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INFORMATION CRITERIA AND HIGHER EIGENMODE ESTIMATION IN MONTE CARLO CALCULATIONS

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ABSTRACT

Recently developed Monte Carlo methods of estimating the dominance ratio (DR) rely on autoregressive (AR) fittings of a computed time series. This time series is obtained by applying a projection vector to the fission source distribution of the problem. The AR fitting order necessary to accurately extract the mode corresponding to DR is dependent on the number of fission source bins used. This makes it necessary to examine the convergence of DR as the AR fitting order increases. Therefore, we have investigated if the AR fitting order determined by information criteria can be reliably used to estimate DR. Two information criteria have been investigated: Improved Akaike Information Criteria (AICc) and Minimum Descriptive Length Criteria (MDL). These criteria appear to work well when applied to computations with fine bin structure where the projection vector is applied.

Key Words: Monte Carlo, information criteria, eigenmode, AICc, MDL

1. INTRODUCTION

Estimations of the ratio of non-fundamental to fundamental mode eigenvalues of the fission source distribution have useful applications in Monte Carlo calculations, such as confidence interval estimation of the fission source distribution [1,2]. Recently, much work has been focused on estimating these ratios using time series analysis techniques [3]. These methods use autoregressive (AR) and autoregressive moving average (ARMA) fittings of a time series computed from the fission source distribution in order to estimate the dominance ratio (DR), the ratio of the largest non-fundamental mode eigenvalue to the fundamental mode eigenvalue. One method in particular, the coarse mesh projection method [4], has proven to be an accurate semi-black-box estimator of DR.

In general, projection approaches to eigenvalue ratio estimation depend on the spatial binning of the fission source distribution. The bin size and shape affects how the eigenvalue ratio estimation converges and what AR order is necessary to estimate it. While it was shown that the coarse mesh projection method only requires a four-bin mesh with a first order AR fitting to reliably estimate DR of a two-dimensional problem, the choice of mesh depended on how the eigenfunction corresponding to the largest non-fundamental mode eigenvalue roughly looked like. A method that does not require such knowledge is desired. Ideally, the projection approach should work with regularly assigned fine bins, such as one bin assigned to each fuel bundle. However, a projection with fine bins will pick up the fluctuating components from higher eigenmodes, leading to inaccurate computation of DR with low order AR fittings. To overcome this, the AR fitting order must be increased. Therefore, it is important to provide a way to determine at what AR fitting order the DR computation has converged if fine bin structure is to be used. One way to do this is by using information criteria [5-7]. Methods such as Improved Akaike Information Criteria (AICc) and Minimum Descriptive Length Criteria (MDL), balance the complexity of the model against the goodness-of-fit to provide the optimal fitting order. This work investigates whether these methods can be reliably used in DR estimation.

2. SCALAR TIME SERIES VIA PROJECTION VECTOR

It has been shown [3] that the fluctuating part of the fission source distribution at the m^{th} stationary cycle, denoted $\vec{e}^{(m)T}$, in an MC iterated source calculation can be represented as

$$\vec{e}^{(m)} = \mathbf{A}_0 \vec{e}^{(m-1)} + \vec{\varepsilon}^{(m)} , \tag{1}$$

where $\mathbf{A_0}$ is the $n \times n$ noise propagation matrix and ε is a $n \times 1$ noise component matrix resulting from source particle selection and the subsequent tracking. In this case, n stands for the number of binning cells. By multiplying both sides of the equation by $\vec{e}^{(m-1)T}$ from the right and taking the expectation we can obtain the explicit expression of the matrix $\mathbf{A_0}$ as

$$\mathbf{A}_0 = \mathbf{L}_1 \mathbf{L}_0^{-1} \tag{2}$$

where

$$\begin{aligned} \mathbf{L}_0 &= E\left[\vec{e}^{(m)} (\vec{e}^{(m)})^T \right] \\ \mathbf{L}_1 &= E\left[\vec{e}^{(m)} (\vec{e}^{(m-1)})^T \right]. \end{aligned} \tag{3}$$

