

# Using scaling-region distributions to select embedding parameters

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## Abstract

Reconstructing state-space dynamics from scalar data using time-delay embedding requires choosing values for the delay  $\tau$  and the dimension  $m$ . Both parameters are critical to the success of the procedure and neither is easy to formally validate. While embedding theorems do offer formal guidance for these choices, in practice one has to resort to heuristics, such as the average mutual information (AMI) method of Fraser & Swinney for  $\tau$  or the false near neighbor (FNN) method of Kennel *et al.* for  $m$ . Best practice suggests an iterative approach: one of these heuristics is used to make a good first guess for the corresponding free parameter and then an “asymptotic invariant” approach is then used to firm up its value by, e.g., computing the correlation dimension or Lyapunov exponent for a range of values and looking for convergence. This process can be subjective, as these computations often involve finding, and fitting a line to, a *scaling region* in a plot: a process that is generally done by eye and is not immune to confirmation bias. Moreover, most of these heuristics do not provide confidence intervals, making it difficult to say what “convergence” is. Here, we propose an approach that automates the first step, removing the subjectivity, and formalizes the second, offering a statistical test for convergence. Our approach rests upon a recently devel-

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<sup>1</sup>These authors contributed equally to this work.

oped method for automated scaling-region selection that includes confidence intervals on the results. We demonstrate this methodology by selecting values for the embedding dimension for several real and simulated dynamical systems. We compare these results to those produced by FNN and validate them against known results—e.g., of the correlation dimension—where these are available. We note that this method extends to any free parameter in the theory or practice of delay reconstruction.

*Keywords:* Delay-coordinate embedding, Nonlinear time series analysis, embedding parameters

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## <sup>1</sup> 1. Overview

<sup>2</sup> Delay-coordinate embedding, [1, 2, 3] the foundation of nonlinear time-  
<sup>3</sup> series analysis,<sup>2</sup> involves constructing  $m$ -dimensional vectors  $\vec{v}(t)$  from a  
<sup>4</sup> scalar time series  $x(t)$ , defined by

$$\vec{v}(t) = [x(t), x(t - \tau), x(t - 2\tau), \dots, x(t - (m - 1)\tau)]$$

<sup>5</sup> for a time-delay  $\tau$ . If this is done correctly, the reconstructed dynamics will  
<sup>6</sup> generically be topologically conjugate to the underlying dynamics that are  
<sup>7</sup> sampled by  $x(t)$ .

<sup>8</sup> There are two free parameters in this procedure: the delay  $\tau$  and the  
<sup>9</sup> dimension  $m$ , both of which are critical to obtain a proper embedding. The  
<sup>10</sup> embedding theorems offer guidance for these choices, but in practice—when  
<sup>11</sup> one has a finite number of potentially noisy data points that are measured  
<sup>12</sup> with finite precision—it is typical to resort to heuristics to choose good pa-  
<sup>13</sup> rameter values. Many strategies have been proposed for these purposes. One  
<sup>14</sup> generally chooses  $\tau$  first, working with some statistic that measures indepen-  
<sup>15</sup> dence of  $\tau$ -separated points in the time series. The first minimum of a plot of  
<sup>16</sup> the average mutual information versus  $\tau$ , as proposed by Fraser & Swinney  
<sup>17</sup> [6], is perhaps the most common such technique. Subsequently one proceeds  
<sup>18</sup> to choose  $m$ , using e.g., the false near neighbor (FNN) method of Kennel *et*  
<sup>19</sup> *al.* [7]. In this approach, embeddings of the data for a sequence of dimensions

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<sup>2</sup>For comprehensive reviews of the theory and practice in this field, including exhaustive citation lists, we refer the reader to [4, 5].

20  $m = \dots, k, k+1, \dots$  are used to compute the nearest neighbor to each point  
21 at dimension  $k$ . A change in the neighbor relationship—when a neighbor in  
22  $k$  dimensions is no longer one in  $k+1$  dimensions—is taken as an indication  
23 that the dynamics had not been properly “unfolded” with  $m = k$  and that  
24  $m$  should be increased.

