

MaxEnt interface summary—January 1999

Maximum Entropy Data Consultants Ltd. (MEDC) supply specialist computer programs for data analysis. Company policy is to provide fully reliable top-of-the-range quality software.

Maximum entropy (MaxEnt) data analysis is designed to estimate additive distributions from incomplete and noisy data. Usually, the distribution in question is positive, although the extensions to arbitrary sign and Fermi–Dirac statistics are included as standard options. Because MaxEnt is founded on rigorous mathematics, the programs do not contain any unnecessary parameters. Also, estimates of the distribution are fully quantified, so that error bars can be found for given features. Furthermore, a series of ‘reasonably plausible’ sample reconstructions can be generated, to illustrate the probabilistic nature of the process, or for use in subsequent numerical analysis. Earlier programs, based on finding just a single “best estimate”, are rendered obsolete by these developments.

MEDC supply a kernel program (`MemSys5`) which performs this data inversion in a very general environment. `MemSys5` is the most advanced program available for this purpose, and is designed to be as simple as possible to use, even for large-scale applications. The program is written in FORTRAN 77, but for user convenience a machine-translated version in C is also available. This is accompanied by a 100-page manual describing both the theory of MaxEnt and the practical application through `MemSys5`. The kernel compiles to approximately 100 kB of code.

Each particular application requires an additional *interface* program which describes the data being analysed, and how they relate to the distribution being measured. Typically, a MaxEnt reconstruction involves a few hundred calls to the interface, and the overall speed of computation depends critically upon its efficient coding.

The principal component of any interface is a routine which models the experimental responses, and computes the data which would have been observed from a particular distribution. Typically, this routine includes one or more user-definable parameters. Because of the internal structure of `MemSys5`, which assumes reasonable continuity properties in order to perform an efficient maximisation, this modelling routine needs to be supplemented by another routine to give the differential response of the data to small changes in the distribution. A third routine which uses the transpose differential response to propagate small data changes back to small changes in the distribution completes the interface.

A complete interface is defined as a subroutine package which accepts a list of data and the corresponding error bars, to be supplied by the user at a specified memory location, and which models the experimental responses in sufficient detail to enable the MaxEnt kernel program to compute the corresponding reconstructed distribution at a different specified memory location. For some applications these memory locations may be disc files if core storage is limited: contact MEDC for specific advice. In order to aid portability, all interface routines are written in standard FORTRAN 77, for which documented source code is supplied. Machine-translated versions of the source code in C are also available. Alternatively, for some applications a complete executable program (without source or object code) can be supplied at a substantial discount.

The interfaces currently available are summarised in the following pages.

Deconvolution, in one or two dimensions

The data \mathbf{D} are a blurred version of the distribution f ,

$$D(x) = \int dy b(x, y) f(y)$$

where b is a specified point-spread function. These types of data occur often, and the interface is used most frequently to deconvolve blurred optical pictures or photographs.

The data and the distribution are digitised with the same cell-size. The convolution operation is normally performed by Fast Fourier Transform, which requires power-of-2 dimension(s) and a spatially invariant point-spread function $b = b(x - y)$. Alternatively, a direct convolution operation can be supplied at slightly higher cost, not subject to these restrictions. The convolution operation is usually assumed to continue into unmeasured areas beyond the edges, so that structure very near the edges can not be fully deconvolved. If appropriate, wraparound periodicity is available as an alternative.

Noise on the data is usually assumed to be Gaussian, independent on each cell, but possibly of different standard deviation in different cells. Alternatively, Poisson statistics can be imposed, as for data obtained by explicitly counting quanta.

Fourier spectroscopy in one dimension

The data are Fourier transform coefficients,

$$D(t) = A(t) \int du \exp i(ut + \phi(u)) f(u)$$

or

$$D(t) = A(t) \int du \cos(ut + \phi(u)) f(u)$$

or

$$D(t) = A(t) \int du \sin(ut + \phi(u)) f(u)$$

where $A(t)$ and $\phi(u)$ are user-supplied functions. For example, in one-dimensional NMR spectroscopy, $A(t)$ might be an exponential decay, and $\phi(u)$ might be linear in u . A few simple enhancements, such as automatic baseline suppression in the data, can be incorporated in the interface. Fourier data are usually band-limited, and for optimal resolution, f is computed on a suitably fine grid, having substantially more points than the number of data. Because of the Fast Fourier Transform, f will have a power-of-2 number of cells.

Noise on the data is assumed to be Gaussian, independent on each datum, but possibly of different standard deviation for each t . This allows erratic data to be effectively discarded, without damaging the reconstructed distribution, by setting their standard deviations to be large.

Fourier spectroscopy in two dimensions

This is a variant of one-dimensional Fourier spectroscopy in which a Fourier transform in a second dimension yields a two-dimensional dataset relating to a two-dimensional distribution $f(u, v)$. The standard interface is designed for NMR spectroscopy, and has the facility to deconvolve simultaneously both “absorption” and “dispersion”, i.e., 0° and 90° phase, distributions.