The eigenvalue problem of $\mathbf{A}_0$ can be written as

$$\begin{aligned} \mathbf{A}_0 \vec{b}_i &= \lambda_i \vec{b}_i \ , i = 1, \ldots, n, \\ \mathbf{A}_0^* \vec{d}_i &= \lambda_i \vec{d}_i \ , i = 1, \ldots, n, \end{aligned} \tag{4}$$

where $\mathbf{A}_0^*$ is the adjoint matrix of $\mathbf{A}_0$ and $\mathbf{A}_0^* = \mathbf{A}_0^T$ because $\mathbf{A}_0$ is real. By the standard results of linear algebra, $\mathbf{A}_0^*$ and $\mathbf{A}_0$ have the same set of eigenvalues with their eigenvectors satisfying

$$\vec{d}_j^T \vec{b}_i = 0 \quad \text{if} \quad \lambda_j \neq \lambda_i . \tag{5}$$

The eigenvalues of $\mathbf{A}_0$ are the ratio of eigenvalues $k_i / k_0, i = 1, 2, \ldots$ of the fission source distribution when $n \gg 1$ and all bins are sufficiently small.

A projection vector is then applied to $\vec{e}^{(m)}$ to create a new time series. An AR or ARMA process can estimate appropriate eigenvalue ratios as the zeroes of the characteristic polynomial. The choice of projection vector guides which eigenvalue ratio is extracted. Original methods used a projection vector $\vec{p}^T = (0,\cdots,0,1,\cdots,1)$ to conduct ARMA fitting of the half domain to draw out the information about DR [3]. The subsequent projection method [4] was very different from original methods. It used the appropriate eigenvector of the adjoint of matrix $\mathbf{A}_0$ as the projection vector. For example, to compute the first eigenvalue ratio DR, the projection vector was chosen as the first eigenvector of the adjoint of matrix $\mathbf{A}_0$. This projection vector was applied to $\vec{e}^{(m)}$ to create a new scalar time series. With this new scalar time series, the AR fitting could then be applied to estimate the eigenvalue ratio. When the projection vector is chosen in this manner and applied to the fluctuating part, the resulting equation becomes [4]

$$y^{(m)} = \lambda_k y^{(m-1)} + z^{(m)} \tag{6}$$

where

$$\begin{aligned} y^{(m)} &= \vec{d}_k^T \cdot \vec{e}^{(m)} \\ z^{(m)} &= \vec{d}_k^T \cdot \vec{\varepsilon}^{(m)} \end{aligned} \tag{7}$$

In particular, the coarse mesh projection method [4] uses a small number of bins to compute $y^{(m)}$ and estimates DR as the autocorrelation coefficient of $y^{(m)}$ based on (6). Typically, the number of bins is two, four and eight for one, two and three dimensional rectangular systems. However, the setting up of bins depends on what the eigenfunction of fission source distribution corresponding to DR roughly looks like. This means that in some cases the coarse mesh projection method might require the knowledge of the non-fundamental mode solutions of a relevant idealized problem. Practically, the projection approach with regular fine bin structure should work without requiring such knowledge. However, since the eigenvector $\vec{d}_1$ of the adjoint of $\mathbf{A}_0$ cannot be exactly computed due to statistical error in the estimation of $\mathbf{A}_0$, the projected series $y^{(m)}$ may also extract eigenmodes not corresponding to DR. In problems with fine bin structure, the small bins would contribute to the extraction of highly oscillating higher modes. For this reason, the AR fitting order in DR computation must be raised. This can be regarded as the cost of becoming independent of the knowledge of a relevant idealized diffusion/transport problem. Thus, a method to determine the proper fitting order is worth studying.

3. INFORMATION CRITERIA

In time series analysis, the relative goodness-of-fit of a statistical model can be determined using information criteria. Among them, two criteria are worth studying: AICc and MDL. Both of these methods attempt to balance the complexity of the model with its goodness-of-fit to the sample data to provide an optimal fitting order. AICc is generally used instead of Akaike Information Criteria (AIC) [5], the predecessor of AICc, as it performs better than AIC when the sample size is small and converges to AIC when the sample size is large [6]. MDL was developed by Rissanen and is consistent for a wider range of problems than AIC methods, including ARMA processes [7].

