Bayesian Data-Analysis Toolbox
Release 4.23, Manual Version 3

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Chapter 25

MaxEnt Density Function Estimation

The Maximum Entropy Method of Moments package, which we will refer to as the MaxEnt package, uses Bayesian Probability theory to compute the posterior probability for the number of Lagrange multipliers need to represent a density function given a set of samples. The input data to this package are the samples drawn from an unknown density function. For example, the samples generated from the run of a Markov chain Monte Carlo simulation might serve as input. Indeed this is exactly what happens when the “Get MaxEnt Histogram” button is activated. For plotting purposes the samples must be numbered, so the input data are a two column Ascii file.

25.1 Using The Package

To use this package, you must do the following:

Select the “MaxEnt Histogram” package from the Package menu.

Load two column Ascii data using the “Files” menu.

Set the number of Lagrange Multipliers to use in the analysis, this can be set to a number or to “Automatic.” The automatic feature will cause the package to compute the posterior probability for the number of Lagrange multipliers.

Set the number of bins in the histogram.

Review the prior probabilities for package. The MaxEnt Histogram package does not allow the user to set prior probabilities.

Select the server that is to process the analysis.

Check the status of the selected server to determine if the server is busy, change to another server.

Run the the analysis on the selected server by activating the Run button.
Figure 25.1: MaxEnt Density Function Estimation Package Interface

To use the Density Function Estimation package:

1. Load a 2 column ascii data set containing samples from the density function in question.

2. Specify the order of the moment expansion used to represent the density function, or leave this combo box set as automatic if the package is to determine the optimal expansion order.

3. Specify the size of the discrete density function using "Size" combo box.

4. Select the server to run the analysis.

5. Run the analysis using the "Run" button.

6. Use "Get Job" to get the results from the server.

Figure 25.1: This is the interface to the MaxEnt Density Function Estimation package. This package will compute the posterior probability for the Lagrange Multipliers using a Maximum Entropy method of moments calculation with a given or unknown number of multipliers. For more on the actual calculations and the widgets see the text.
Get the results of the analysis by activating the Get Job button. If the analysis is running, this button will return the Accepted report containing the status of the current run. Otherwise, it will fetch and display the results from the current analysis.

Output from the package consists of an McMC Values report, See Fig. 25.2. The First part of the McMC Values report, not shown, details the parameter settings that were input to the analysis. After the parameter file values, the McMC Values Report has the first few moments of the data. These moments show up in the Bayesian Calculation as sufficient statistics, i.e., the only functions of the data needed to perform the inference calculations. Next there is a bar chart of the posterior probability for the number of multipliers needed to represent the data. This is followed by the Lagrange multipliers that had maximum posterior probability. Finally, the Lagrange multipliers computed as the mean and standard deviations of the Markov chain Monte Carlo.

There is also a console log, Figure 25.3 which contains counts of the number of simulations having one, two, etc Lagrange multipliers. This report shows the convergence of the simulations on the number of multipliers. The MaxEnt Density Function Estimation package outputs a running count of the number of simulations having one, two, etc. Lagrange multipliers to the console. This count is the unnormalized posterior probability for the number of Lagrange multipliers as a function of the annealing parameters. When the annealing parameter is small, the simulations distribute themselves according the the prior probability for the number of multipliers, Eq.(25.19) below, which is an $\exp(-m)$. So if there are 33 simulations having 0 multipliers, just on the prior one would expect 12 having 1 and about 3 having 2. As one can see, at small values of the annealing parameter, the simulations are distributed according the prior probability for the model. As the annealing parameter increases the data become increasingly important and the by the time the annealing parameters has reached 0.015 the simulations are definitely heading for a model containing 2 multipliers.

In addition to the McMC Values report and the console log, The interface also makes considerable use of Ascii Plot Viewer. The package outputs a number of plots unique to this package. The first of these is the posterior probability for the number of multipliers, Fig. 25.4. The horizontal axis is the number of Lagrange Multipliers and the vertical axis is the probability for indicated number of multipliers. In this problem, this probability was zero everywhere except when the number of multipliers was two and then the probability was one.

There are three other plots unique to this package, the estimated density function with error bars, Fig 25.12, is discussed in the following sections. In this package the “Data, Model and Residuals” plot is a unique and we will discuss that plot shortly. Finally, a gray scale plot of the density function with the samples also plotted, Fig. 25.5. This scatter plot is meant to illustrate how well the actual samples conform to the inferred Maximum Entropy method of moments density function. The data used in this plot are from the Bayesian Analysis test data, the Histogram subdirectory and the HistFreqW data set. These data samples are from an analysis run using the Bayesian Analysis software and then viewing one of the output histograms and finally activating the “View Samples” button and saving the samples. This particular set of samples is vary Gaussian like. Consequently, there is a bright area in the center of Fig. 25.5 which tapers off symmetrically as you move away from the mean. The horizontal axis is just the repeat simulation number from the Markov chain Monte Carlo simulations. The vertical axis is the parameter value from that simulation.

