

Bayesian Data-Analysis Toolbox
Release 4.23, Manual Version 3

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Appendix H

Outlier Detection

From a Bayesian perspective one must define what is meant by an outlier and then apply the rules of Bayesian probability theory to compute the appropriate posterior probabilities. In the calculations done in the Bayesian Analysis software, all of the Ascii models are of the form

$$d_i = G(\Omega, t_i) + n_i \quad (\text{H.1})$$

where d_i represents a single data item sampled at time t_i , $G(\Omega, t_i)$ is a model function containing some parameters Ω to be estimated and the data are contaminated by additive noise n_i of some unknown standard deviation σ .

By an outlier we mean that for some times t_j this model does not apply, rather at these times the data and the model are related by

$$d_j = A_j + n_j \quad (\text{H.2})$$

where A_j is the value of the outlier at time t_j . These two models can be combined to obtain a model that includes both the parameters and the outliers:

$$d_i = G(\Omega, t_i)(1 - \delta_i) + \delta_i A_i + n_i \quad (\text{H.3})$$

where δ_i is the probability that the i th data value is an outlier and A_i is the outlier value.

In practice, we simply assume that $\delta_j = 0$ for the vast majority of the data, i.e., there are only a few outliers in a given data set. So when the Markov chain Monte Carlo simulations are running they propose a change in the number of outliers. This change could be an increase or a decrease in the number of outliers. If its a decrease, the Markov chain Monte Carlo simulation chooses one of the outliers at random and proposes that it was not an outlier after all. If its an increase, the proposed change is to change the δ_i corresponding to the largest residual to one. Here the residual means the difference between the data and the model, and the model is $G(\Omega, t_i)$ where there is no outlier and its A_j when there is an outlier. When proposing an outlier, one must propose a value for the A_j and the obvious choice is to set A_j to d_j and then simulate A_j like any other parameter. Using this proposed model, all of the parameters in the the Markov chain Monte Carlo simulation are varied until they reaches equilibrium. Finally, the proposed updated simulation is accepted or rejected according the the acceptance rules for a Metropolis-Hastings algorithm.

In a typical data set, the number of outliers is zero. Additionally, the computational burden introduced by turning on outlier detection is substantial, often doubling the time required to run an

