counter-clockwise from the X-axis) of a vertex of the polygon: 0 gives a vertex at 3 o'clock, 45 a vertex at 1:30, 90 a vertex at 12:00 and so on. The default value depends on the number of sides of the polygon, and gives "conventional" orientations (triangle pointing straight up, square with sides parallel to the X and Y axes, pentagon pointing straight up...).

If you enter the number of sides of the polygon as a negative value, the polygon will be drawn "puckered in" at each side, so the result is a "star"-shaped figure. For example, if you specified the number of sides as -5 instead of just 5, the plotting symbol will be a 5-pointed star.

PLOTTING SYMBOLS THAT INDICATE ERRORS

There are three plotting symbols that you can use to show the errors of the points on the plot: error box, error cross, and error ellipse. If you select one of these symbols, the program will need estimated errors for each of the data points. If you select the error ellipse symbol, the ISOPLOT will also need values for the X-Y error correlations. If you don't know how to estimate an error correlation, use this equation:

$$\text{Rho} = (E_x^2 + E_y^2 - E_z^2) / (2E_x E_y)$$

or:

$$E_z^2 = E_x^2 + E_y^2 - 2E_x E_y \text{Rho}$$

where Rho is the correlation between the X and Y errors, E_x , E_y , and E_z are the percent errors in X, Y and Z, and where $Z=Y/X$. For example, if X were $^{206}\text{Pb}/^{204}\text{Pb}$ and Y were $^{207}\text{Pb}/^{204}\text{Pb}$, then Z would be $^{207}\text{Pb}/^{206}\text{Pb}$. Or, if X were $^{207}\text{Pb}/^{235}\text{U}$ and Y were $^{206}\text{Pb}/^{238}\text{U}$, then Z would be

$R^{207}\text{Pb}/^{206}\text{Pb}$ ($R = \text{natural } ^{235}\text{U}/^{238}\text{U}$). Error correlations are zero if the error in Y doesn't tend to increase with the error in X. If the error correlations are much greater than about 0.5, don't use error box or error cross symbols, because these symbols will convey a misleading impression as to the actual area of uncertainty around the data point.

ENTERING DATA FROM THE KEYBOARD

As soon as you select a plotting symbol, the screen will change to:

Enter datafile sets as first#, last#, *; break series w. semicolon
(example: 2,12;14,16* for sets 2 thru 12 + 14 thru 16)
Errors are 2-sigma, in percent

Set#	Name	$^{87}\text{Rb}/^{86}\text{Sr}$	%err	$^{87}\text{Sr}/^{86}\text{Sr}$	%err	Rho
------	------	---------------------------------	------	---------------------------------	------	-----

SET# 1 - ENTER X [,%err,], Y [,%err [,err-correl.]] (ENTER when done)

F9 Recall F7 All Points F8 Datafile F10 Alpha/Graphics

The axis names and plotting symbols shown above are only examples, of course, and the information about datafile sets will appear only if you've loaded a datafile into memory.

To enter the X- and Y-values for your data points, type in the two numbers, separated by a comma, then press the ENTER key. To include the errors with the points (you'll need to include errors for plotting symbols that reflect errors or for Yorkfits), enter 4 values separated by commas, in the format X, X-error, Y, Y-error. Remember to use the correct error-format (percent or absolute, at the 2-sigma/95%-confidence level), which you specified from the starting screen. If no error correlations are entered (as the optional 5th value), they're assumed to be zero. If the errors for all of the points are going to be the same, don't bother entering them at this point -- you can enter them as a group later. You can look at the last several entries you've

made, incidentally, by pressing the **RECALL** key (**F9**).

When you've entered all of the points that you want plotted with the plotting-symbol or color that you chose earlier, press **ENTER**. If you're using an error-symbol (error box, error cross, or error ellipse) as the plotting symbol and you didn't enter error-values for some or all of the samples, **ISOPLOT** will ask you for blanket errors:

ENTER X-errs, Y-errs, [,Err.-Corr.] for sets with unassigned errors...

Enter the 2 or 3 values requested. Note that, again, the error correlation is an optional value, and note also that the assigned errors must be nonzero.

The screen will then display a list of the data-point values that you just entered, and query:

ENTER Set# to be edited? (ENTER when done):

Check the displayed list for mistakes. If there are any, enter the set# (shown to the left of the X- and Y-values) of one of the incorrect data-points. Enter the correct values, when requested, then continue with the editing process until all of the values are correct. Press **ENTER**, and the data points will be plotted.

THE ADD POINTS SCREEN

After the data points are plotted, this screen will appear:

A Plot more points, adding to existing set

R " " " , replacing " "

Esc Start a new plot

E End ISOPLOT

Y Yorkfit

F9 PolyFit

F6 Splines

F7 Connect Symb

F4 Label

F5 Dump Graphics

F8 Datafile

F10 Alpha/Graphics

At this point, you can choose to plot more points, do a Yorkfit, abandon the current plot and start a new one, or perform some operations on the plotted data. You can toggle between the graphics display and the alphanumeric display (shown above) with the F10 key. If you press R, the program will return to the **SELECT PLOTTING SYMBOL** screen, and any additional data-points that you enter will be counted as a new batch for any subsequent regressions.

But if you want to plot more points (perhaps with a different plotting-symbol or color) that are to be pooled with the just-plotted points for a later Yorkfit (or other regression), press A.

CONNECTING DATA POINTS WITH A LINE

You can connect each data point on your plot with a straight line by invoking the "Connect-the-dots" function from the **ADD POINTS** screen (press F7). The data points will be connected from the smallest X-value to the largest X-value.

LABELING WORDS OR PHRASES ON THE PLOT

You can have ISOPLOT put a phrase anywhere on the plot by pressing F4 from the SELECT PLOTTING-SYMBOL screen or from the ADD POINTS screen. Type in the phrase, then locate the phrase using the arrow-keys (shifted for gross movement, unshifted for fine movement). Press ENTER to fix the phrase on the plot, or Esc to cancel.

STORING AND RETRIEVING DATA FROM DATA FILES

You can use ASCII files to store data that ISOPLOT can read, provided that you use the following format:

- 1) data must use a row-column format where the rows are used for data for different samples, and the columns for different parameters or measurements for those samples;
- 2) the column-width must be 9 characters (the LOTUS default);
- 3) the column names must appear above any data, and directly overlie a line of repeating equals-signs (=====). There must be 9 equals-signs for each column;
- 4) the column names may occupy up to 18 characters;
- 5) the first 18 characters can be used for sample names only;
- 6) no more than 50 columns and 150 rows are allowed;
- 7) the first row of the file can be used as a file title (up to 80 characters) to identify the file;
- 8) the file must be stored with a left-margin of 0 and a right-margin large enough to include all of the columns of data;
- 9) the file must have the extension *.PRN (the Lotus default for ASCII files).

ACCESSING DATAFILES

To get data from a datafile, press the function key labeled GET DATAFILE from either the starting screen or the SELECT PLOTTING SYMBOL screen. The screen will then show a catalogue of all of the *.PRN files in the current drive\path. If there are no *.PRN files in the current disk\path, you'll have to specify the correct one. When the screen shows a list of the *.PRN files for the drive\path that you specified, select a file with the cursor keys and ENTER.

Once you've chosen a datafile, the computer will search for and display a list of all of the column-names (column headings) for that file. Select either 2 columns (X and Y; or, if doing weighted averages, Y and Y-error), 4 columns (X, X-error, Y, Y-error), or 5 columns (X, X-error, Y, Y-error, X-Y error-correlation).