25 This type of heuristic reasoning is difficult to implement as a formal com-  
26 putational procedure. For example, the depth of a minimum in a discrete  
27 plot that is required, the distance that defines a false neighbor, and the max-  
28 imum fraction of FNN that signals a proper unfolding can all be subjective.  
29 In the face of these uncertainties, best practice suggests an iterative method:  
30 one of these heuristics is used to choose a good first guess for the correspond-  
31 ing parameter. An “asymptotic invariant” approach is then used to firm up  
32 the value. In this procedure, the value of some dynamical invariant—e.g.,  
33 correlation dimension or Lyapunov exponent—is computed over a parameter  
34 range to look for convergence. This process can also be subjective, however,  
35 since these computations often involve identifying a *scaling region*. In a plot  
36 of the correlation sum or distance growth, for example, such scaling regions  
37 are generally selected by eye, a process that is not immune to confirmation  
38 bias. (Of course, if one simply fits a line to the full results of the calculation  
39 without regard to the plot shape, the resulting value of the computed dy-  
40 namical invariant is typically not correct.) The notion of convergence with  
41 increasing embedding dimension, too, is problematic: is one significant figure  
42 in the correlation dimension enough? Or does one need two? These issues  
43 are exacerbated by the fact that when the embedding dimension is large, the  
44 nearest neighbors tend to be far away, giving incorrect results [8, 9]. More-  
45 over, larger embedding dimensions can introduce spurious effects for data  
46 sets that are small or noisy.

47 In this paper, we address these subjectivities and informalities using a  
48 recently developed method for automated scaling-region selection [10] that  
49 offers statistical confidence intervals on the results. A sketch of the algorithm  
50 is as follows:

- 51 1. On the two-dimensional plot, perform linear fits to segments of the data  
52 using every possible combination of left and right endpoints.
- 53 2. Calculate a weight for each linear fit that is directly proportional to  
54 the length of the segment and inversely proportional to the square of  
55 the least-squares fit error.
- 56 3. Using the ensemble of fits, generate a histogram of all slopes, taking

57 into account the calculated weights.

58 4. Generate a probability distribution function (PDF) of slopes from the  
59 histogram using a kernel density estimator. The mode of this PDF is  
60 the most likely estimate of the scaling region slope, and its full width  
61 at half maximum provides confidence bounds.<sup>3</sup>

62 This technique can be used as the core of an effective methodology, de-  
63 scribed in Section 2, for automating the asymptotic invariant procedure. The  
64 algorithm outlined in the steps above not only removes the subjective identi-  
65 fication and extraction of the scaling regions; it also supports calculation of  
66 statistical estimates of convergence, computed using an appropriate metric  
67 on the PDFs. As a proof of concept for these claims, we apply this method-  
68 ology in Section 2 to data from a number of real and simulated dynamical  
69 systems to select values for the embedding dimension. We then compare the  
70 results—both the embedding dimension and the dynamical invariants—to  
71 those produced by other methods.

72 While we focus here primarily on estimating  $m$ , it is easy to use this  
73 methodology to estimate good values for  $\tau$ —or, indeed, for any parameter  
74 in a procedure for calculating dynamical invariants. One could also use a  
75 straightforward two-parameter extension of our method to estimate  $m$  and  
76  $\tau$  simultaneously, as in [11].

## 77 2. Automating the asymptotic invariant procedure

78 Our goals in this section are to outline a systematic procedure for selecting  
79 good values for the free parameters in the delay-reconstruction process and  
80 to demonstrate the procedure in the context of the embedding dimension,  
81  $m$ . We do this with several synthetic and real data sets that are described  
82 in Section 2.1, first estimating the delay,  $\tau$  using the method of Fraser &  
83 Swinney [6], then embedding the data for a range of  $m$  and computing the  
84 correlation sums using TISEAN [12, 13]. Using the method of Deshmukh *et*  
85 *al.* [10] on the resulting plots and the Wasserstein metric [14] on the resulting  
86 distributions, we establish the embedding dimension at which the correlation  
87 dimension converges; see Section 2.2. These results are compared to the

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<sup>3</sup>The algorithm in [10] returns two additional distributions that provide information about boundaries of the scaling region(s). The approach proposed in this paper does not rely on those distributions.

88 dimension given by the false near neighbor method [7]. We also compare the  
 89 correlation dimension results to the known values, where they exist. Finally,  
 90 in Section 2.3 we apply these ideas to computation of Lyapunov exponents.  
 91 We will note that algorithms to compute different dynamical invariants might  
 92 work best using different embedding dimensions.