Figure H.1: The Posterior Probability For The Number of Outliers

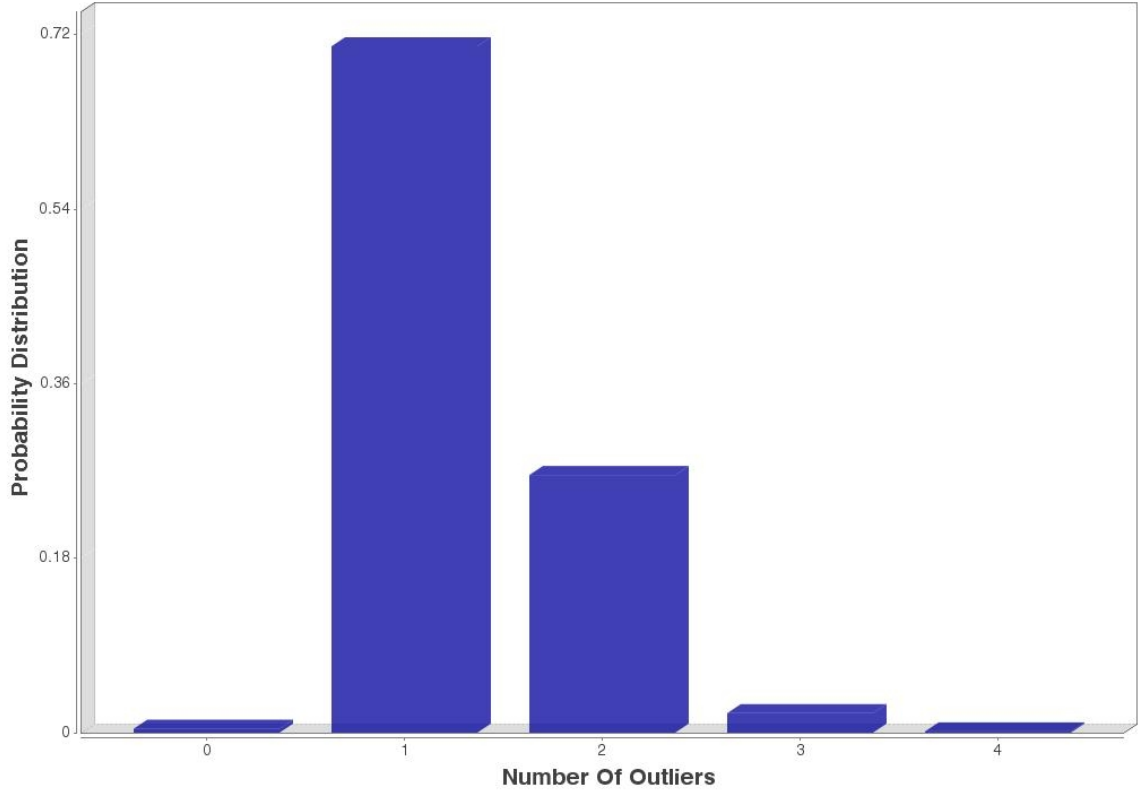


Figure H.1: When outlier detection is enabled in a Markov chain Monte Carlo simulation, a set of extra parameters are added to the model. These parameters include the number, location and value of each outlier. As a result, the posterior probability for the number of outliers is added to the outputs. Additionally, the expected values of these parameters are written into the McMC values report.

analysis. Consequently, we do not look for outliers unless the “Find Outliers” check box is toggled on, i.e., you have pretty good evidence that there is an outlier in the data.

When outlier detection is turned on there is one additional output plot, the posterior probability for the number of outliers. This plot is illustrated in Fig. H.1. The way this posterior probability is generate is to simply count the number of simulations having zero outliers, one, two, etc. and then normalize the posterior by dividing by the total number of simulations. From the plot shown in Fig. H.1, its pretty obvious that about 70% of the simulations had at least one outlier and another 30% had two or three.

When we are computing the means and standard deviations of the output parameters when outlier detection is activated, none of this makes any difference. We simply compute the mean value

of a parameter using all of the McMC simulations and output its value. This is written formally as:

$$\langle \Omega \rangle = \frac{1}{N} \sum_{j=1}^N \Omega_j \quad (\text{H.4})$$

where Ω is the parameter being estimates and Ω_j is the value of the parameter in the j th Markov chain Monte Carlo simulation. Suppose that some fraction of the simulations had one outlier, lets call that fraction r . We are free to split the simulations into two sets, one set of $(1-r)N$ simulations having zero outliers, and one set of rN simulations having one outlier. Lets adopt the notation Ω_k for the parameter in k th simulations having no outliers, and $\hat{\Omega}_j$ for the parameters in j th simulations having one outlier. Then the expected value of the parameter can be written as:

$$\begin{aligned} \langle \Omega \rangle &= \frac{1}{N} \left[\sum_{j=1}^{rN} \hat{\Omega}_j + \sum_{k=1}^{(1-r)N} \Omega_k \right] \\ &= \frac{rN}{rN^2} \sum_{j=1}^{rN} \hat{\Omega}_j + \frac{(1-r)N}{(1-r)N^2} \sum_{k=1}^{(1-r)N} \Omega_k \\ &= \frac{rN}{N} \bar{\hat{\Omega}} + \frac{(1-r)N}{N} \bar{\Omega} \\ &= r\bar{\hat{\Omega}} + (1-r)\bar{\Omega} \end{aligned} \quad (\text{H.5})$$

where $\bar{\hat{\Omega}}$ is the average value of the Ω parameter in the simulations having an outlier, and similarly $\bar{\Omega}$ is the average value of the Ω parameter in simulations having no outliers. So the expected value of the parameter is a weighted average of the parameters estimates having zero and one outliers where the weights are just the probability for the number of number of outliers. We mentioned earlier when we computed the average value of a parameter across the simulations that no attempt was made to account for the presence of an outlier, and the reason now becomes obvious. The relative weighting of the various simulations has already been taken care of when the posterior probability for the number of outliers was computed.