ISOPLOT will retrieve the data for those columns from the disk, and display the data on the screen¹. If you had pressed F6 (PRINTER OUTPUT) before loading the file, the data would also be printed out.

USING DATA FROM DATAFILES

To plot from a datafile, you'll need to specify which data-points by with "set numbers", where the set number of a data point corresponds to its row in the spreadsheet (the first row below the double-equals signs is for set number 1), and is printed out when the datafile is first accessed by the program. For example, after you've selected a plotting symbol, the screen will show:

Enter datafile sets as first#, last#, *; break series w. semicolon
(example: 2,12;14,16* for sets 2 thru 12 + 14 thru 16)

To plot the data for set number 5, enter 5*. To plot data for sets 5, 6, 7, 8, and 9, enter 5,9*. To plot data for sets 5, 6, 7, 8 and 11 and 15, 16, 17, enter 5,8;11;15,17*. In other words, indicate continuous sequences of sets with a comma, separate different continuous sequences (or individual sets) with a semicolon, and always add an asterisk at the end. It's OK to mix data from datafiles and typed-in input. You can also plot data from several different datafiles by pressing A(dd) after each plot, then switching datafiles.

¹To save time after recovery of a long file, you can suppress the display of the sample names and data by pressing any key as the data are being displayed.

If you want to plot all of the datafile's data, press F7 (All Points) or F6 (same as F7, but doesn't display the data for the points on the screen).

YORKFITS OF DATA

YORKFIT "MODELS"

A "Yorkfit" refers to a linear regression using the general algorithm developed by Derek York (York, 1969). This algorithm weights each point according to both its X- and Y-errors, and also takes into account the X-Y error-correlations. ISOPLOT uses both the original York algorithm, and also a few modifications, depending on the type of data you're working with and the amount of scatter of the data. Each of these modifications, called MODELS by the program, makes different assumptions about the reason for the scatter of the points about a straight line.

MODEL-1 Yorkfits: -- The MODEL-1 Yorkfit is York's original algorithm, and assumes that the only cause for scatter from a straight line are the assigned errors. The points are therefore weighted proportional to the inverse-square of these errors. A test of the MODEL-1 assumption is provided by the **PROBABILITY OF FIT** value calculated by the program. If this value is reasonably high (more than 15% to 20%), then the MODEL-1 assumptions are probably (but not certainly) justified. If this probability is low (less than 20% or so), however, you may choose another model. The MODEL-1 errors are calculated using the maximum-likelihood algorithm of Titterton and Halliday (1979).

If you select the MODEL-1 fit even though the **PROBABILITY OF FIT** is close to zero, you are in effect requesting that the actual errors be calculated from the observed scatter (thus invoking the use of the Student's-t multiplier to convert from estimated errors to 95%-confidence errors), and you are also specifying that the true errors and error-correlations of the data points are for some reason directly proportional to the ones you have assigned to them. This is an important point, though seldom acknowledged.

ISOPLOT will always attempt a MODEL-1 fit first. In the print-out, the A PRIORI errors are the errors in the slope and intercept calculated by propagating only your assigned errors for the points; no matter how much the points scatter, the A PRIORI errors will not increase. The INCLUDING SCATTER errors, however, are calculated from the actual scatter of the points from a line, and are independent of the

assigned errors. These errors, given at the 1-sigma level, are provided mainly for comparison purposes with the output of other, simpler implementations of York's algorithm. *The only geologically useful errors are the ones given as 95% CONFIDENCE-LIMIT errors.*

How the 95% confidence-limit errors are calculated depends on the probability that the assigned errors for the points can account for the observed scatter. If the probability is greater than 0.15, the 95% confidence-limit errors are simply 1.96 times the A PRIORI errors (1.96 is the Student's-t value for an infinite number of points -- the reason for this is discussed by Brooks and others, 1972).

MODEL-2 Yorkfits: -- A **MODEL-2** Yorkfit assigns equal weights and zero error-correlations to each point. This is probably seldom justified by any real mechanism, but at least avoids the mistake of weighting the points according to analytical errors (see above discussion on Model-1 regressions) when it is clear that, in fact, some other cause of scatter is involved. The 95% confidence-limit errors are calculated from t times the INCLUDING SCATTER errors. If you know little or nothing about the dominant cause of the scatter of the points, and about the statistical form of that cause, you should probably use this model.

MODEL-3 Yorkfits: -- A **MODEL-3** Yorkfit assumes that the scatter is due to a combination of the assigned errors plus a normally-distributed variation (of unknown magnitude) in the Y-values. This model (which is similar to the Model-3 algorithm of McIntyre and others, 1966) may be realistic in the case of Rb-Sr and other isochron data for rocks whose initial ratios were variable. For this model, the program will solve for the unknown Y-variation as well as for the best-fit line, so you can judge whether or not the solution is realistic.

Remember, though, that it is physically quite possible (perhaps even likely) that the initial ratios of the samples were significantly correlated with their Rb/Sr (or other parent/daughter ratio), in which case the **MODEL-3** assumptions are not valid. For a good example of such a case, see Juteau and others, 1984.

MODEL-3 is offered as an option if the program recognizes, from numbers in the axis names, that you're plotting isochron data for Rb-Sr, Sm-Nd, U-Pb (either 206/204-238/204 or 207/204-235/204), or Th-Pb. The 95% confidence-limit errors are calculated from t times the INCLUDING SCATTER errors.

MODEL-4 Yorkfits: -- A **MODEL-4** Yorkfit is used only for U-Pb isotope data on a concordia diagram. This model assumes that the points scatter due to a combination of the assigned errors plus "geological" errors in the $^{207}\text{Pb}/^{206}\text{Pb}$ ratios. These "geological" errors are assumed to increase linearly from the upper concordia-intercept to the lower

concordia-intercept (or vice-versa; see below). This model (see Davis, 1982, for another approach to this problem) may be appropriate for cases where a multi-episodic disturbance is suspected (in which case the closer the point to the upper intercept the greater its weight), and for cases where a significant degree of inheritance of older zircons is suspected (in which case the closer the point to the lower intercept the greater its weight). You may choose whether the lower concordia-intercept (press L for Model-4 LI) or the upper concordia-intercept (press U for Model-4 UI) is to be the age of interest.

The MODEL-4 Yorkfit is offered only for data sets with 6 points or more. The 95% confidence-limit errors are calculated by multiplying the INCLUDING SCATTER errors by the t value for $N'-2$ degrees of freedom, where N' is a number that is in general less than the actual number of points. This approach is necessary because of the way in which the MODEL-4 algorithm weights the points -- the more concordant that point, the greater its weight. In the extreme case, with 2 nearly-concordant points plus any number of much less concordant points, the algorithm will in effect pay attention only to the two most-concordant points and ignore the others. Obviously, in this case the true degrees of freedom are much less than the apparent degrees of freedom. To compensate for this effect, N' is calculated by assigning each of the two most-concordant points a "point value" of 1, and the assigning the remaining points a fractional "point value" based on their MODEL-4 weights; the less their MODEL-4 weight, the smaller a fraction of a whole "point" is assigned.

The effect of this procedure is to drastically reduce the degrees of freedom assigned to many data sets, especially if 1 or 2 of the points in the set are much more concordant than the rest. So the data sets which are most appropriate for the MODEL-4 approach are those with a large number of points that are relatively evenly-spaced along a linear trend. Data sets with few points will tend to have MODEL-4 errors that are very large, due to the large (up to several tens or even hundreds) Student's-t multiplier invoked. You can tell the value of N' used by the algorithm from the printout, which refers to the NUMBER OF EQUIVALENT "POINTS".