The “Data, Model and Residual” plot in the Maximum Entropy method of moments package, Fig. 25.6, is unusual for the following reasons: in most packages the data are a continuous function of time and don’t actually change all that much from one point to the next. However, in this package the data are a random sample out of an unknown underlying density function and smooth continuous
Figure 25.2: The MaxEnt Method Of Moments McMC Values Report

McMC Values Report for the Density Function Estimation Package

<table>
<thead>
<tr>
<th>Number</th>
<th>Moment</th>
<th>Cumulant</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-3.19602056E+02</td>
<td>-3.19602056E+02</td>
</tr>
<tr>
<td>2</td>
<td>1.02145560E+05</td>
<td>8.56739829E-02</td>
</tr>
<tr>
<td>3</td>
<td>-3.26459857E+07</td>
<td>-1.43628567E-04</td>
</tr>
<tr>
<td>4</td>
<td>1.04337504E+10</td>
<td>-1.29381267E-04</td>
</tr>
<tr>
<td>5</td>
<td>-3.33465926E+12</td>
<td>-3.27148438E-02</td>
</tr>
<tr>
<td>6</td>
<td>1.06576843E+15</td>
<td>-2.33284416E+01</td>
</tr>
</tbody>
</table>

Probability For The Number of Multipliers

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15

Given 2 Multipliers

The parameters that Maximized the posterior probability are:

<table>
<thead>
<tr>
<th>Description</th>
<th>Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>LogZ given 2</td>
<td>4.83560181E+00</td>
</tr>
<tr>
<td>Lagrange Multiplier 1</td>
<td>3.95924945E-01</td>
</tr>
<tr>
<td>Lagrange Multiplier 2</td>
<td>-3.82316203E+00</td>
</tr>
</tbody>
</table>

The expected parameter values given a 2 Multiplier Model:

<table>
<thead>
<tr>
<th>Parameter Description</th>
<th>Mean Value</th>
<th>Std. Dev.</th>
<th>Peak Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>LogZ given 2</td>
<td>4.83560181E+00</td>
<td>4.62284E-02</td>
<td>4.83560E+00</td>
</tr>
<tr>
<td>Lagrange Multiplier 1</td>
<td>3.95924945E-01</td>
<td>7.68460E-02</td>
<td>3.95925E-01</td>
</tr>
<tr>
<td>Lagrange Multiplier 2</td>
<td>-3.82316203E+00</td>
<td>1.24154E-01</td>
<td>-3.82316E+00</td>
</tr>
</tbody>
</table>

Figure 25.2: The MaxEnt Density Function Estimation Package outputs a standard McMC Values report. The First part of this report, not shown, details the parameter settings that were input to the analysis. After the parameter file values, the McMC Values Report has the first few moments of the data. These moments show up in the Bayesian Calculation as sufficient statistics, i.e., the only functions of the data needed to perform the inference calculations. Next there is a bar chart of the posterior probability for the number of multipliers needed to represent the data. This is followed by the Lagrange multipliers that had maximum posterior probability. Finally, the Lagrange multipliers computed as the mean and standard deviations of the Markov chain Monte Carlo samples.
Figure 25.3: The MaxEnt Density Function Estimation Package Console Log

| Phase | Annl Parm | <Likelihood> | <StdDevLike> | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | ...
|-------|-----------|--------------|--------------|---|---|---|---|---|---|---|---|---|---|
| Annealing | 45E-06 | -1.2847E+04 | 1.2319E+04 | 33 | 11 | 2 | 2 | 0 | 0 | 0 | 0 | 0 |...
| 2 | 12E-05 | -8.7576E+03 | 2.9464E+03 | 40 | 5 | 3 | 0 | 0 | 0 | 0 | 0 | 0 |...
| 3 | 46E-05 | -8.0843E+03 | 1.1540E+03 | 40 | 4 | 2 | 2 | 0 | 0 | 0 | 0 | 0 |...
| 4 | 0.001 | -7.8142E+03 | 1.3536E+02 | 45 | 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 |...
| 5 | 0.008 | -7.6652E+03 | 3.2444E+02 | 37 | 1 | 5 | 3 | 2 | 0 | 0 | 0 | 0 |...
| 6 | 0.011 | -7.4675E+03 | 4.3092E+02 | 27 | 1 | 3 | 5 | 2 | 0 | 0 | 0 | 0 |...
| 7 | 0.013 | -7.2545E+03 | 4.1095E+02 | 14 | 1 | 2 | 2 | 4 | 6 | 0 | 0 | 1 | 0 |...
| 8 | 0.015 | -7.1117E+03 | 3.7322E+02 | 9 | 0 | 2 | 7 | 5 | 5 | 0 | 0 | 1 | 1 |...
| 9 | 0.018 | -6.9616E+03 | 2.3343E+02 | 2 | 0 | 3 | 5 | 4 | 0 | 0 | 1 | 1 |...
| 10 | 0.022 | -6.8851E+03 | 6.3603E+01 | 0 | 0 | 4 | 0 | 5 | 3 | 0 | 0 | 0 | 0 |...