In addition to the plot containing the posterior probability for the number of outliers, we also modify the data, model and residual plots. This modification is illustrated in Fig. H.2 where we have placed a large red dot at the location of an outlier. If multiple outliers had been present, the multiple red dot would be present. Note one last thing on this plot, when we compute the model having an outlier, the point at which the outlier is present is the outlier value not the value computed from the model equation. In this example, the model equation is an exponential plus a constant and such a function could never exhibit the dip seen in Fig. H.2.

Figure H.2: The Data, Model and Residual Plot With Outliers

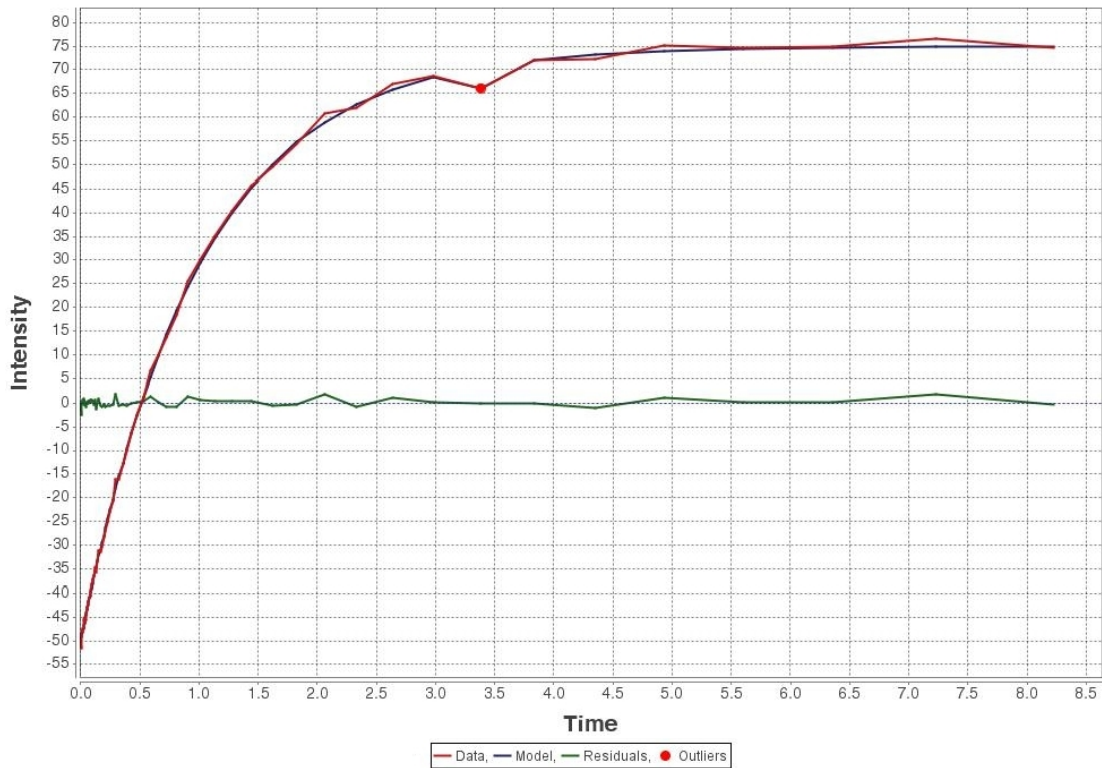


Figure H.2: The Data, Model and Residual plot is also modified when an outlier is present. The modification is pretty simple, at the point where an outlier is present we mark the location with a large red dot. Also note that the outlier value replaces the value computed from the model equation, in this case the exponential model is replaced by the outlier value at the location of the outlier.

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