OBTAINING ISOCHRON AGES FROM YORKFIT LINES

If your plot is an isochron plot (including Rb/Sr, Sm/Nd, $^{207}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$, $^{207}\text{Pb}/^{206}\text{Pb}$ - $^{204}\text{Pb}/^{206}\text{Pb}$, $^{206}\text{Pb}/^{204}\text{Pb}$ - $^{238}\text{U}/^{204}\text{Pb}$, $^{207}\text{Pb}/^{204}\text{Pb}$ - $^{235}\text{U}/^{204}\text{Pb}$, and $^{208}\text{Pb}/^{204}\text{Pb}$ - $^{232}\text{Th}/^{204}\text{Pb}$), the computer will automatically calculate an isochron age and error from the Yorkfit results. The decay constants used are those recommended by the I.U.G.S. Subcommittee on Geochronology (Steiger and Jäger, 1977), though you can change them if you wish (see CHANGING DECAY CONSTANTS

AND MODEL-AGE PARAMETERS). Sm-Nd isochron regressions will also yield the calculated ϵ_{CHUR} for the initial ratio.

A WORD ABOUT 3-POINT ISOCHRON

You should be aware that the actual uncertainties of isochron ages for regression lines with only 3 or 4 data points and no apparent "geological" scatter can be significantly greater than the uncertainties calculated by most regression algorithms, including that of ISOPLOT. The reason for this is that with only 1 or 2 degrees of freedom (3 or 4 data points), the probability of getting an MSWD¹ of close to 1 even though some "geological" scatter exists in the population is significantly greater than zero. For such data sets, the lack of statistical resolution of this "geological" scatter can be expected to occur in a significant number of cases, and, because the use or non-use of a very large (12.7 for N=3) Student's-t multiplier is involved, can lead to a large underestimate of the true isochron uncertainties. For this reason, you should avoid the use of 3-point isochrons or concordia chords if possible.

WHY ARE ISOPLOT'S ERRORS FOR CONCORDIA-INTERCEPT AGES SO LARGE?

Occasionally, a user will comment that the concordia-intercept errors from ISOPLOT seem unreasonably high, especially compared to published errors calculated by other methods. The answer usually is that the other methods involve invalid assumptions or incomplete methods, such as:

- 1) Confusion between whether a given regression program is asking for 1-sigma or 2-sigma/95%-confidence errors.

If one responds with 1-sigma errors when the program is expecting 2-sigma errors, and if the MSWD of the regression is not much more than one, the resulting errors will be too low by a factor of 2.

- 2) Incorrect assignment of error correlations.

Normally, data on the concordia diagram are very highly cor-

¹MSWD = Mean Square of Weighted Deviates. This does not refer to porcine perverts; essentially, it is the ratio of the observed scatter of the points from the best-fit line to the scatter predicted by the assigned errors of the points. If the assigned errors are the only cause of scatter, the MSWD will be near 1.

related - typically in the range of 0.99 to 0.99999. If some arbitrary value such as 0.7 or 0.9 or even (God forbid) 0 is used, the mathematics of the York algorithm will, in effect, assume a much larger radiogenic $^{207}\text{Pb}/^{206}\text{Pb}$ than is probably the case. For example, if X- and Y-errors of 1% are assigned together with an error-correlation of 0.7, the implicit error in the radiogenic $^{207}\text{Pb}/^{206}\text{Pb}$ is 0.77% -- much larger than the typical errors of .05% - .10%. As a result, the MSWD of the regression may be grossly underestimated (with especially dramatic possible effects on 3- or 4-point chords).

Pb-isotope data are also usually very highly correlated, with the exception of data for those 207/206 versus 204/206 plots where the 204/206 ratio is much less precise than the 207/206 ratio. Note that this is not the case for 207/206-204/206 data for common Pb, where almost all of the errors generally arise from the mass-fractionation uncertainty of the analysis.

- 3) Use of 2-sigma (or even worse, 1-sigma) regression uncertainties instead of 95%-confidence limit.

It seems to be a little-appreciated fact that "1-sigma" errors for small ($n < 10$) data-sets do not in themselves say anything about a confidence limit. They are not even the "true" standard deviations of the regression parameters (slope, intercept...) -- just the best estimate of the standard deviations for that data set, and in fact have a significant uncertainty in themselves. The smaller the data set, the larger the this uncertainty becomes.

Statisticians dealt with this problem long ago by using only confidence limits for small data-sets to indicate the real uncertainty in a derived parameter. Confidence limits are obtained by multiplying the estimated "1-sigma" errors by a numerically-derived fudge-factor ("Student's-t"). Student's-t factors are a function of the degrees of freedom of the data-set (N-2 for a linear regression) and the confidence level of interest. For a large number of points, the 95%-confidence limits and the 2-sigma errors become very similar. By scientific convention, this confidence limit is usually at the 95% level (so the true value will lie outside the 95%-confidence limits only 1 time out of 20). It is my contention, as well as that of many other careful workers, that use of "1-sigma" regression errors for small data-sets borders on deliberate deception. In the worst case (a 3-point regression), the 1-sigma errors are a factor of almost 13 smaller than the 95%-confidence errors, and offer little in the way

of useful geologic constraints.

- 4) Calculation of the concordia-intercept uncertainties from only the propagated slope error, while ignoring the contribution from the propagated intercept or centroid error.

This error was common in the past, and still occurs from time to time. Its effect is greatest for data points whose centroid lies close to the concordia curve (if one ignores the centroid uncertainty, then no matter how much scatter exists, if the centroid falls on concordia the calculated intercept-error will be zero).

- 5) Calculation of the slope- and intercept-errors from only the propagated analytical errors but ignoring the scatter of the points.

If one is sure that the only reason for the scatter of the points can be the analytical errors, then it is true that the appropriate way of estimating the regression-line errors are by simply propagating the analytical errors, without even the application of the Student's-t factor (though Student's-t should have been used in the calculation of the analytical errors!). In many real-world instances, however, it is quite clear that the analytical errors are not the cause of most of the scatter (the probability figure shown in ISOPLOT's print-out can be used as a guide). In such cases, it is evident that the precision of the regression line should reflect the actual scatter of the points, for example by multiplying the a priori errors by the square root of the MSWD parameter. There are still programs in use, however, which ignore the scatter of the points even when this scatter grossly exceeds that predicted by the analytical errors. Such a procedure is almost literally nonsense.

FITTING A CURVE TO DATA

POLYNOMIAL CURVES

To request a polynomial regression on data you've just plotted, press **F9** from the ADD POINTS or SELECT PLOTTING SYMBOL screens and specify the order of the polynomial for regression (1 to 6). This regression (Figure 1) weights the points equally, uses the Y values as the dependent variables and the X values as the independent variables.

SPLINE CURVES

If a polynomial curve doesn't adequately describe the trend of the data, you may want to try fitting a spline curve (**F6** from the ADD DATA or SELECT PLOTTING SYMBOL screens). Examples of spline curves are shown in Figures 2 and 3. The SPLINES menu offers the options below:

F1 HELP	F2 Akima Spline		
F3 Normal Spline	F4 Smooth Spline	F5 Sr Ages	F10 Alpha/Graphics

A spline curve is a collection of cubic polynomials that connect a set of X-Y points without breaks in slope. Two disadvantages of spline curves are that (1) there is no convenient analytical expression for them (because they're a collection of many different polynomials), and (2) there is no really satisfactory analytical expression for the

error of the curve.