Two-dimensional absorption or emission tomography

The data are line integrals,

$$D(h, \theta) = \int \int dx dy \delta(x \cos \theta + y \sin \theta - h) f(x, y)$$

where h is an offset at orientation θ . The standard interface assumes that the orientations are distributed uniformly around the circle $(0, 2\pi)$, and that the required distribution f lies within a concentric disc of given radius.

Noise on the data can be Gaussian, as for X-ray absorption tomography, or Poisson as for positron emission tomography.

Raman spectroscopy

This is a variant of one-dimensional deconvolution, in which the required distribution is superposed upon a large unknown (but fairly smooth) background. MaxEnt is used here to estimate simultaneously both the background and the required distribution.

$$D(x) = \int dy b(x - y) f(y) + \text{Background}(x)$$

The blurring function can be specified as Lorentzian, Gaussian, or other form, and the noise is assumed to be Gaussian.

Fourier transform ion cyclotron spectroscopy

This is a variant of one-dimensional Fourier spectroscopy in which the distribution $f(u)$ is excited by a frequency “chirp”.

“MASQUERADE” quasi-elastic light scattering

The data are autocorrelation measurements in homodyne-detected quasi-elastic light scattering, i.e., light-beating spectroscopy, photon correlation spectroscopy, dynamic light scattering, sometimes known as QLS or PCS.

$$D(t) = \left(\int d\tau f(\tau) \exp(-t/\tau) \right)^2 + \text{Background}$$

The noise is assumed to be Gaussian for each datum, as from a large number of detector counts, though the nonlinear nature of the data is important, and is treated correctly. The data can come from single autocorrelations or banks of multiple “log-spaced” autocorrelator boards as commonly found in modern hardware. As with all MemSys5 interfaces, this terminates automatically when the data are properly fitted, so that non-random autocorrelator errors do not seriously damage the reconstructions. The interface can be converted to handle heterodyne-detected QLS data.

“FAME” time-resolved and dynamic fluorescence spectroscopy

The data are pulsed fluorescent decays

$$D(t) = E(t) * \int d\tau f(\tau) \exp(-t/\tau)$$

where $E(t)$ is the shape of the exciting pulse (or a reference sample decay of known half-life), and $*$ is convolution. Detection may be through a polariser set at the magic angle, or, using two separate decays, through a polariser set vertically and then horizontally. The excitation may be either vertically polarised or unpolarised. The program can allow for continuing fluorescent decay from previous pulses if the excitation has a period which is small compared with the decay time. The noise is assumed to be Poisson, and the method of allowing for dark current counts from the detector and blank sample counts is statistically correct. The program has several additional options, such as channels for scattered light ($\tau = 0$) and background ($\tau = \infty$).

Extensions to the FAME interface will be made available for a media handling charge. Those being developed include:

1. Recovery of decay times, rotational correlation times and initial anisotropy amplitudes from a global analysis of the two polarised components using a three-dimensional program FAME3.
2. Treatment of excitation transfer between fluorescent species.

Contact MEDC for current details.

Flash photolysis

The data are the transient absorption of the sample after photo-dissociation:

$$D(t) = \int f(k) \exp(-kt) dk.$$

This is a variant of pulsed-fluorimetry spectroscopic analysis.

“PHAME” frequency-domain fluorescence spectroscopy

The data are phase shifts and modulation ratios at various frequencies of sinusoidal excitation.

$$\phi(\omega) = \arctan(P(\omega)/Q(\omega))$$

$$M(\omega) = \left(P^2(\omega) + Q^2(\omega)\right)^{1/2}$$

with

$$P(\omega) = \frac{\int dt \int_0^\infty d\tau f(\tau) \exp(-t/\tau) \sin \omega t}{\int_0^\infty d\tau f(\tau) \exp(-t/\tau)}$$
$$Q(\omega) = \frac{\int dt \int_0^\infty d\tau f(\tau) \exp(-t/\tau) \cos \omega t}{\int_0^\infty d\tau f(\tau) \exp(-t/\tau)}$$

where $\phi(\omega)$ is the angular shift between fluorescence and excitation signals and M is the modulation ratio.

The program can handle a large number of frequencies, and automatic scaling of the noise is a standard option, as well as channels for scattered light ($\tau = 0$) and background ($\tau = \infty$).

“MADAME” drug absorption and disposition kinetics

The data consist of measurements of the concentration of the drug in blood at various times after dosing. Given a knowledge of the drug’s disposition kinetics, the rate at which it reaches the systemic circulation from an unknown input, such as an oral dose, can be estimated. The total amount absorbed, and other associated quantities can also be determined, together with their error estimates.

If the data are obtained after a known input of the drug, such as an intravenous bolus or infusion, the disposition kinetics may be characterised by an impulse response function

$$R(t) = \int d \log \lambda f(\log \lambda) \exp(-\lambda t)$$

where $f(\log \lambda)$ is obtained, effectively by inverse Laplace transformation, from the data. All the usual pharmacokinetic parameters, such as clearance and volume of distribution, can be obtained from $f(\log \lambda)$, together with error estimates.