93 *2.1. Data sets*

94 We use four data sets in this work.

95 • The  $x$  coordinate of a 90,000-point trajectory from the canonical Lorenz  
 96 system [15]:

$$\begin{aligned}\dot{x} &= 10(y - x), \\ \dot{y} &= x(28 - z) - y, \\ \dot{z} &= xy - \frac{8}{3}z,\end{aligned}$$

97 with the initial condition  $(0, 1, 1.05)$ . This is obtained using a fourth-  
 98 order Runge-Kutta algorithm for  $10^5$  points with the time step  $\Delta t =$   
 99  $0.01$ . We discard the first  $10^4$  points to remove transient behavior and  
 100 focus on the attractor. For this well-studied system the correlation  
 101 dimension and largest Lyapunov exponent are well-known (approximately  
 102 2.05 and 0.91, respectively) [16, 17, 18].

103 • The first coordinate of a 990,000-point trajectory from the 14-dimensional  
 104 Lorenz-96 system [19]:

$$\frac{dx_k}{dt} = (x_{k+1} - x_{k-2})x_{k-1} - x_k + F \quad (1)$$

105 for  $k = 1, \dots, 14$  with  $x_{k \pm 14} = x_k$ . The trajectory for the initial condition  
 106 [6, 5, 5, ..., 5] is obtained using the fourth-order Runge-Kutta  
 107 algorithm with time step  $\Delta t = \frac{1}{64}$ . We discard the first  $10^4$  points from  
 108 the million point trajectory to remove the transient. This example is  
 109 included because its dynamics are high dimensional: the Kaplan-Yorke  
 110 dimension is estimated to be 6.93 by [20].

111 • Two 80,000-point data sets from experiments on a Photonic Integrated  
 112 Chip (PIC) distributed feedback laser that was developed as part of  
 113 the European Commission PICASSO project, sampled at 40 GHz [21].  
 114 These examples are included to validate our method on experimental  
 115 data for which there are established values for delay-reconstruction  
 116 parameters and correlation dimension.

117 *2.2. Correlation Dimension*

118 In this section, we demonstrate how to choose good values of the em-  
119 bedding dimension,  $m$ , for the four data sets described in Section 2.1 using  
120 automated asymptotic invariant analyses on correlation-sum plots.

121 Results for the classic Lorenz-63 system are shown in Figure 1. The first  
122 three panels show the standard steps in the delay-reconstruction process.  
123 From the time series, shown in panel (a), TISEAN’s `mutual` command gives  
124 the average mutual information versus  $\tau$ , shown in panel (b). We select  
125 the first minimum at  $\tau = 18$  for the rest of the analysis. To estimate the  
126 embedding dimension  $m$ , we then run TISEAN’s `false_nearest` command;  
127 panel (c) shows the percentage of false near neighbors plotted versus  $m$ .  
128 Using a 10% threshold, as is common in practice, the FNN results suggest  
129  $m = 3$ .<sup>4</sup>

130 The bottom three panels of Figure 1 demonstrate our methodology using  
131 the correlation dimension as an asymptotic invariant. The correlation sums,  
132  $C(\epsilon)$ , are found from TISEAN’s `d2` command for a range of  $m$  values. Here  
133  $\epsilon$  is the size of the balls used to cover the set during the calculation of the  
134 Grassberger-Procaccia algorithm [22]. Panel (d) shows  $\ln C(\epsilon)$  versus  $\ln \epsilon$ . If  
135 this plot has a scaling region, its slope is the correlation dimension.

136 It is common practice to choose the endpoints of a scaling region by eye,  
137 and then compute the slope using a linear fit. In this case, if the slopes were  
138 to converge as  $m$  increases, it is thought that the  $m$ -embedded attractor is  
139 properly unfolded and that the value of the correlation dimension is correct.  
140 Figure 1(d) shows clear scaling regions whose slopes behave as expected:  
141 when  $m$  is too low, the attractor is not properly unfolded and the computed  
142 correlation dimensions—i.e., the slopes of the blue ( $m = 1$ ) and orange ( $m =$   
143 2) traces—are artificially low. As  $m$  increases, the slopes increase and then  
144 appear to converge.

145 We formalize this procedure using the method of Deshmukh *et al.* [10],  
146 which uses slope distributions to identify scaling regions and the Wasserstein  
147 distance to establish convergence of the distributions with increasing  $m$ . As  
148 a first step, we compute potential scaling regions corresponding to an ensem-  
149 ble of intervals, varying the left and right endpoints. We set the minimum

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<sup>4</sup>In this paper we leave TISEAN’s many algorithmic parameters at their default values unless otherwise mentioned. For Lorenz-63, we increased the default range of  $\tau$  in `mutual` to see the first minimum in Figure 1(b).