In each case, the goal is the minimization of the criteria. The criteria are expressed as follows [6,7]:

$$\text{AICc} \equiv N \cdot \ln(\xi) + N \frac{1 + k/N}{1 - (k+2)/N} \tag{8}$$

$$\text{MDL} \equiv \xi \left[1 + \frac{k}{N} \ln(N) \right]. \tag{9}$$

where N is the number of active cycles, ξ the residual variance, and k is the AR fitting order. The first term on the right hand side is proportional to the goodness-of-fit. The second term deals with the complexity of the model.

4. RESULTS

Results are presented for two problems. The first problem is the one-energy group checkerboard problem shown in Figure 1. The macroscopic cross section data are $\Sigma_t = 1.0$, $\Sigma_s = 0.7$, and $\nu\Sigma_f = 0.39$ (type H), 0.24 (type C), all in cm^{-1} in units. The reference value of DR is 0.9581, calculated by the discrete ordinates method [3]. The simulation parameters were 80,000 particles/cycle, 40,000 active cycles, and 400 inactive cycles.

H	C	H	C	H	C
C	H	C	H	C	H
H	C	H	C	H	C
C	H	C	H	C	H
H	C	H	C	H	C
C	H	C	H	C	H

$H: \Sigma_t = 1.0 cm^{-1}, \Sigma_a = 0.3 cm^{-1}, \nu\Sigma_f = 0.39 cm^{-1}$
$C: \Sigma_t = 1.0 cm^{-1}, \Sigma_a = 0.3 cm^{-1}, \nu\Sigma_f = 0.24 cm^{-1}$

Each unit is a square of 4 cm by 4 cm.

Vacuum at exterior boundaries.

Figure 1: Description of Problem 1

DR was estimated using a source mesh of one source bin per cell. Two different projection vectors were used: the binary half-domain projection vector $(0, \ldots, 0, 1, \ldots, 1)$ (zero for the first half of bins and unity for the second half of bins), and the eigenvector of the adjoint noise propagation matrix; the projection with fine bins. The order predictor results are shown in Fig. 2 & 4 and the estimated DR are shown in Fig. 3 & 5.