Akima Splines (Akima, 1970) will yield a curve that may bend sharply towards the next point, as the curve proceeds from left to right. This type of curve is especially suitable if you believe that data-points strongly constrain the local location of the curve. The **Akima Spline** option will also construct curves through the upper and lower Y-error limits if you specified errors when you plotted the data. The X-errors will be ignored, though.

Normal Splines tend to curve less sharply than the **Akima Splines**, though at the expense of possible overshoots and oscillatory artifacts. Try both types of splines to see which is the most useful for your data.

If you don't want the spline to be forced through every point, because you've plotted a large number of points that scatter about any reasonable curve, use the **Smooth Spline** option. A **Smooth Spline** is constructed through the points in a least-squares sense, and is especially useful for data sets with significant scatter due to geological or analytical error.

You'll have to specify the minimum X-interval over which the curve-segments will "pay attention" to the data, and the minimum number of points to be used for each segment. The curve is constructed as a sort of moving average, in which only a quarter of the curve-segment is drawn for each least-squares fit. The larger the X-interval specified and the larger the minimum number of points for each interval, the more "smoothed" the curve will be. Experiment.

You also have the option of plotting the "error-envelope" of the smoothed spline. This "error envelope" is another pair of spline curves that should enclose most of the data points defining the smoothed spline, and will pinch and swell according to the local scatter of points along the spline. This envelope does not have rigorous statistical significance, however, and should be used mainly as a visual guide to the precision of the curve.

CREATING CONCORDIA PLOTS

If your plot is a conventional concordia plot (Figure 4), with $^{206}\text{Pb}/^{238}\text{U}$ plotted against $^{207}\text{Pb}/^{235}\text{U}$, you'll find a few differences from the normal X-Y plotting routines. To select a concordia plot, press C from the starting screen. You can then either specify the plot limits in terms of minimum and maximum ages to be shown, or (by pressing F1) define the limits of the concordia plot in terms of its X- and Y-limits.

When you request a Yorkfit through data on a Concordia plot, the program will automatically calculate the intercepts of the Yorkfit line with the concordia curve, and the uncertainties of those intercepts. These uncertainties are calculated using the algorithm developed by Ludwig (1980), and are printed out in two forms: symmetrical but approximate uncertainties, and the more accurate, asymmetric uncertainties. You can choose which to use.

FORCING A YORKFIT LINE THROUGH A SPECIFIED AGE

You can force a Yorkfit through a specified age on the concordia curve from the **ADD POINTS** screen by pressing F (forced Yorkfit) instead of Y. **ISO PLOT** will ask you what age (in Ma) to force the next Yorkfit through, and what uncertainty to assign to this forcing age. The uncertainty value is optional -- if you enter only one value, the uncertainty in the forcing age will be assumed to be zero. If you do enter an uncertainty value, the program will calculate the Yorkfit line and concordia intercepts three times, forcing the line through not only the forcing age but also the forcing age plus and minus its assigned uncertainty. The propagated uncertainties in the unforced intercept arising from this procedure will be included in the final age-uncertainties of the unforced intercept.

The uncertainty in the forcing age is assumed to be symmetric; that is, you can't enter a forcing age with uncertainties of +100 Ma and -50 Ma.

After any Yorkfit regression, the program will calculate the concordia intercepts of the Yorkfit line and its associated uncertainties, using the algorithm of Ludwig (1980). These intercepts will be labeled on the lower-right corner of the plot, with the labels for each successive solution for a given plot stacked on top of the previous labels.

CONSTRUCTING A CONTINUOUS-DIFFUSION CURVE FOR COUPLED LOSS OF RADIOGENIC-Pb AND ^{238}U RADIOACTIVE DAUGHTERS

Some systems -- notably low-temperature uranium ores and low-temperature uraninite (pitchblende) and coffinite -- continuously leak both radiogenic-Pb and one or more of the several radioactive daughters of uranium. I have noted that for many such systems, the ratio of the leakage of Pb to the radioactive daughters must have been roughly constant over the age of the material, so that a particular type of continuous-diffusion curve can be useful in evaluating the age of the material (Ludwig, Simmons, and Webster, 1984).

To construct such a curve, press F9 from the SELECT PLOTTING-SYMBOL or ADD POINTS screens. ISOPLOT will ask you to specify the age of the system and the ratio of diffusion constants for Rn compared to Pb, divided by 10^{10} . Radon may not, in fact, have been the actual daughter that was leaking out of the system (Radium seems to be the dominant wanderer in many cases), but the shape of the curve is the same for any daughter. Try diffusion-constant ratios in the range of .5 to 10 ($\times 10^{10}$) to get a feeling for the shape of the curves. For any specific set of data points, you'll have to find the best-fit curve by a trial-and-error process of varying the assumed age of the system and the assumed diffusion-constant ratio. There is no provision for estimating errors.

OBTAINING GROWTH CURVES FOR Pb-ISOTOPE PLOTS

If your plot is either for $^{207}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$ or for $^{208}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$, and you want ISOPLOT to construct a single-stage Pb-isotope growth curve on the plot (Figure 5), press F9 (Growth Curve) from the SELECT PLOTTING-SYMBOL screen. You must then select:

-
- S Stacey-Kramers Growth-Curve
 - O Other Growth-Curve (you specify)
 - Esc No Growth-Curve
-

If you press S, the program will draw a single-stage Pb-isotope growth-curve using the constants suggested by Stacey and Kramers (1975). If you press O, the program will ask you to define your own single-stage growth curve, requesting: (1) the starting age of the system, (2) the initial isotope ratios, (3) the μ^1 of the source, and, for $^{208}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$ plots, (4) the Th/U of the source. The screen will look like this:

SINGLE-STAGE Pb-ISOTOPE GROWTH-CURVE

```

                206/204 at start of growth .... 11.152
                208/204 at start of growth .... 31.230
    Mu (present-day 238/204) of source ==> 9.74
                Present-day 232/238 or source .... 3.78
    Time before present (Ma) at start of growth .... 3700
    (add an asterisk to specify a starting-
     age on the current growth-curve)
  
```

```

F5 Restore Stacey-Kramers
F9 Recall   Esc Exit Form   ENTER Enter Response   CTRL-ENTER Done
  
```

Use the arrow-keys to move the cursor to the value you want to change, type in the value and press ENTER. You needn't change values which are already acceptable. To restore the values in the form to the standard Stacey-Kramers values (Stacey and Kramers, 1975), press F5.

If you want to start a new growth curve at some particular age on the growth curve defined by the parameters first appearing on the screen, you can have the program calculate the appropriate 206/204 and 207/204 or 208/204 ratios for this age by entering the age with an asterisk in the "Time...at start of growth" cell. For example, if you wanted to construct a growth curve that started from the Stacey-Kramers curve at 2700 Ma and evolved with a μ of 12, you would:

- 1) press F5 to restore the Stacey-Kramers values (if the initial values on the screen were not the Stacey-Kramers values);
-

¹ μ is defined as the $^{238}\text{U}/^{204}\text{Pb}$ of the system, normalized for U-decay to the present day.

- 2) type in 2700* in the "Time..." cell and press CTRL-ENTER. The 206/204 and 207/204 or 208/204 values immediately change to the values defined by a 2700 Ma age on the Stacey-Kramers growth curve;
- 3) enter a value of 12 in the "Mu" cell and press CTRL-ENTER.