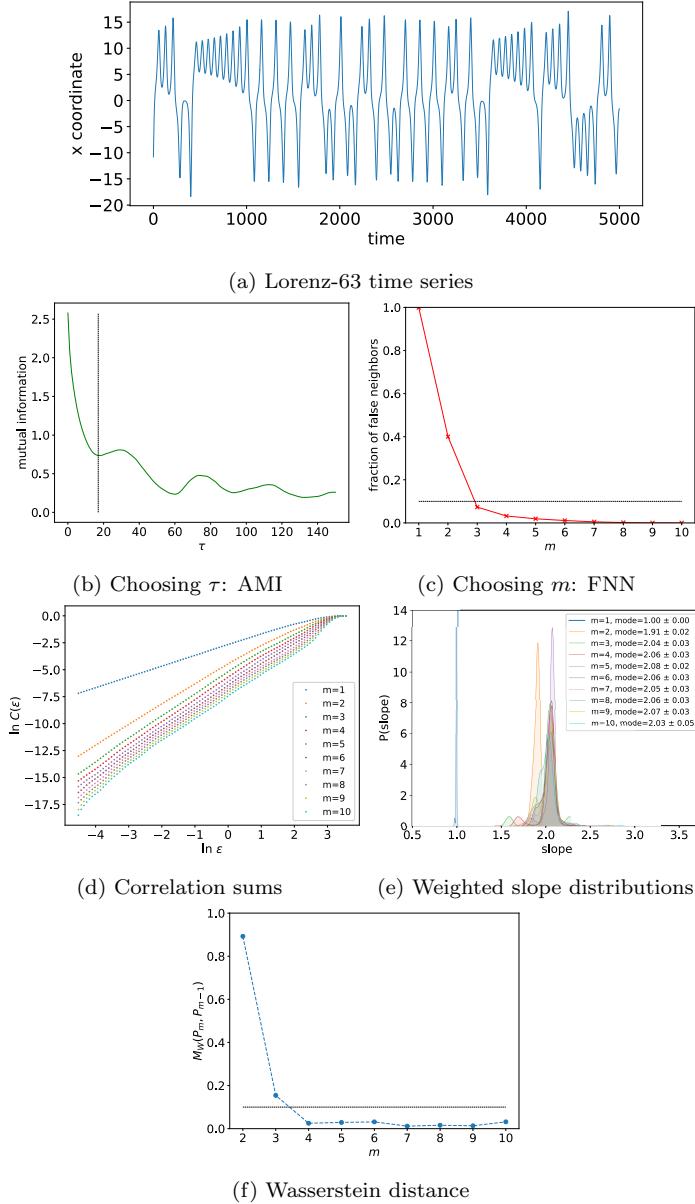


Figure 1: Lorenz-63 example. (a) Time series for the  $x$  coordinate. (b) Average mutual information as a function of  $\tau$ . (c) Percentage of false near neighbors as a function of the embedding dimension  $m$ . (d) Correlation sum plots for  $\tau = 18$  and  $m \in [1, 10]$ . (e) Weighted slope distributions generated from an ensemble of fits in different intervals from panel (d). (f) Wasserstein distance between successive slope distributions.

150 number of points for the fitting interval to be 10, but allow all possible com-  
151 binations otherwise. This choice is discussed in [10]. In panel (d) there are  
152 100 values of  $\ln(\epsilon)$  as possible endpoints; using a minimal width of 10 points  
153 then gives 4005 potential scaling regions. For each  $m$  in Figure 1(d), we  
154 then generate a distribution of slopes,  $P_m$ , from least-squares fits for each  
155 interval. The goodness of the fit is included by weighting each result by the  
156 length of the fitting interval and inversely by square of the fit error. We show  
157 kernel density estimates for these distributions in panel (e), calculated using  
158 python’s `scipy.stats.gaussian_kde` function.

159 The geometry of these distributions brings out the salient information  
160 quite effectively, including both the existence of one or more scaling regions  
161 and their slopes. Unimodal slope distributions, as in Figure 1(e), suggest  
162 the presence of a single, wide scaling region for  $d2$ .<sup>5</sup> The mode of  $P_m$  is an  
163 estimate of the slope of the scaling region and the width of the distribution  
164 around that mode width gives an indication of precision. More formally, we  
165 calculate a confidence interval by computing the standard deviation,  $\sigma$ , of  
166 the ensemble members within the full width at half maximum (FWHM) of  
167 the mode. For the  $m = 2$  case (orange),  $\sigma = 0.02$ , giving the estimated slope  
168  $1.92 \pm 0.02$ .