Figure 25.3: The MaxEnt Density Function Estimation Package outputs a running count to the console. This count is the unnormalized posterior probability for the number of Lagrange multipliers as a function of the annealing parameters. When the annealing parameter is small, the simulations distribute themselves according to the prior probability for the number of multipliers, Eq. (25.19) below, which is an exp(−m). So if there are 33 simulations having 0 multipliers, just on the prior one would expect 12 having 1 and about 3 having 2. As one can see, at small values of the annealing parameter, the simulations are distributed according to the prior probability for the model. As the annealing parameter increases the data become increasingly important and by the time the annealing parameters has reached 0.015 the simulations are definitely heading for a model containing 2 multipliers.

The problem of density estimation occurs in many disciplines. For example, in MRI it is often necessary to classify the types of tissues in an image. To perform this classification one must first identify the characteristics of the tissues to be classified. These characteristics might be the intensity of a T1 weighted image and in MRI many other types of characteristic weightings (classifiers) may be generated. In a given tissue type there is no single intensity that characterizes the tissue, rather there is a distribution of intensities. Often this distributions can be characterized by a Gaussian,
Figure 25.4: The first output generated by the MaxEnt Density Function Estimation package is a plot of the posterior probability for the number of Lagrange Multiples needed to represent the Maximum Entropy density function. Here that probability indicates that the data are Gaussian, i.e., all probabilities were zero except the 2 Lagrange multiplier model and its probability was one.
Figure 25.5: The Model Averaged Density Function And Samples

After the model averaged density function, the package outputs a gray scale plot of the posterior probability and the samples from the Markov chain Monte Carlo simulations. The horizontal axis is just the repeat simulation number from the Markov chain Monte Carlo simulations. The vertical axis is that simulations corresponding parameter value. This plot is meant as a visual aid in seeing how well the estimated density function and the samples agree.
Figure 25.6: In addition to the contour/scatter plot, the Maximum Entropy Method Of Moments package outputs a plot of the data, the model and the residuals. Because the data are a random sample drawn from an unknown underlying density function, we have plotted a binned histogram of the data samples, red line. The blue line is the estimated density function inferred by this package. Finally, the difference between the binned histogram and the estimated density function are shown in green. Note the fit in the wings is always much smaller in the wings and increases until you get to the center of the estimated histogram.
but just as often it is much more complicated. Either way, estimating the distribution of intensities is an inference problem. In the case of a Gaussian distribution, one must estimate the mean and standard deviation. However, in the Non-Gaussian case the shape of the density function itself must be inferred. Three common techniques for estimating density functions are binned histograms [52, 23], kernel density estimation [53, 51], and the maximum entropy method of moments [58, 43]. In the following section, the maximum entropy method of moments will be reviewed. Some of its problems and conditions under which it fails will be discussed. Then in later sections, the functional form of the maximum entropy method of moments probability distribution will be incorporated into Bayesian probability theory. It will be shown that Bayesian probability theory solves all of the problems with the maximum entropy method of moments. One gets posterior probabilities for the Lagrange multipliers, and, finally, one can put error bars on the resulting estimated density function.

In the problem being formulated, one has a data set consisting of samples drawn from an unknown density function. Figure 25.7 displays an illustrative set of such data samples, these data samples (gray circles) were generated in a Markov chain Monte Carlo simulation; although the source of the data samples is unimportant for the problem considered here. The horizontal axis is sample number and the vertical axis is the sample value. There are 2500 samples shown in this figure. The problem is to estimate both the density function and the uncertainty in the estimated density function. Often such data samples can be characterized by a Gaussian density function, but just as often the density function is more complicated. Either way, estimating the distribution of intensities is an inference problem. In the case of the Gaussian, one must estimate both the mean and standard deviation. However, in the Non-Gaussian case, the shape of the density function itself must be inferred. Three common techniques for estimating density functions are binned histograms [52, 23], kernel density estimation [53, 51], and the maximum entropy method of moments [58, 43]. In the following section, the maximum entropy method of moments will be reviewed and some of its problems and conditions under which it fails will be discussed. Then in the following sections, the functional form of the maximum entropy method of moments probability distribution will be incorporated into Bayesian probability theory. Because the resulting Bayesian calculations never solve for the Lagrange multipliers, probability theory never encounters the difficulties involved in solving the maximum entropy method of moments functional equations. As a Bayesian calculation, one gets posterior probabilities for both the number and values of the Lagrange multipliers as well as error bars on the resulting density function. The solid line in Fig. 25.7 is an example of the estimated density function with error bars generated using the techniques and procedures described in this paper.

25.3 Review of The Maximum Entropy Method Of Moments

Claude Shannon [58] derived the Shannon entropy as a measure of the information content of a discrete probability distribution. If this discrete probability distribution is represented by \( f_j \), then the Shannon entropy, \( S \), is given by

\[
S = -\sum_{j=1}^{n} f_j \log(f_j) \quad (0 \leq f_j \leq 1) 
\]

where \( n \) is the number of discrete probabilities in the distribution. The entropy \( S \) is a measure of the information content of a probability distribution. It reaches its maximum value when all \( f_j = 1/n \).
Figure 25.7: In the density estimation problem addressed here, one as a set of samples (open circles) drawn from some unknown density function and one wishes to infer the distribution of the samples (solid line with error bars). This density function was estimated using Bayesian probability theory to determine what probabilities must be assigned. The maximum entropy method of moments was then used to assign the indicated probabilities. Finally, a Markov chain Monte Carlo simulation was used to draw samples from the posterior probability for the density function, see the text for the details.
and $S = \log(n)$, and it reaches its minimum value when one of the $f_j = 1$, and then $S = 0$. Thus the Shannon entropy maps discrete probability distributions onto the interval $0 \leq S \leq \log(n)$, with $S = \log(n)$ the completely uninformative state, and $S = 0$ the state of certainty. Everything in between represents increasing knowledge for decreasing entropy.