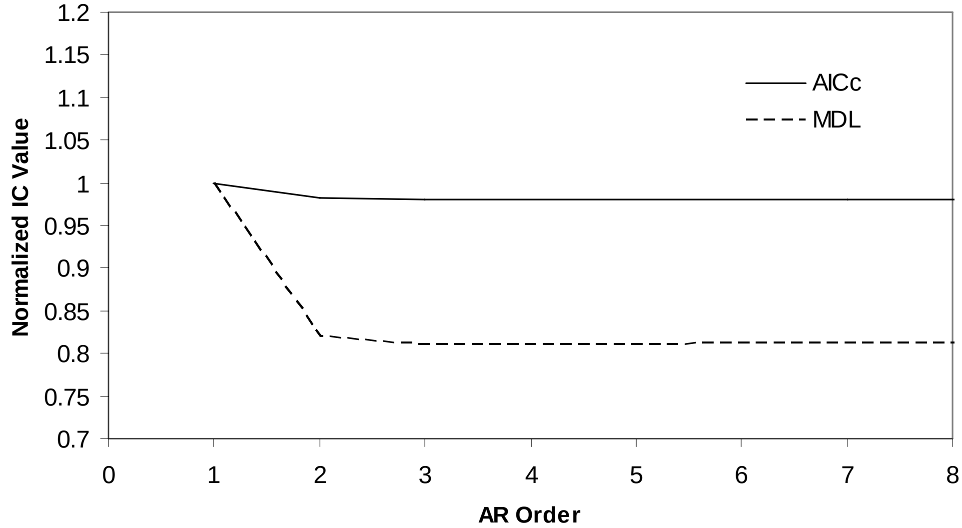

Figure 2: Order prediction for binary projection applied to Problem 1

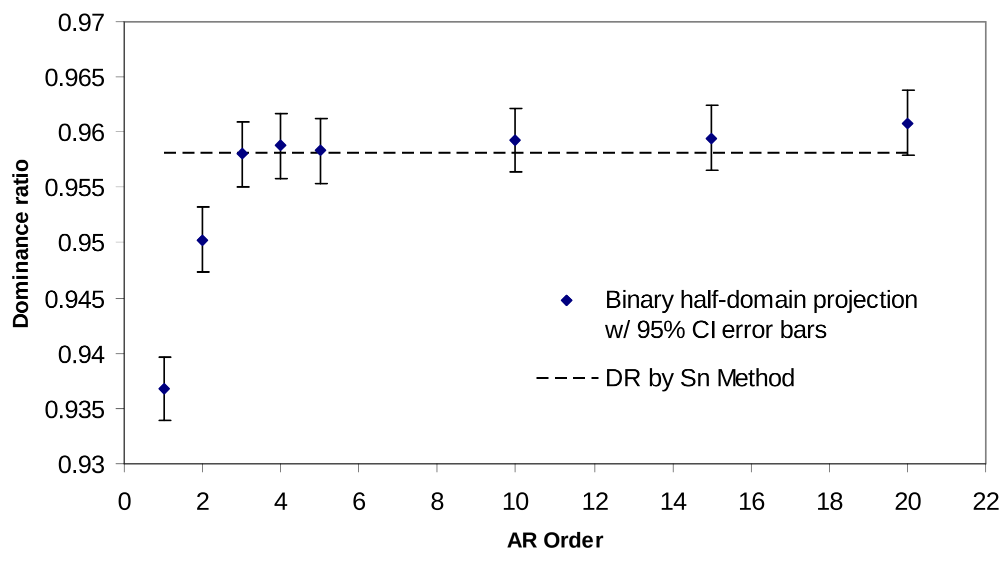

Figure 3: Binary half-domain projection applied to Problem 1

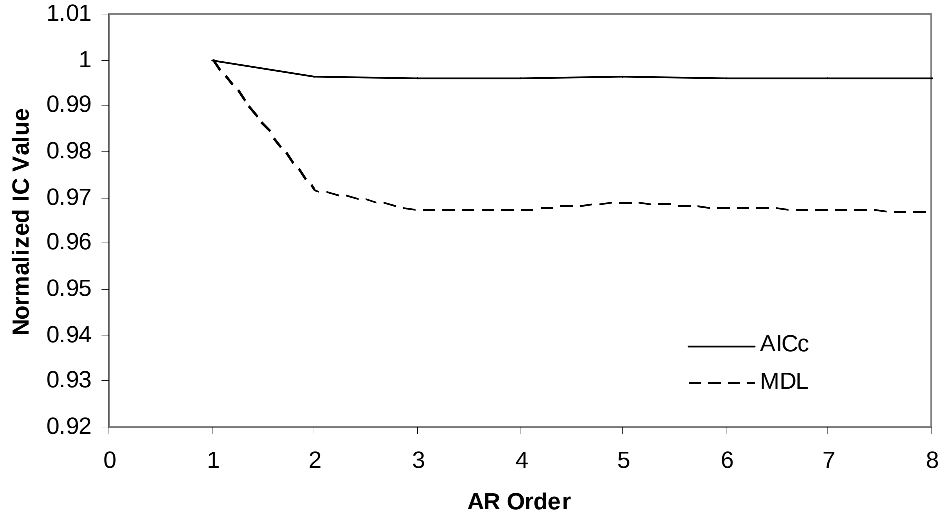

Figure 4: Order prediction for projection w/ fine bins applied to Problem 1

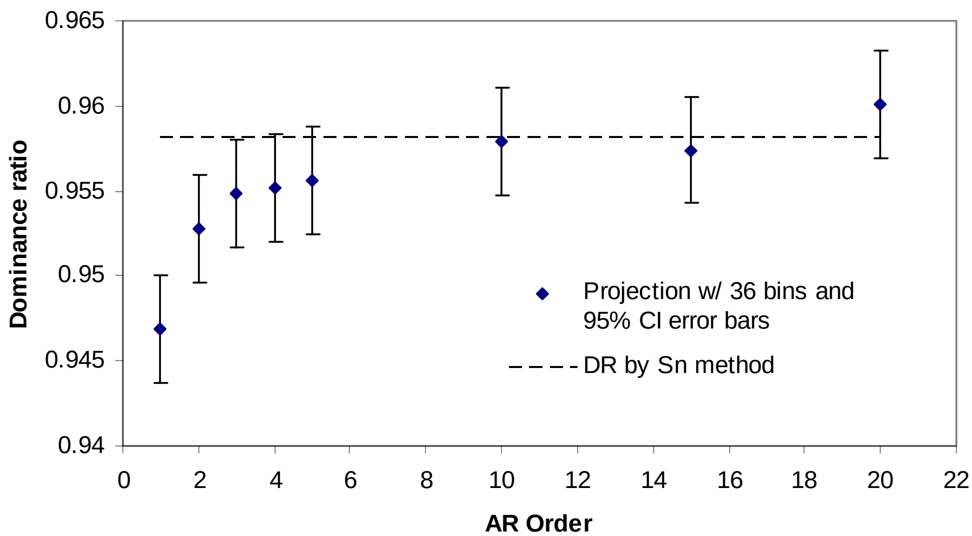

Figure 5: Projection w/ fine bins applied to Problem 1

As can be seen in Fig. 2, the decreasing trends of AICc and MDL end at order two. In Fig. 4 AICc ceases to decrease at order two and MDL at order three. The AR order at which the estimated DR (95% CI) contains the reference value for the first time is three in Fig. 3 and four in Fig. 5. The information criterion does seem to provide an estimate of the appropriate fitting order. If one chooses the order one or two larger than the order at which AICc and MDL cease to decrease, DR computation will be reliable.