169 If there were **no** scaling region in the plot, the distribution would be  
170 wide and the corresponding confidence interval large. For Figure 1, the  
171 trajectory samples the attractor cleanly and thoroughly, resulting in small  
172 error estimates. However, this is not the case for all of the examples below.  
173 Moreover, if the plot contains *multiple* scaling regions, the distributions will  
174 be multi-modal. This may occur, for example, for  $d2$  when  $\epsilon$  is larger than  
175 the diameter of the attractor, or for noisy data when  $\epsilon$  is small [10]. The  
176 possibility of such multi-modal distributions is why we use the mode rather  
177 than the mean.

178 The choice of the smallest embedding dimension that gives an accurate  
179 and valid calculation of the correlation dimension is the critical matter at  
180 issue here. We assert that this  $m$  corresponds to the smallest value for  
181 which the slope distributions “converge.” In Figure 1(d), this convergence is  
182 apparent to the eye: the  $P_1$  (blue) and  $P_2$  (orange) distributions reflect the  
183 low correlation dimensions of an incompletely unfolded attractor; however,

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<sup>5</sup>Note that all distribution plots in this paper have the same vertical scale for the purposes of comparison, and may be truncated.

184 the  $P_m$  for  $m \geq 3$  largely overlap. This suggests that  $m = 3$  or  $4$  would be a  
185 good choice.

186 To formalize the notion of convergence, we use the Wasserstein metric  
187 [14],  $M_W$ , to compare sequential pairs  $P_m$  and  $P_{m-1}$ . As a metric,  $M_W = 0$  if  
188 and only if the distributions are identical, or—as we are using it for samples—  
189 if and only if the weighted sample values are the same. Figure 1(f) shows  
190  $M_W(P_m, P_{m-1})$  for the Lorenz-63 d2 slope distributions, calculated using the  
191 `python scipy.stats.wasserstein_distance` function. For this noise-free,  
192 low-dimensional case, the distance  $M_W(P_m, P_{m-1})$  monotonically decreases  
193 with  $m$ .

194 For real-valued data, it is known that the  $L_1$  Wasserstein distance for a  
195 sample of size  $N$  from a distribution approaches zero as  $N^{-1/2}$  under some  
196 technical assumptions [23]. In our experiments,  $N = \mathcal{O}(10^3)$  is the number  
197 of selected left and right endpoint pairs for the linear fits. The theoretical  
198 error is also proportional to the width of the PDF, which in our applications  
199 tends to be  $\mathcal{O}(1)$ . We make the null hypothesis that the PDFs are the same  
200 if

$$M_W(P_m, P_{m-1}) \lesssim 0.1.$$

201 In Figure 1(f) this threshold, shown as the dashed line, first occurs at  $m = 4$   
202 where  $M_W(P_4, P_3) = 0.025 < 0.1$ , so we choose this embedding dimension.  
203 This then gives  $d_2 = 2.06 \pm 0.03$ , which is in reasonable agreement with the  
204 known value of  $\approx 2.05$ .

205 Our approach bears some similarities to other methods for choosing  $m$ ,  
206 but the  $M_W$  threshold is mathematically justifiable. By contrast, there ap-  
207 pears to be no such justification for the selection of a threshold for the per-  
208 centage of false nearest neighbors. The suggestion of [7] is that “a physicist  
209 might well choose to accept this threshold to make more efficient any further  
210 computations performed on the data,” a reason based only on convenience.  
211 Moreover, the percentages of FNN can vary widely with  $\tau$  and  $m$ , and also  
212 are sensitive to noise [9]. This further complicates the selection of a threshold  
213 for the FNN heuristic. Similarly, Cao [24] proposes a method to automate  
214 the asymptotic invariant approach by comparing quantities calculated from  
215 embeddings at successive dimensions. The quantities are derived from dis-  
216 tances between points that are neighbors in space ( $E1(d)$ ) or in time ( $E2(d)$ ).  
217 However, the paper does not formalize a threshold on  $E1$  and  $E2$  to indicate  
218 that the correct embedding dimension has been reached.