After deriving the entropy function, Shannon proceeded to use the entropy function as a way of assigning maximally uninformative probability distributions that are consistent with some given prior information. In the maximum entropy method of moments, the Shannon entropy is constrained by the power moments. Suppose the probabilities $f_j$ are defined on a set of discrete points $x_j$. In this case, the expected value of the power moments is given by

$$\langle x^k \rangle = \sum_{j=1}^{n} x_j^k f_j \quad (k = 0, 1, \ldots, m) \quad (25.2)$$

where $k = 0$ is the normalization constraint. Because this is an equality, one can move the sum to the left-hand side of the equation, and because this equation is equal to zero one can multiply through by a constant, called a Lagrange multiplier, and the equation will still be zero:

$$\lambda_k \left[ \langle x^k \rangle - \sum_{j=1}^{n} x_j^k f_j \right] = 0. \quad (25.3)$$

Additionally, if one has more than one constraint, one can sum over the constraints and the sum is still zero:

$$\sum_{k=0}^{m} \lambda_k \left[ \langle x^k \rangle - \sum_{j=1}^{n} x_j^k f_j \right] = 0. \quad (25.4)$$

Because this equation is zero, it can be added to the Shannon entropy without changing its value:

$$S = -\sum_{j=1}^{n} f_j \log(f_j) + \sum_{k=0}^{m} \lambda_k \left[ \langle x^k \rangle - \sum_{j=1}^{n} x_j^k f_j \right]. \quad (25.5)$$

To assign numerical values to the $f_j$, Eq. (25.5) is maximized with respect to variations in the $f_i$. The resulting equations can be solved for the functional form of the probability. Taking the derivative with respect to $f_i$ and solving, one obtains:

$$f_i = Z(m, \lambda)^{-1} \exp \left\{ \sum_{k=1}^{m} \lambda_k x_i^k \right\} \quad (25.6)$$

where $Z(m, \lambda)$ is a normalization constant that is a function of both the number of Lagrange multipliers and their values. This equations gives the functional form of the maximum entropy method of moments probability distribution in terms of the Lagrange multipliers $\lambda_j$, but one must also satisfy the constraints, namely:

$$\langle x^k \rangle = \sum_{i=1}^{n} x_i^k f_i \quad (k = 1, \ldots, m). \quad (25.7)$$

Equations (25.6) and (25.7) are a system of coupled nonlinear equations for the Lagrange multipliers. To solve for the values of the Lagrange multipliers that maximize the entropy, one typically uses
Figure 25.8: The First 10 Power And Central Moments

<table>
<thead>
<tr>
<th>Moment</th>
<th>Power</th>
<th>Central</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>9.96127964E-01</td>
<td>0.00000000E+00</td>
</tr>
<tr>
<td>2</td>
<td>9.92317063E-01</td>
<td>4.61424576E-05</td>
</tr>
<tr>
<td>3</td>
<td>9.88566722E-01</td>
<td>1.95337184E-08</td>
</tr>
<tr>
<td>4</td>
<td>9.84876378E-01</td>
<td>6.64319953E-09</td>
</tr>
<tr>
<td>5</td>
<td>9.81245478E-01</td>
<td>1.06175263E-11</td>
</tr>
<tr>
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<td>9.77673479E-01</td>
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</tr>
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<td>9.74159848E-01</td>
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<tr>
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<td>5.63247606E-16</td>
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<td>9.67305611E-01</td>
<td>1.15656817E-18</td>
</tr>
<tr>
<td>10</td>
<td>9.63963991E-01</td>
<td>2.38918537E-19</td>
</tr>
</tbody>
</table>

Figure 25.8: The first 10 power and central moments computed from the samples shown in Fig. 25.7.

A Newton-Raphson [50] searching algorithm. This searching algorithm Taylor expands Eq. (25.5) about the current estimated values of the Lagrange multipliers to second order, and then solves for the values of the change in Lagrange multipliers that makes the derivatives go to zero. The procedure must be iterated a few times and, when it converges, it typically converges quadratically.

To make this more concrete, suppose one computes the first 10 moments, of the samples shown in Fig. 25.7 and uses them in a maximum entropy method of moments calculation. What would happen to the maximum entropy distribution as more and more moments are incorporated into the calculation? The first 10 moments are shown in Fig. 25.8. Two sets of moments are shown, the power moments and the central moments. The power moments are given by

\[
\langle \text{Power Moment } k \rangle = \frac{1}{N} \sum_{i=1}^{N} d_i^k
\]  

(25.8)

and the central moments are given by

\[
\langle \text{Central Moment } k \rangle = \frac{1}{N} \sum_{i=1}^{N} (d_i - \bar{d})^k
\]  

(25.9)

where \( N \) is the total number of data values and \( \bar{d} \) is the mean data value.