The second problem is illustrated in Fig. 6: a one-group isotropic inhomogeneous and symmetric reactor system. The macroscopic cross section data are $\Sigma_t = 1.0$, $\Sigma_s = 0.7$, and $\nu\Sigma_f = 0.24$ (type 1), 0.3 (type 2), 0.39 (type 3), all in cm^{-1} in units. This system was designed to roughly model a large BWR with alternate fuel placement of different fuel assemblies and a high DR. The medium fuel (type 2) was arranged to decouple the quadrants, which artificially raises DR for computational research purposes. The reference value of DR is 0.9993 ± 0.0004 (2σ by recently established ARMA methodologies) [3]. The simulation parameters were 200,000 particles/cycle, 50,000 active cycles, and 500 inactive cycles. These parameters are not unrealistic since the real standard deviations of the sources are more than five times of the apparent standard deviations for most cells.

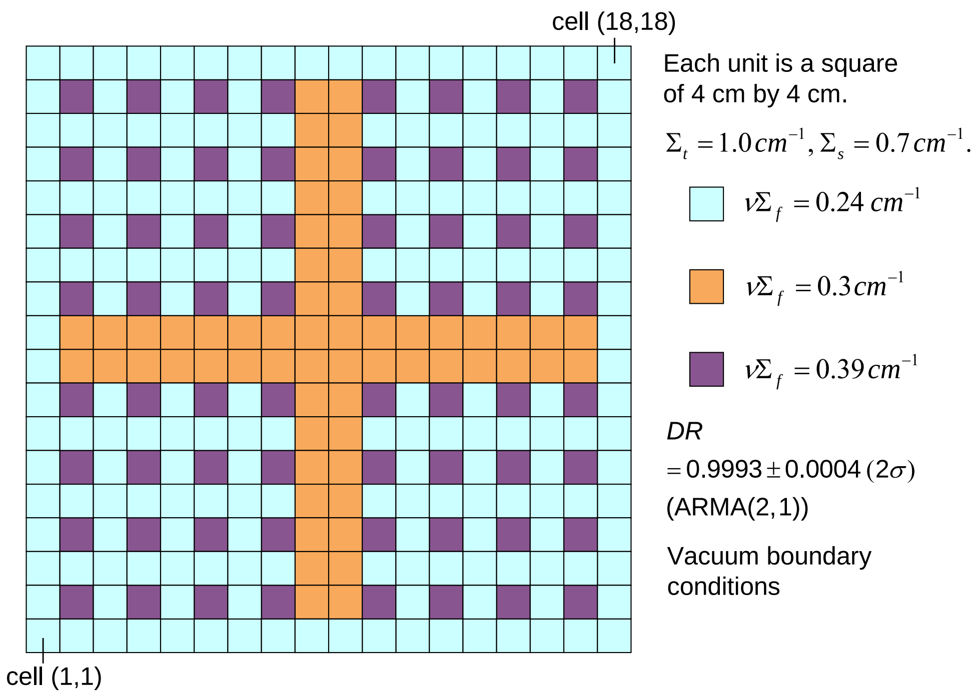

Figure 6: Description of Problem 2

Again, DR was estimated using a source mesh of one source bin per cell and the same two types of projection vectors were used. The order predictor results are shown in Fig. 7 & 9 and the estimated DR are shown in Fig. 8 & 10.