Once you select a growth curve the screen will show:

- T Suppress Ticks and Tick-Labels
- L Suppress Tick-Labels Only
- C Draw a Complete Curve with Labeled Ticks
- Esc No Growth-Curve

Because the plot may become too "busy" if the age-ticks and age-tick labels of the growth curve are included, you can select how much labeling you want to include.

If you request a Yorkfit for data on a $^{207}\text{Pb}/^{204}\text{Pb}$ - $^{206}\text{Pb}/^{204}\text{Pb}$ plot that contains a growth curve, ISOPLOT will solve for the growth-curve intercepts as well as the $^{207}\text{Pb}/^{206}\text{Pb}$ age of the Yorkfit line.

CALCULATING WEIGHTED AVERAGES OF A SINGLE VARIABLE

You can use ISOPLOT to calculate weighted averages of a single variable by pressing A from the starting screen. ISOPLOT will then ask for data and errors for only one variable rather than two, will use the Y-axis to show that variable, and use the X-axis to show the "set number" of the data points (Figure 6).

You can use data from a datafile just as for X-Y plots, except that you'll be asked to specify two and only two columns (the values and their errors) of data. Request datafile access after you've specified a weighted-averages plot (otherwise, the X-values could be used as the variable to average with the Y-values the errors).

If there is no excess scatter of the data being averaged (that is, the MSWD is not much greater than 1), the weighted averages algorithm simply weights each point by its inverse variance and calculates the uncertainty in the average value from the assigned uncertainties for each point. If there is excess scatter (MSWD>1), the average is

calculated by assuming that the data scatter due to a combination of their assigned errors plus an unknown, "external" variance that has a normal (Gaussian) distribution¹. In these cases, the most probable value of the "external sigma" arising from the external variance is also calculated.

UTILITY FUNCTIONS FOR ISOTOPIC DATA

Several utility functions can be invoked from the starting-screen of ISOPLOT. These functions (press U to see a list) include:

- 1) **Calculation of Radiogenic $^{207}\text{Pb}/^{206}\text{Pb}$ ages:** -- Press R. Enter the radiogenic $^{207}\text{Pb}/^{206}\text{Pb}$ ratio together with the percent error in the ratio (optional) and the time that radiogenic Pb-isotope growth ended (also optional). If the second optional value is not entered, a value of zero is assumed (yielding the usual radiogenic 207/206 age).
- 2) **Calculation of Model-Pb age and Mu:** -- Press P. Enter the $^{206}\text{Pb}/^{204}\text{Pb}$ and $^{207}\text{Pb}/^{204}\text{Pb}$ ratios of the isotopic composition of interest. The program will calculate a model age and Mu^2 assuming a Stacey-Kramers single-stage growth-curve.
- 3) **Calculation of Model-Nd age:** -- Press N. Select whether you want the model age calculated assuming a chondritic source with constant Sm/Nd or a depleted source. Enter the $^{147}\text{Sm}/^{144}\text{Nd}$ and $^{143}\text{Nd}/^{144}\text{Nd}$ ratios of the sample.
- 4) **Calculation of Model-Sr age:** -- Press S. Similar to the calculation of a model-Nd age, except that the depleted-source option is not offered.

CALCULATION OF AGES FROM MARINE-CARBONATE SR-ISOTOPE RATIOS

A fifth utility function can be invoked from the **Splines** menu, provided that you've just plotted data for a global-marine trend of Sr-

¹The algorithm for this approach was developed by Brent Troutman of the U.S. Geological Survey.

²Ratio of $^{238}\text{U}/^{204}\text{Pb}$ normalized for U-decay to the present day.

isotope ratios versus age. These data can be either in the form of $^{87}\text{Sr}/^{86}\text{Sr}$ versus age, or as some simple function of $^{87}\text{Sr}/^{86}\text{Sr}$ (such as delta-values relative to modern seawater) versus age. The data-set for this trend is of your own choosing.

For convenience, the data sets of Koepnick and others (1986), Hess and others (1986), DePaolo (1986), and Capo and DePaolo (1986) have been put on the **ISOPLLOT** disk and stored as files named **EXXON~SR**, **HESS~SR**, and **UCLA~SR**, respectively. The latter file contains combined data from DePaolo (1986), Capo and DePaolo (1986), and Richter and DePaolo, 1987 (diffusion-corrected data). The Sr-isotope data are expressed in two ways in these files -- as measured $^{87}\text{Sr}/^{86}\text{Sr}$, and as Delta- ^{87}Sr , where the latter is the difference in parts per thousand between the sample $^{87}\text{Sr}/^{86}\text{Sr}$ and modern-seawater $^{87}\text{Sr}/^{86}\text{Sr}$.

From the **SPLINES** menu, select the **SR AGES** option. Specify a **Perfect Fit** or a **Smoothed Curve** to the global-marine trend data.

If you specify a **Perfect Fit**, the routine will fit an Akima-method spline to the data, where the curve is forced through each data-point on the trend. This is appropriate for relatively sparse, very-high precision data-sets such as that of DePaolo (1986). You should include the analytical errors of the reference data-set if you specify a **Perfect Fit**.

For large global-marine-trend data-sets with resolvable non-analytical scatter, such as those of Koepnick and others (1985) or Hess and others (1986), you should specify a **Smoothed Curve**. For a **Smoothed Curve**, the analytical errors of the reference data-set are irrelevant. The attributes of both of these curve-types are briefly described in the section on **FITTING A CURVE TO DATA**.

ISOPLLOT will ask you to enter the $^{87}\text{Sr}/^{86}\text{Sr}$ value of the unknown-age sample and the uncertainty in that value. Again, you can use other ways of expressing the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio such as delta-values, so long as the form of the ratio is the same as that used for the global-marine trend. The procedure is as follows:

- 1) All ages (intercepts) along the global-marine trend (spline curve) that have the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of your unknown are determined. If there is only one such age, it is used as the best age-estimate. If there are several such ages, their average is used.
- 2) The intercepts of the upper and lower limits (from your assigned error) on the sample $^{87}\text{Sr}/^{86}\text{Sr}$ ratio with the global-marine trend are located. The differences between the resulting maximum and minimum ages and the best age-estimate

are used to calculate variances in the positive and negative age directions, and assigned to a sample-error variance.

- 3) The intercepts of the sample Delta-⁸⁷Sr with the spline curve constructed through all of the upper limits of the calibration curve are determined, then the intercepts of the spline curve constructed through all of the lower limits of the calibration curve. In the case of a normal spline or Akima spline calibration curve (that is, a curve passing through each of the calibration points), the upper and lower limits are taken to be spline curves constructed through the upper and lower error-limits of the points. In the case of a smooth spline, the limits reflect the 2-sigma statistical error about the curve. The differences between the maximum and minimum ages from these intercepts and the best age estimate are used to calculate variances in the positive and negative age-directions, and assigned to a global-marine-trend variance.
- 4) The upper and lower errors on the best age-estimate are determined by taking the square roots of the sums of the variances from sample error and from global-marine-trend error. Because the upper and lower errors are determined separately, they will generally not be symmetric about the best age estimate.

CHANGING THE DECAY CONSTANTS AND MODEL-AGE PARAMETERS

The default decay constants used by **ISOPLLOT** are those recommended by the I.U.G.S. Subcommittee on Geochronology (Steiger and Jäger, 1977). You can change those constants, however, as well as the Rb-Sr and Sm-Nd model-age parameters¹. From the starting screen, switch to the Radiogenic-Isotope Utilities screen by pressing **U**. Press **ALT-C** to bring up the form containing the decay constants and model-age parameters being used by **ISOPLLOT**. Select the parameters that you want to change with the Up/Down arrows, type in the new values, and press **ENTER**. Press **CTRL-ENTER** when you've completed the changes.