If one incorporates the power moments one at a time into a maximum entropy method of moments calculation, the distributions shown in Fig. 25.9 result. The flat line marked with inverted triangles is the zeroth moment, i.e., a uniform distribution. The tilted line marked with closed triangles is an exponential distribution, and because the samples are far from exponentially distributed, this distribution is almost a uniform distribution. Finally, the remaining curves (solid unmarked lines) are the maximum entropy method of moments distributions corresponding to power moments two through seven. Note that these distributions are nearly identical, differing only near the peak values.

In Fig. 25.8, a total of 10 moments were given, however, in Fig. 25.9 only eight maximum entropy method of moment distributions are shown, corresponding to \( k = 0, 1, \ldots, 7 \). The reason for this is that the numerical calculation failed to converge when more than the 7 nontrivial moments
Figure 25.9: The maximum entropy moment distributions as a function of increasing numbers of moments. The flat line with open triangles is a normalized uniform density resulting from using only the zeroth moment. When the first moment is incorporated (line with closed triangles), not much changes because an exponential distribution cannot represent the distribution of samples shown in Fig. 25.7. However, for second and higher moments (dotted unmarked lines) all of the maximum entropy method of moments distributions closely resemble each other with only minor variations. Only density functions corresponding to moments zero through 7 are shown, the numerical algorithm failed to converge for power moments greater than 7.
were incorporated into the calculation. This is typical of the numerical calculations used in solving maximum entropy method of moments problems. Above some number of moments, the searching algorithm fails to converge or the numerical values of the moments were incompatible and no maximum entropy solution exists, see Meed and Papanicolaou [43] for the conditions under which the maximum entropy method of moments can fail.

This completes this review of the maximum entropy method of moments. Here is a short list of some of the problems with this technique:

1. The maximum entropy method of moments did not use the data samples shown in Fig. 25.7; rather one must compute a number of moments from the samples and use these moments in the calculations. From a Bayesian standpoint this is a rather ad hoc thing to do and has no justification whatsoever. By its very nature, Bayesian probability theory uses the raw data; not the moments, and if the moments are needed, they will show up automatically, they won’t have to be artificially forced into the problem.

2. There is no way to determine how many moments, Lagrange multipliers, are needed. That is to say, the maximum entropy method of moments has an arbitrary component to it: one must guess the number of moments, or simply continue adding moments until the procedure fails.

3. There is no way to consistently find the maximum entropy method of moments solution. From a finite data sample, the moments can be mutually incompatible and, consequently, no solution may exist [43]. And even if the maximum entropy solution exists, searching algorithms such as Newton-Raphson, which is commonly used on this problem [43, 50], may not be able to find it.

4. There is no way to put error bars on the Lagrange multipliers. Because the maximum entropy method of moments picks out an extremum, the question of putting error bars on the Lagrange multipliers almost does not make sense. After all, maximum entropy picks out a single point. Nonetheless, from a Bayesian perspective, for a finite amount of data one should be able to put error bars on the multipliers, or, better yet, compute the posterior probability for the Lagrange multipliers given the data and the prior information.

5. The same comments apply to the assigned density function. Because the maximum entropy method of moments picks out a single value, there is no way to determine how uncertain one is of the estimated density function. As far as maximum entropy is concerned, there is only a single density function. But from a Bayesian standpoint, this is simply false. From a finite sample, probability theory would never pick out a single density function; rather, probability theory will indicate a range of values that the density function could take on that are consistent with the available data and prior information.

When the maximum entropy method of moments works, it gives a good representation of the underlying density function that quickly converges as a function of the number of constraints (moments). However, the maximum entropy method of moments is not a Bayesian techniques: it does not use the raw data, there is no way to determine how uncertain one is of the resulting density function, and it is not uncommon for the maximum entropy method of moments to fail because the set of moments are incompatible. A true Bayesian calculation does none of these things. It would always give a results in terms of the calculated posterior probability distributions for the number and value of the Lagrange multipliers, and it would do this even if the calculated moments are incompatible.
25.4 The Bayesian Calculations

To resolve these difficulties, Bayesian probability theory will be applied to compute the posterior probability for the number of Lagrange multipliers. The posterior probability for the number of multipliers \( m \) given all of the data \( D \) is computed using Bayes’ theorem [1]:

\[
P(m|D) = \frac{P(m|I)P(D|mI)}{P(D|I)} \tag{25.10}
\]

where \( P(m|I) \) is the prior probability for the number of Lagrange multipliers, \( P(D|mI) \) is a marginal direct probability for the data given the number of multipliers. Finally, \( P(D|I) \) is a normalization constant and is computed using the sum and product rules of probability theory:

\[
P(D|I) = \sum_{m=1}^{\nu} P(D|mI) = \sum_{m=1}^{\nu} P(m|I)P(D|mI) \tag{25.11}
\]

where \( \nu \) is some given upper limit on the number of Lagrange multipliers.