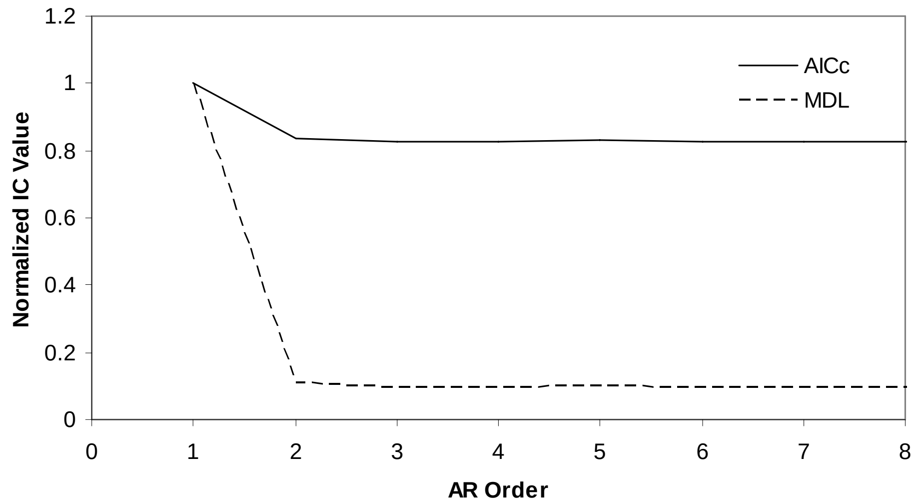

Figure 7: Order prediction for binary projection applied to Problem 2

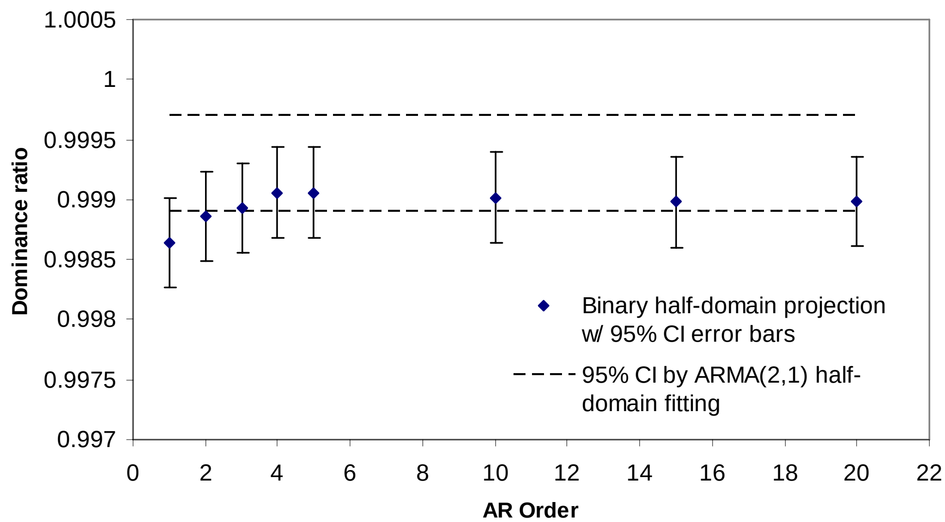

Figure 8: Binary half-domain projection applied to Problem 2

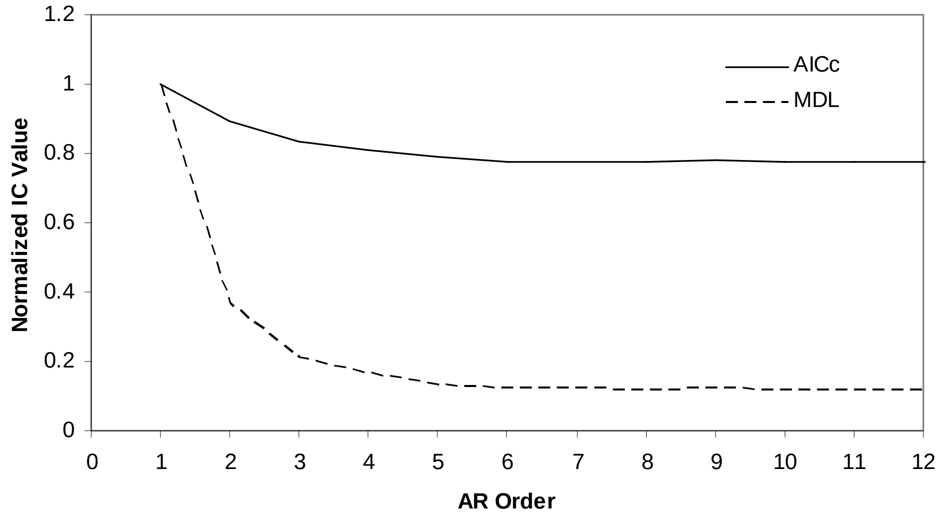

Figure 9: Order prediction for projection w/ fine bins applied to Problem 2

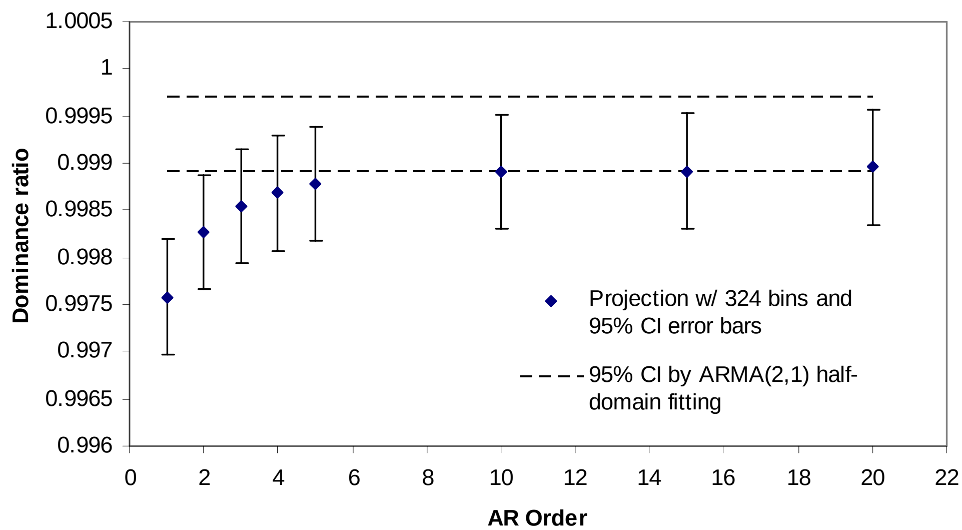

Figure 10: Projection with fine bins applied to Problem 2

Fig. 7 shows the information criteria cease to decrease at order 2 for the binary half-domain projection method, while Fig. 9 indicates an order 6 for the projection with fine bins. For the binary half domain projection vector, the estimated DR in Fig. 8 contains the reference value (the center of reference confidence interval) at order 3 for the first time. When using the projection with fine bins, the reference DR is contained at order 5 for the first time. Again, it appears that these information criteria will provide an estimate of the necessary fitting order, and though not always exact. However, choosing a fitting order one or two greater than the order indicated by the information criteria seems to work well.

5. CONCLUSIONS

Information criteria can be used to determine AR fitting order necessary for the convergence of DR estimation. The projection method with fine bin structure will work if the projection vector is chosen to be the eigenvector corresponding to the largest eigenvalue of the adjoint of the fission source noise propagation matrix and if the AR fitting order is chosen one or two greater than the order at which the decreasing trends of AICc and MDL end. AICc and MDL generally plateau well before order ten. Therefore, the projection method with fine bin structure can be developed for practical use. The projection method with binary half-domain projection will also work similarly. However, since previous work [3] showed that the selection of half-domain needed some care to prevent the cancellation of the eigenfunction corresponding to DR from occurring, the success of binary half-domain projection depends on the knowledge of higher eigenmodes, perhaps gleaned from a relevant idealized diffusion/transport problem. On the other hand, such knowledge is not required in the projection method with fine bin structure. In this respect, more research on the projection method with fine bin structure is encouraged.

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