¹Note that by changing the constants for either Rb-Sr or Sm-Nd model ages, you can get model ages for any other parent-daughter pair, such as Lu-Hf or K-Ca. Be sure to restore the original values when you're done, though, otherwise the calculation of isochron ages will be affected.

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ISOPLOT will store the edited values in the CONSTS.ISO file, which is (and should remain) on the same disk and path as the ISOPLOT program. From now on, every time you load ISOPLOT, these new constants will be used.

ACKNOWLEDGEMENTS

ISOPLOT uses several algorithms that were adapted in whole or in part from other sources. The polynomial regression and "normal" spline algorithms were adapted from Numerical Recipes (Press and others, 1987), and the "Akima" spline algorithm was adapted from Akima (1970). The sorting algorithm is a modified version of the Shell Sort sub-program supplied with the Quick Basic 4.0 language. Jim Quick of the U.S.G.S. supplied the Epson printer-dump algorithm, and Brent Troutman of the U.S.G.S. developed the analytical expression for the external variance of a weighted average. George Cumming provided the algorithm for construction of error ellipses. The Model-1 Yorkfit is, of course, derived from York (1969) with uncertainties calculated using the algorithm of Titterton and Halliday (1979), and the Model-2 Yorkfit is a modification of the "equal weight" model of McSaveney (Faure, p. 427-434).

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FIGURE CAPTIONS

- Figure 1: Example of X-Y plot with polynomial regression curve to the data points (boxes).
- Figure 2: Example of X-Y plot with spline curves fit to the Sr-isotope data of Capo and DePaolo (1986). The narrow boxes indicate the data with errors; spline curve (Akima method - see text) is constructed for both the best-estimate data-points and their error extremes.
- Figure 3: Example of X-Y plot with spline curves fit to the Sr-isotope data (boxes) of Koepnick and others (1985). The curves were constructed with the Smoothed Spline option, and indicate roughly the uncertainty at any point in the curve.
- Figure 4: Example of a concordia plot for data with large errors (error ellipses).
- Figure 5: Example of a plot of common-Pb data, with single-stage evolution curve. Ages and intercepts were calculated by the program.
- Figure 6: Example of screen for a weighted averages plot. Empty boxes indicate rejected points.

