Updates to the PET

(PMF Evaluation Tool)

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PMF:
The Answer to Life, the Universe, and Everything!
A data matrix is decomposed into an arbitrary number of factors, each of which is represented by a constant mass spectrum and a contribution time series. There is usually some residual of fit.

The PMF Approach: Weighted Least Squares

- in many dimensions, called

\[ Q = \sum_{i=1}^{m} \sum_{j=1}^{n} \left( \frac{\text{resid}_{ij}}{\sigma_{ij}} \right)^2 \]

estimated error of each point

- If all points are fit as well as we know them, the \( Q \)-contribution from each point is \( \sim 1 \)

\[ Q = \sum_{i=1}^{m} \sum_{j=1}^{n} \left( \frac{\sim \sigma_{ij}}{\sigma_{ij}} \right)^2 = \sum_{i=1}^{m} \sum_{j=1}^{n} (\sim 1)^2 \]

and the total Q is \( \sim \) the size of the matrix.
The PMF Approach: Weighted Least Squares

• Let’s normalize the total $Q$ to $Q_{exp}$, then if all points are fit to $\sim \sigma$, $Q/Q_{exp} \sim 1$

\[
Q/Q_{exp} = \frac{m}{\sigma} \sum_{i=1}^{m} \sum_{j=1}^{n} \left( \frac{\text{resid}_{ij}}{\sigma_{ij}} \right)^2 / m \times n
\]

• Adding factors decreases $Q$, but may not give meaningful factors!

(Please utilize) PMF Resources!

• (There’s a wiki.)

• On the wiki you’ll find links to
  – Publications about the method
  – Full description of how to install the PET
  – Description of preparing matrices for the PET
  – What’s going on when you press the button
  – Troubleshooting tips

What, you don’t want to carry a 17” laptop?

Panel with Just the Buttons

Already in v2.03!

New graphs!

Fraction of measured organic (time series)

More time-averaging plots
- Day of Week
- Weekday/Weekend
- Monthly
New graph capability for Scatter Panel

Color correlations by a different variable

Do you use the Scatter Panel?

a) Yes: love it
b) Yes: but it’s a pain
c) No: didn’t know about it
d) No: don’t know how it works
e) No: Can’t make it work
Scatter Panel for Mass Spectra

Send some Spectra!

* The fabulous Donna Sueper made you a button and a panel, and so it’s really very easy and so you have to come up with a better excuse if you don’t want to share and you don’t want people to compare to your brilliant previous results and cite your fabulous papers and bring you fame (if not fortune) for all time.
Updates to Calculations

- Diurnal calculations updated
  – parallel to updates made in Squirrel

- Do more calculations after PMF execution to reduce calculations when you update the panel, for faster panel updates
  – Residuals, Scaled residuals, Diurnal

HR database only has 3 (lonely) spectra!
Version 2.04 coming in ~1 week

• Will send mail to the AMS Users list

• Should be back-compatible for existing experiments (no need to re-run PMF)