In Eq. (25.10), the Lagrange multipliers do not appear. Consequently, Eq. (25.10) is a marginal posterior probability where the Lagrange multipliers have been removed from the right-hand side using the sum rule of probability theory:

\[
P(m|DI) \propto P(m|I) \int P(D|\lambda_1 \cdots \lambda_m|mI)d\lambda_1 \cdots d\lambda_m \tag{25.12}
\]

where \( P(D|\lambda_1 \cdots \lambda_m|mI) \) is the joint probability for all of the data \( D \equiv \{d_1, \ldots, d_N\} \) and the Lagrange multipliers given the number of multipliers \( m \) and the prior information \( I \). Note that the normalization constant has been dropped, the equal sign has been replaced by a proportionality sign, and this probability distribution must be normalized at the end of the calculation. Applying the product rule to the right-hand side of this equation results in:

\[
P(m|DI) \propto P(m|I) \int P(\lambda_1 \cdots \lambda_m|mI)P(D|\lambda_1 \cdots \lambda_m I)d\lambda_1 \cdots d\lambda_m. \tag{25.13}
\]

Assuming logical independence of the data samples, the right-hand side of this equation can be factored:

\[
P(m|DI) \propto P(m|I) \int P(\lambda_1 \cdots \lambda_m|mI) \prod_{i=1}^{N} P(d_i|\lambda_1 \cdots \lambda_m I)d\lambda_1 \cdots d\lambda_m. \tag{25.14}
\]

Finally, assuming logical independence of the Lagrange multipliers, \( P(\lambda_1 \cdots \lambda_m|mI) \) may also be factored to obtain

\[
P(m|DI) \propto P(m|I) \int \left[ \prod_{j=1}^{m} P(\lambda_j|mI) \right] \left[ \prod_{i=1}^{N} P(d_i|\lambda_1 \cdots \lambda_m I) \right] d\lambda_1 \cdots d\lambda_m. \tag{25.15}
\]

The direct probability for the data given the number of Lagrange multipliers and their values, \( P(d_i|m\lambda_1 \cdots \lambda_m I) \), is the maximum entropy method of moments probability given in Eq. (25.6).
Substituting Eq. (25.6) into Eq. (25.15) one obtains

\[ P(m|DI) \propto P(m|I) \int \left[ \prod_{j=1}^{m} P(\lambda_j|mI) \right] \left[ \prod_{i=1}^{N} \frac{1}{Z(m, \lambda)} \exp \left\{ \sum_{k=1}^{m} \lambda_k d_i^k \right\} \right] d\lambda_1 \cdots d\lambda_m \]  

(25.16)

as the posterior probability for the number of Lagrange multipliers given the data and the prior information. Expanding the products gives

\[ P(m|DI) \propto P(m|I) \int \frac{P(\lambda_1|I) \cdots P(\lambda_m|I)}{Z(m, \lambda)^N} \exp \left\{ \sum_{k=1}^{m} \sum_{i=1}^{N} \lambda_k d_i^k \right\} d\lambda_1 \cdots d\lambda_m, \]

(25.17)

and evaluating the sum over the data values results in

\[ P(m|DI) \propto P(m|I) \int \frac{P(\lambda_1|I) \cdots P(\lambda_m|I)}{Z(m, \lambda)^N} \exp \left\{ \sum_{k=1}^{m} \lambda_k N \bar{d}^k \right\} d\lambda_1 \cdots d\lambda_m \]  

(25.18)

where the \( \bar{d}^k \) are the power moments of the samples defined in Eq. (25.7).

The functional form of Eq. (25.18) is interesting in several ways. First, the data do not appear in this equation, rather there are \( m \) power moments of the data. These power moments are called sufficient statistics. They are sufficient in that they are the only quantities needed for the inference; the data itself are irrelevant. Only maximum entropy distributions have sufficient statistics. In this case, the constraint functions are simple polynomials, \( x^k \), so the sufficient statistics are the power moments calculated using the data samples. Second, every term in the sum in Eq. (25.18) is of the form \( \lambda_k N \bar{d}^k \), which can always be driven to infinity by choosing \( \lambda_k \) suitably. So one might think that this could not possibly be a well-behaved probability density function. However, this is not the case, because this is a fully normalized probability density function and the normalization constant is a function of both the number of Lagrange multipliers and their values. Any attempt to drive the exponent to infinity simply results in a larger normalization constant that keeps everything finite.