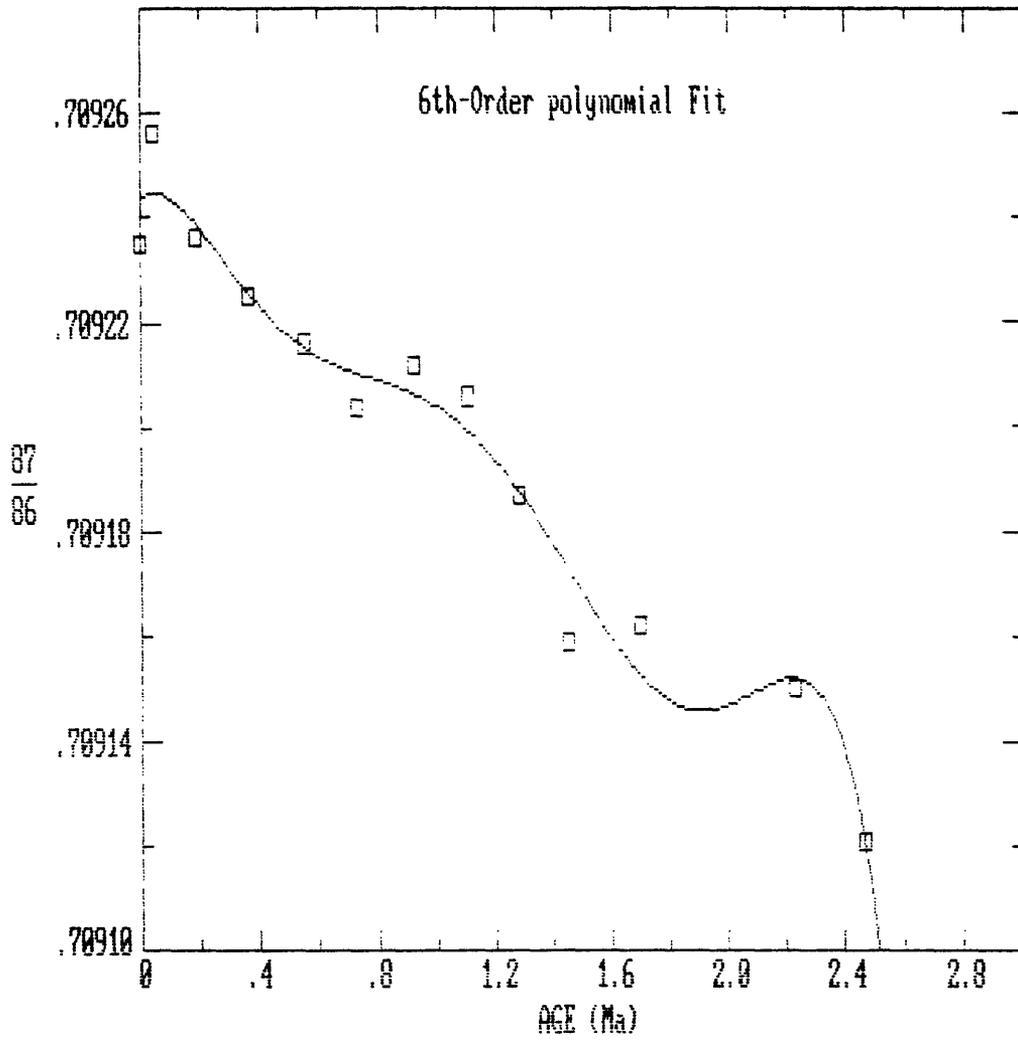


fig. 1

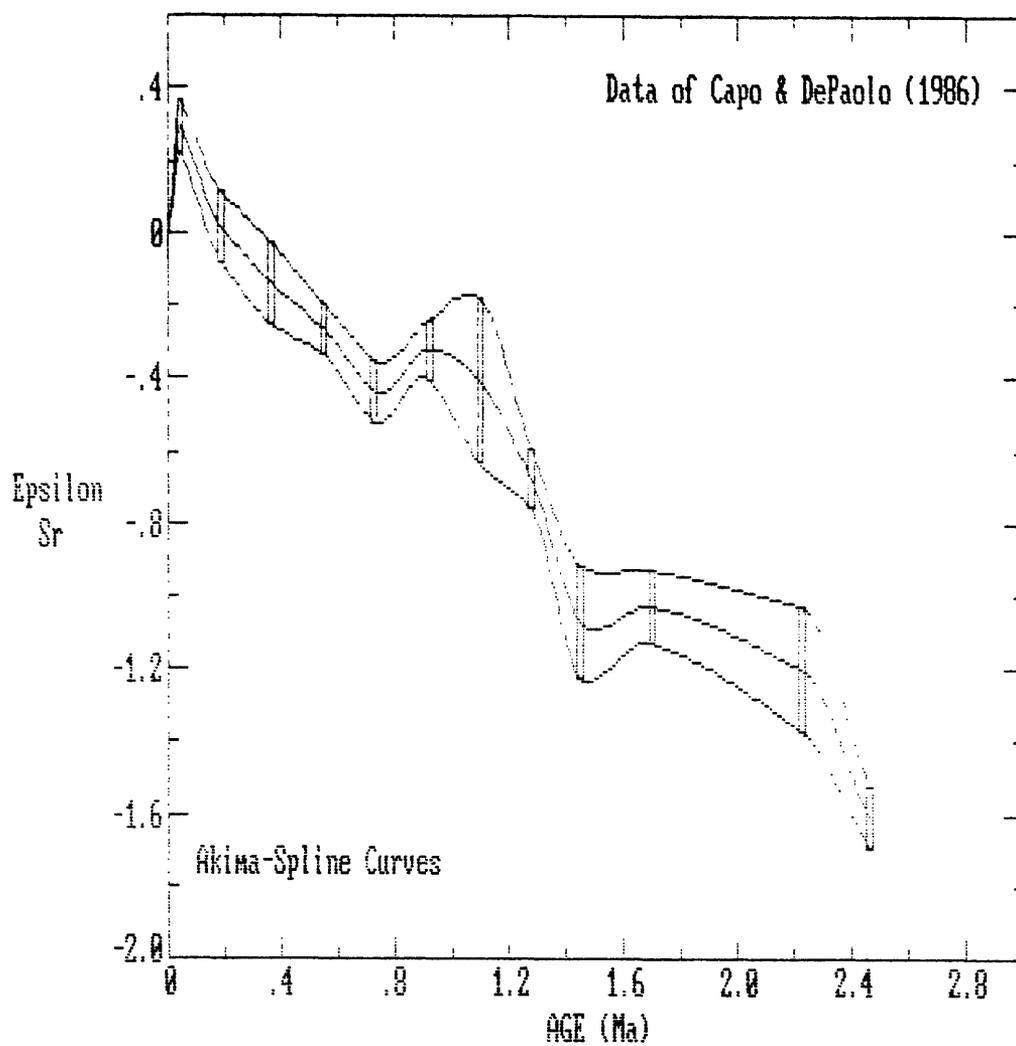


fig. 2

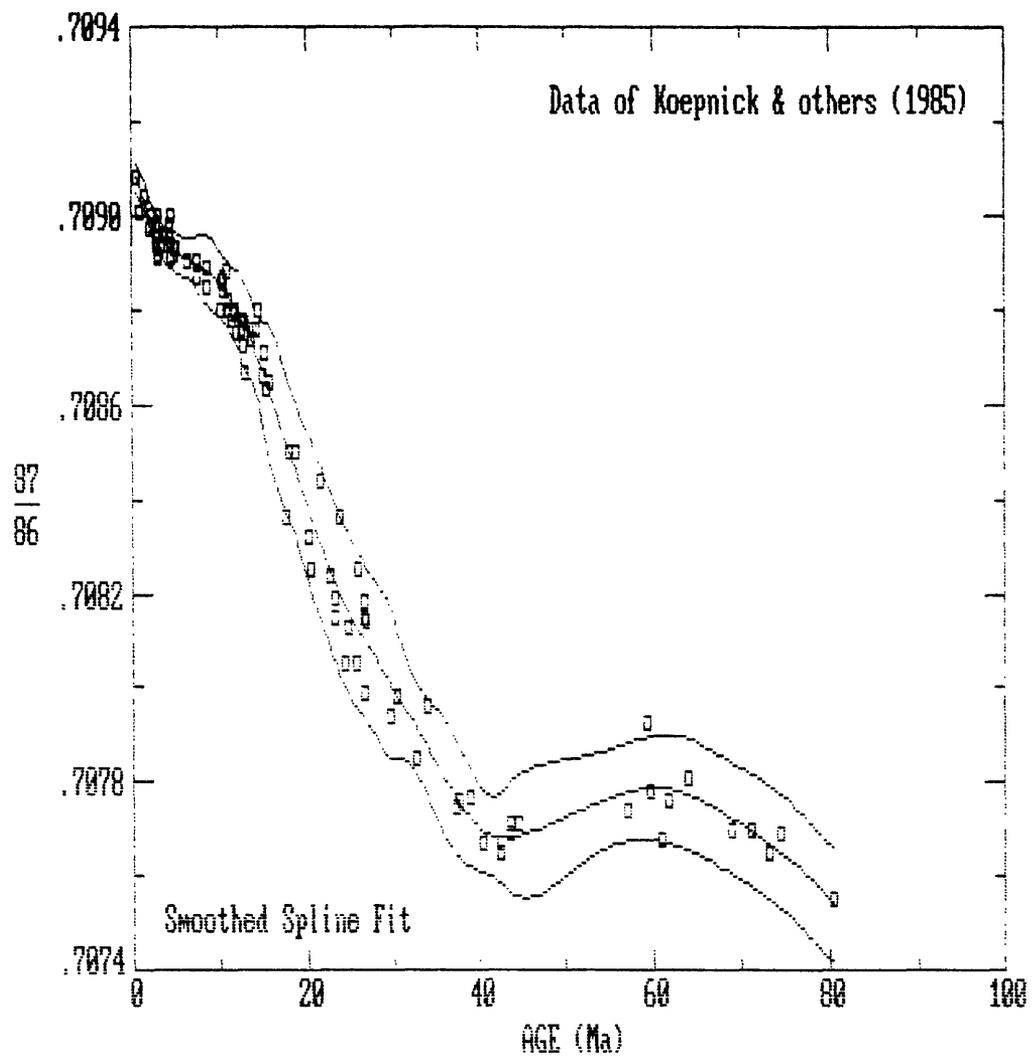


fig. 3

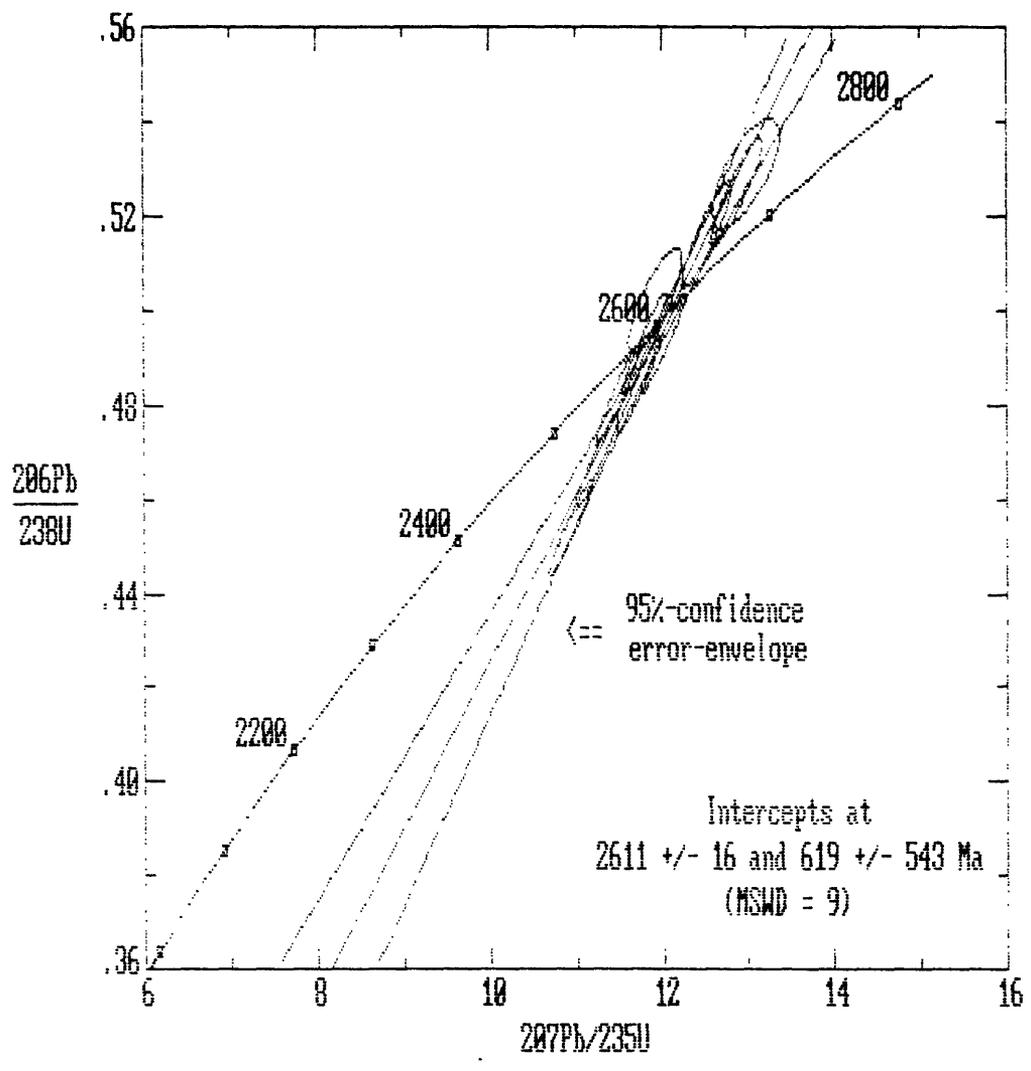


fig. 4

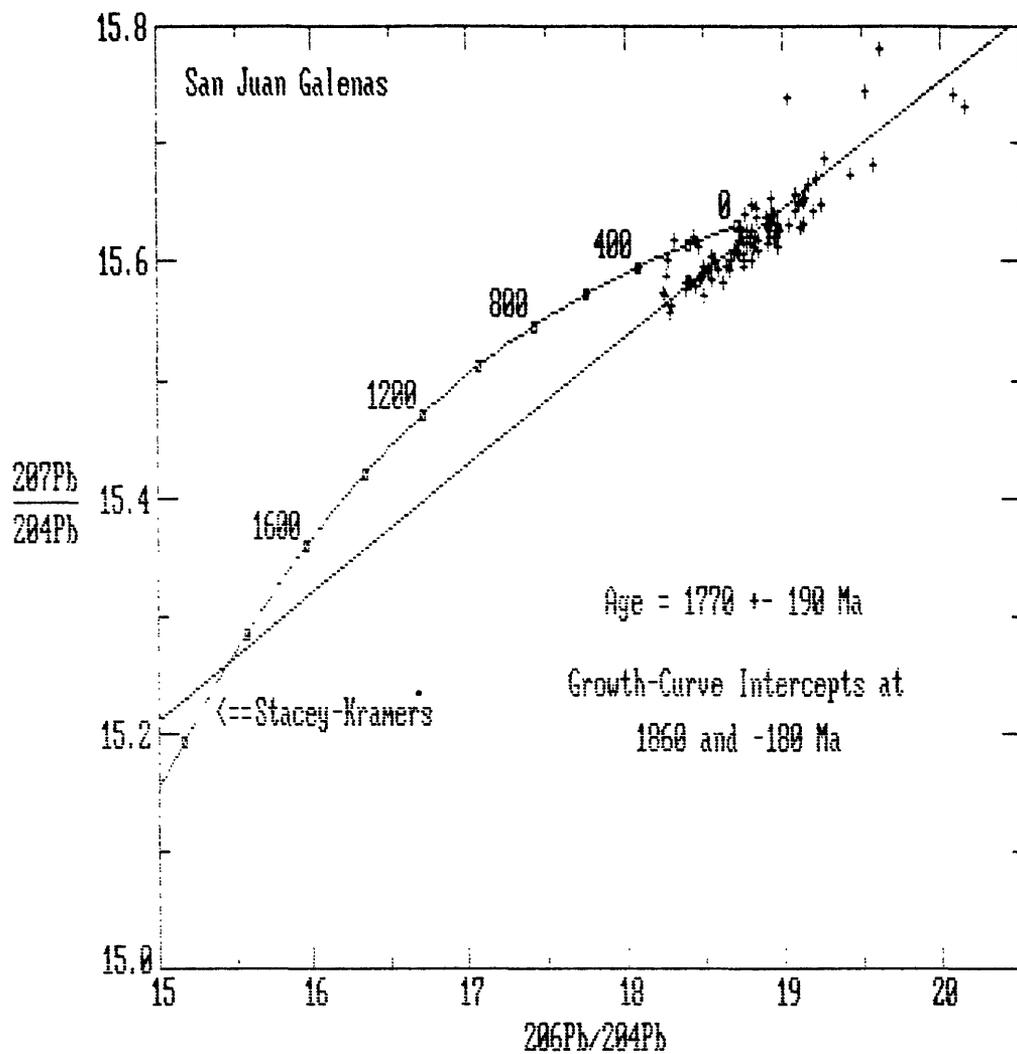