219 For the second example, we use the Lorenz-96 trajectory described in

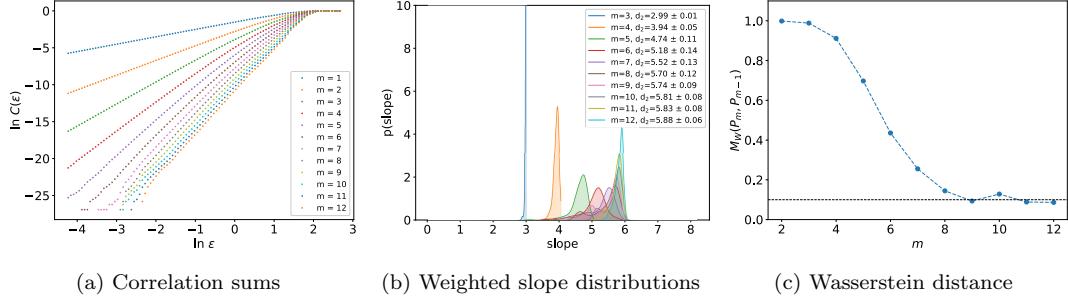


Figure 2: Lorenz-96 example. (a) Correlation sum plots for embeddings for  $\tau = 23$  and  $m \in [3, 12]$ . (b) Weighted slope distributions generated from an ensemble of fits in different intervals from panel (a). (c) Convergence of slope distributions.

220 Section 2.1 to give a time series sampled from an attractor in a 14D state  
 221 space. In this case, AMI (not shown here) does not give a good estimate for  
 222  $\tau$  because it has broad, almost-flat region with a first minimum at  $\tau = 145$ , a  
 223 value that produces an over-folded embedding. Instead, we use the curvature-  
 224 based heuristic of [25] to select  $\tau = 23$ . The resulting correlation sums from  
 225 TISEAN for a range of embedding dimensions are shown in Figure 2(a). The  
 226 corresponding slope distributions, panel (b), exhibit the same behavior as the  
 227 Lorenz-63 example: they peak at artificially low slopes when the dimension  
 228 is too small, and appear to converge with increasing  $m$ . The Wasserstein  
 229 metric, panel (c), confirms this and suggests  $m = 9$  is sufficient. This gives  
 230  $d_2 = 5.74 \pm 0.09$ . This is in accord with the Kaplan-Yorke dimension,  $d_{KY} =$   
 231 6.93 according to [20], for this system, which is an upper bound on  $d_2$  for  
 232 multifractal sets.

233 For this trajectory, the FNN method would require a larger value,  $m =$   
 234 11, giving only a slightly larger estimate of the correlation dimension. The  
 235 difference between the two estimates stems from what each method is trying  
 236 to do. FNN performs an aggregate calculation of neighbor relationships  
 237 across the attractor, with the goal of identifying false trajectory crossings  
 238 created by inadequate unfolding. Elimination of such crossings is sufficient  
 239 for computing the correct dimension, but not necessary [9]. By contrast, our  
 240 method uses the convergence of the desired invariant as the primary criterion,  
 241 which is more appropriate given that this is the goal.

242 Moving beyond synthetic examples, we now consider two PIC laser data  
 243 sets from McMahon *et al.* [21]. These were gathered from the same device

244 but under different conditions and, as noted in the paper, lead to quite  
245 different dynamics; see Figure 3(a) and (b). McMahon *et al.* first estimate  
246  $\tau$  using AMI then calculate the correlation sums over a fixed range of  $m \in$   
247  $[5, 10]$ . They apply a “minimum gradient detection” algorithm to find scaling  
248 regions. This method gives  $d_2 = 1.27 \pm 0.05$  and  $1.01 \pm 0.06$ , respectively.  
249 The paper does not note a “best” value for  $m$ , as their goal is calculation of  
250 the correlation dimension and not the embedding dimension.

251 The results of applying our methodology to this data are shown in Figure  
252 3(c)-(h). The minimum AMI occurs at  $\tau = 3$  for both cases. The  
253 correlation sum for a range of  $m$  values is shown in panels (c) and (d). Pan-  
254 els (e) and (f) show the corresponding slope distributions, and (g) and (h)  
255 show the Wasserstein distances. For the data in the left column, the slope  
256 distributions are multimodal for  $m \in [1, 4]$ , reflecting the distinct linear re-  
257 gions in panel (c). The PDFs in (e) are far broader than those in Figures 1  
258 and 2, indicating less certainty. Nevertheless, the Wasserstein distance in  
259 panel (g) does drop below 0.1 for  $m = 5$ , implying  $d_2 = 1.37 \pm 0.05$ . This  
260 is in agreement with the quoted results of McMahon *et al.*, though it should  
261 be noted that their confidence interval is calculated differently.