The only remaining steps in the calculation are to assign the prior probabilities appearing in Eq. (25.18) and to perform the indicated calculations. In the numerical calculations that are done, all probability assignments are discretely normalized to ensure that one has probability distributions, not density functions. Probability density functions can be larger than one, and because of the functional form of the posterior probability, Eq. (25.18), this is not allowed. The prior probabilities were assigned as follows. The prior probability for the number of multipliers, \( P(m|I) \), was assigned using an exponential prior probability:

\[ P(m|I) \propto \frac{1}{Z_m(\nu)} \exp \left\{ -m \right\} \quad (1 \leq m \leq \nu) \]  

(25.19)

were the \( \nu \) is the upper limit on the number of moments and expresses a belief that the number of multipliers should be small, rather than large. The normalization constant \( Z_m(\nu) \) was computed as

\[ Z_m(\nu) = \sum_{m=1}^{\nu} \exp \left\{ -m \right\} = \frac{1 - e^{-\nu}}{e - 1} \]  

(25.20)

and ensures that the prior probability for the number of Lagrange multipliers is normalized and always less than one.
The prior probability for each Lagrange multiplier was assigned using a Gaussian of the form:

$$P(\lambda_j | I) \propto \frac{1}{Z_{\lambda j}} \exp \left\{ -\frac{\lambda_j^2}{2\sigma^2_{\lambda}} \right\} \quad (\lambda_{\text{Min}} \leq \lambda_j \leq \lambda_{\text{Max}})$$  \hspace{1cm} (25.21)

where $\sigma_\lambda$ is the standard deviation of this Gaussian, $\lambda_{\text{Min}}$ is the smallest value the Lagrange multipliers can take on, $\lambda_{\text{Max}}$ is the largest, and $Z_{\lambda j}$ is the normalization constant for the prior probability for the $j$th Lagrange multiplier. The standard deviation, $\sigma_\lambda$, was set so that the prior decayed to 7 $e$-foldings at $\lambda_{\text{Min}}$ and $\lambda_{\text{Max}}$. This prior probability distribution was normalized discretely. To compute the normalization constant, the prior range was divided into 500 intervals and then summed. In this sum, the $k$th discrete value of the $j$th Lagrange multiplier is given by

$$\lambda_{jk} = \lambda_{\text{Min}} + d\lambda (k-1) \quad (1 \leq k \leq 501)$$  \hspace{1cm} (25.22)

with

$$d\lambda = \frac{(\lambda_{\text{Max}} - \lambda_{\text{Min}})}{500}. \hspace{1cm} (25.23)$$

The normalization constant was computed as

$$Z_{\lambda j} = \sum_{k=1}^{501} \exp \left\{ -\frac{\lambda_{jk}^2}{2\sigma^2_{\lambda}} \right\}. \hspace{1cm} (25.24)$$

It is this normalization constant that is used in Eq. (25.21).

The last normalization constant that must be set is $Z(m, \lambda)$, the normalization constant associated with the maximum entropy method of moments probability density function. Again, this probability density function was discretely normalized so that a probability distribution was actually used in the numerical calculations. Thus, all values computed using Eq. (25.6) will strictly be probabilities, not probability densities. The normalization constant is computed using the range of the data samples. If the minimum and maximum data value are represented by $d_{\text{Min}}$ and $d_{\text{Max}}$ respectively, then

$$x_i = d_{\text{Min}} + dx (k-1) \quad (1 \leq k \leq 501)$$  \hspace{1cm} (25.25)

with

$$dx = \frac{(d_{\text{Max}} - d_{\text{Min}})}{500} \hspace{1cm} (25.26)$$

and

$$Z(m, \lambda) = \sum_{i=1}^{501} \exp \left\{ \sum_{k=1}^{m} \lambda_k x_i^k \right\}. \hspace{1cm} (25.27)$$

Again, this normalization constant ensures that Eq. (25.6) is a probability distribution and sums to one on the $x_i$. The posterior probability for $m$ is obtained by substituting Eqs. (25.19, 25.21 and 25.27) into Eq (25.18) to obtain:

$$P(m|DI) \propto \int \frac{\exp \left\{ -m \right\}}{Z_m Z_{\lambda} Z(m, \lambda)^N} \exp \left\{ -\sum_{j=1}^{m} \frac{\lambda_j^2}{2\sigma^2_{\lambda}} \right\} \exp \left\{ \sum_{k=1}^{m} \lambda_k N d_k^k \right\} d\lambda \hspace{1cm} (25.28)$$
where \( d\lambda \) means the integral over all \( m \) Lagrange multipliers. Equation (25.28) is the posterior probability for the number of Lagrange multipliers.

In addition to computing the posterior probability for the number of Lagrange multipliers, the posterior probability for \( \lambda_j \) given the number of Lagrange multipliers and the data is also needed. However, this calculation is so similar to the one just given that it will not be repeated. Rather, note that the integrand of Eq. (25.28) is the joint posterior probability for all of the parameters, \( P(m\lambda_1 \cdots \lambda_m | DI) \), and can be used to generate the posterior probability for any one of the Lagrange multipliers by applying the sum rule of probability theory:

\[
P(\lambda_j | mDI) \propto \int \frac{1}{Z^m Z(m, \lambda)^m} \exp \left\{-\sum_{j=1}^{m} \frac{\lambda_j^2}{2\sigma^2}\right\} \times \exp \left\{\sum_{k=1}^{m} \lambda_k N d_k\right\} d\lambda_1 \cdots d\lambda_{j-1} d\lambda_{j+1} \cdots d\lambda_m.
\]  

To arrive at this result, eliminated the prior probability for the number of Lagrange multipliers, since this probability is a constant when \( m \) is given. Additionally, all the Lagrange multipliers, except \( \lambda_j \), were removed using marginalization. This results in the posterior probability for the single remaining Lagrange multiplier, \( \lambda_j \).