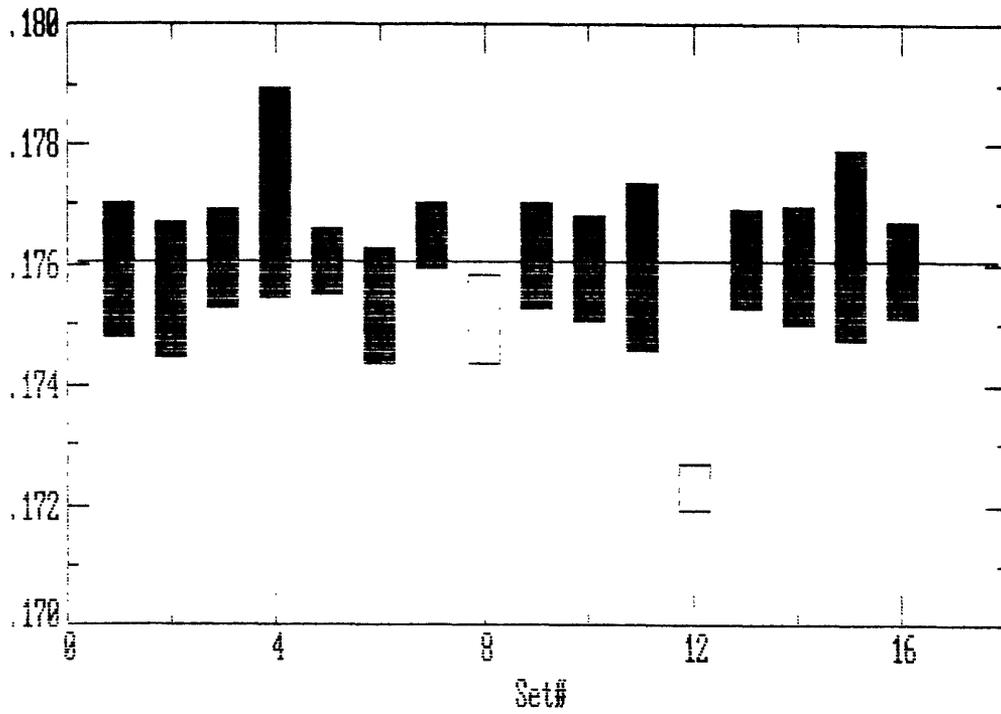


fig. 5



WEIGHTED AVERAGE = .17687 +/- .00019 (.11%) (95% Conf. Limit)
 M.S.W.D. = .594 Probability = .96

REJECTED: .1723 .1751

fig. 6

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