262 The story is quite different for the second case. The distributions in  
263 Figure 3(f) do not appear to converge with increasing  $m$ ; this is corroborated  
264 by the Wasserstein metric in panel (h). Indeed, the curves in panel (d)  
265 are clearly problematic from the standpoint of time-series analysis. The  
266  $m = 1$  and  $m = 2$  results do have scaling regions—indicated by the strong,  
267 unimodal peaks in the blue and orange distributions in panel (f)—but the  
268 slopes of these regions give spurious  $d_2$  values because the attractor is not  
269 reconstructed properly for such low dimensions (as is clear from the change  
270 in slope with increasing  $m$  in this range). When  $m > 2$ , none of the  $d_2$  curves  
271 have clear scaling regions. Our slope distributions bring this out clearly: the  
272 Wasserstein distance never falls below 0.1, indicating low confidence in the  
273 correlation dimension. This is not in accord with the asserted value in [21],  
274 perhaps because computing a gradient from noisy data, as is done in that  
275 paper, is notoriously problematic.

276 A number of methods have been proposed to automate the estimation of  
277  $d_2$ : see, for example, [26, 27, 28]. These papers essentially use the follow-  
278 ing workflow: calculate a local gradient of the correlation sum, generate a  
279 histogram of the slopes, and then locate the peak value. Numerical differen-  
280 tiation can, of course, be problematic unless the data points are noise free.  
281 Our method is designed to avoid this issue. Since we weight the linear fits by