A Markov chain Monte Carlo simulation with simulated annealing was used to draw samples from the integrand of Eq. (25.28) using the data shown in Fig. 25.7. In a typical run, 50 simulations are run simultaneously and in parallel, and 50 samples from each simulation are gathered, so there are 2500 total Markov chain Monte Carlo samples for the number of multipliers and their values. Monte Carlo integration was then used to compute the posterior probability for the number of Lagrange
multipliers given the data and the prior information. The posterior probability for the number of multipliers is shown in Fig. 25.10(A). Note that this posterior probability indicates that only two Lagrange multipliers are needed to represent the density distribution of the data. Consequently, Bayesian probability theory strongly indicates that the data shown in Fig. 25.7 are Gaussianly distributed.

After determining that the number of Lagrange multipliers was two, the joint posterior probability for the two Lagrange multipliers was sampled. These Markov chain Monte Carlo samples are shown in Fig. 25.10(B). Each dot in this figure is one sample from one of the 2500 Markov chain Monte Carlo simulations. By using Monte Carlo integration, one can obtain samples from the posterior probability for each Lagrange multiplier, Fig. 25.11. These one dimensional samples can be used to compute mean and standard deviation estimates of the Lagrange multipliers. However, a means of visually displaying the samples is also desirable. A binned histogram could be used, but even with 2500 samples such histograms are often very rough. Consequently, the program that implements this calculation uses a Gaussian kernel density estimation procedure to generate its histograms.

The 51 bin histograms shown in Fig. 25.11 were generated using a Gaussian kernel that decays to 3 e-foldings over 6 bins. This kernel was centered on each Markov chain Monte Carlo sample and then added to the histogram by evaluating the kernel at each value of the histogram’s x-axis. As a consequence, each of the 2500 samples was smeared out over a 6 bin interval using the Gaussian kernel. Finally, the normalization is set so that the sum over the 51 bins was one. As can be seen from this figure, Lagrange multiplier 1 is estimated to be approximately 0.65 ± 0.08 and multiplier number 2 is approximately −4.4 ± 0.14. Note that these probability density functions for the Lagrange multipliers are not very compact, and the standard deviation of these probability density functions are 0.08 and 0.14, respectively. Given that there are about 2000 data values and the data are noiseless, this is not a very good determination. Thus, while maximum entropy gives one Lagrange multiplier for each moment, it does not indicate how uncertain one is of these values and the uncertainty in the value of the Lagrange multipliers can be large. In the example given here, they have a relative uncertainty of about 20% for multiplier 1 and about 7% for multiplier 2.

Each of the 2500 Markov chain Monte Carlo samples of the Lagrange multipliers shown in
Figure 25.12: The model averaged density function with error bars. A Markov chain Monte Carlo simulation was used to draw samples from the joint posterior probability for the number of multipliers and their values. A total of 2500 samples were drawn. Each sample corresponds to a density function that is consistent with the data and the prior information. The solid line in this plot is the mean value of the 2500 density function estimates and the error bars are the standard deviation of the estimates.

Fig. 25.10(B) corresponds to a density function estimate that is consistent with the given data and prior information. One can use the Lagrange multiplier samples to compute the unknown density function. For example, one could compute the density function at the values specified by Eq. (25.25). For each $x_i$, there are 2500 samples of the density function. For a given $x_i$, one can compute the mean and standard deviation. This mean and standard deviation are shown in Fig. 25.12. At each point in this plot, the mean is the solid line and the standard deviation is shown as the error bar. These error bars are a direct measure of the amount of uncertainty in the Lagrange multipliers and thus directly reflect the uncertainty in the underlying density function.

### 25.5 Summary and Conclusions

The maximum entropy method of moments is fraught with difficulties. It is computationally unstable. One cannot use the raw data; rather one must compute an unknown number of moments using the data and then use those moments in the maximum entropy method of moments. There is
no way to determine how many moments are needed and, finally, there is no way to determine how uncertain one is of the estimated density function.

However, if one uses the maximum entropy formalism to assign the probability for the data given both the number of moments and the value of the Lagrange multipliers, then maximum entropy will assign Eq. (25.6) as the functional form of the probability distribution. One can then use the rules of Bayesian probability theory to compute the posterior probability for the parameters, including the number of Lagrange multipliers. Because the Bayesian calculations are all computed using a forward calculation, i.e., given the values of the parameters, compute a probability, and never attempt to solve for the values of the multipliers that satisfy the constraints, Eq. (25.7), one never runs into computational difficulties. Additionally, the final results are all expressed as probability distributions, so one always knows how uncertain one is of all of the parameters. Finally, because the calculations are implemented using a Markov chain Monte Carlo simulation, one has samples from the joint posterior probability for all of the parameters appearing in Eq. (25.28). These samples can be used to form a mean and standard deviation estimate of each point in the unknown density function, thus putting error bars on the unknown density functions value.
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