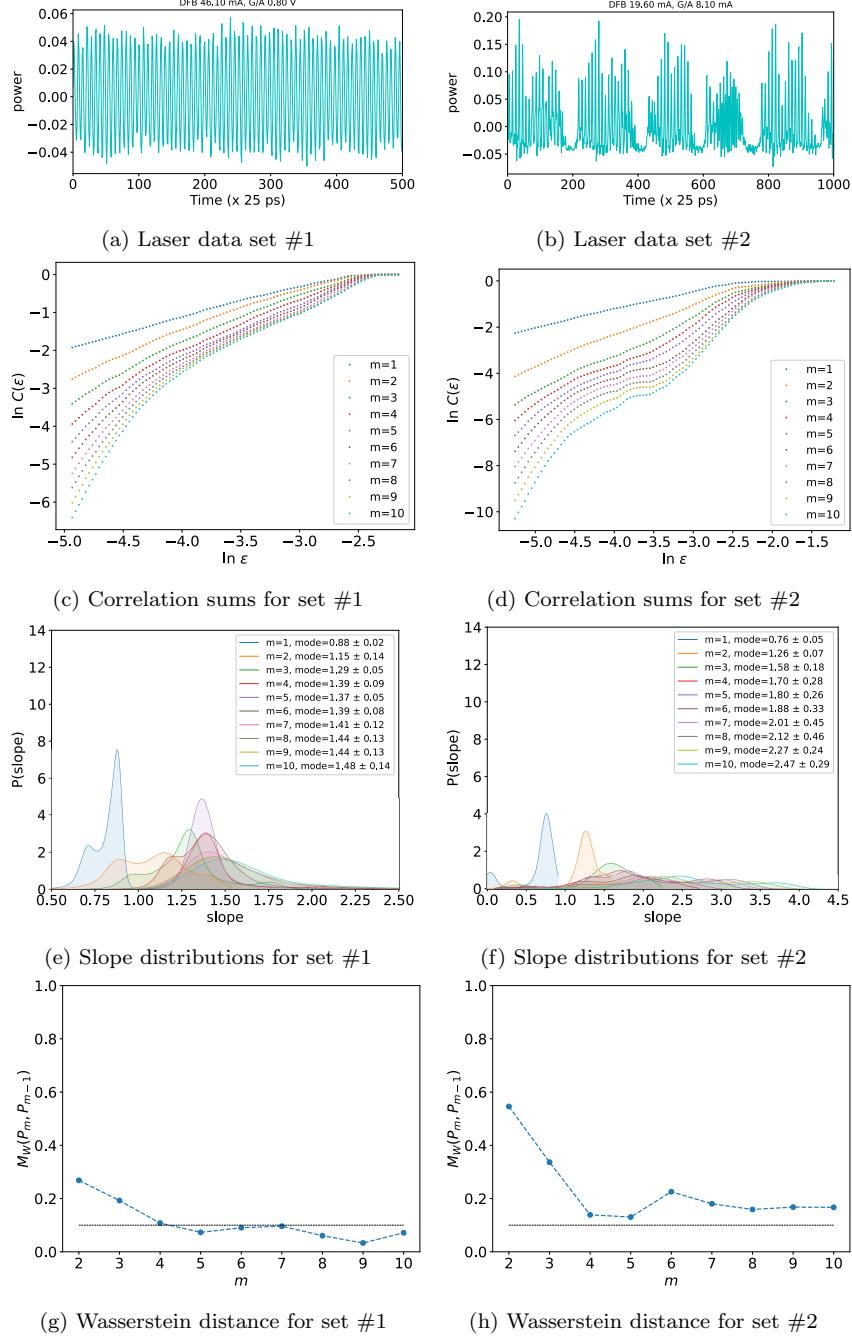


Figure 3: Extracting scaling regions for data from two laser experiments, segments of which are shown in the top two panels. Below each time series are the correlation sums, slope distributions, and convergence measures for the corresponding data.

282 their length, we favor longer fits, thus de-emphasizing small-scale noise. Our  
283 choice of the mode of the slope distribution provides a slope that is common  
284 to a range of endpoint choices. Another important difference between our  
285 method and those in the cited papers is generality. The primary focus of  
286 those papers is an automatic estimate of the correlation dimension. The ob-  
287 jective of our method is to select a good value of the embedding dimension;  
288 the `d2` calculation is only the vehicle. Any other dynamical invariant would  
289 be just as good, as we show next.

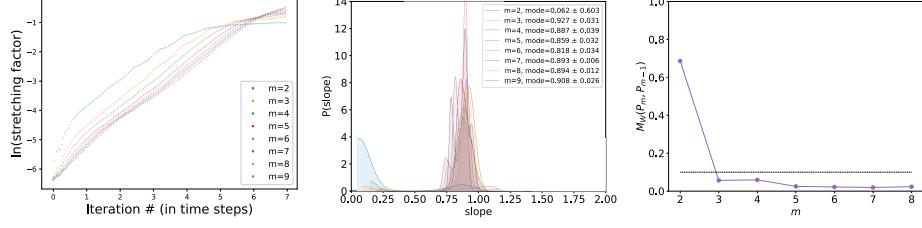
290 *2.3. Other invariants*

291 Correlation dimension is not the only dynamical invariant that involves  
292 fitting a line to a scaling region. Another important quantity is the largest  
293 Lyapunov exponent,  $\lambda_1$ , which can be computed by the widely used Kantz  
294 [29] and Rosenstein [30] algorithms. These calculate a “stretching factor”  
295  $S(\Delta n)$  between nearby trajectory points. This computation also gives a  
296 scaling region to which our method can be applied. This, in turn, pro-  
297 vides another opportunity for an automated asymptotic invariant approach  
298 to choose embedding parameter values.

299 Figure 4 shows the results of this approach applied to the Lorenz-63  
300 dataset from Section 2.1, using TISEAN’s `1yap_k` command. The Wasser-  
301 stein metric, panel (c), suggests that  $m = 3$  is adequate. With this choice,  
302 we estimate  $\lambda_1 = 0.927 \pm 0.031$ , close to the value 0.91 computed from inte-  
303 grating the ODEs [16].

304 Note that this embedding dimension is smaller than the  $m = 4$  in Sec-  
305 tion 2.2, which was obtained using `d2` calculations. This brings out an inter-  
306 esting point: different values of the embedding dimension may be sufficient  
307 for the calculation of different invariants. This is likely due to a combination  
308 of dynamical and algorithmic effects. The `1yap_k` algorithm analyzes how the  
309 dynamics deform the state space by tracking the forward images of points  
310 in an initial  $\epsilon$ -ball that stretches along the most unstable manifold. Our  
311 results suggest that this effect can be tracked effectively in  $m = 3$ , whereas  
312 the `d2` algorithm, which counts points in  $m$ -dimensional  $\epsilon$ -balls, requires a  
313 more fully unfolded reconstruction. In other words, both the nature of the  
314 invariant and the algorithm play a role. This is not the first observation of  
315 this effect, of course, see for example [31, 32].

316 On a related note: default range for the initial  $\epsilon$ -ball in the `1yap_k` calcu-  
317 lation is set, by default, to five values between 0.001 and 0.01 of the span of  
318 the data, and  $S(\Delta n)$  is computed for each  $\epsilon$ . Data limitations can make the



(a) Stretching factor  $S(\Delta n)$  (b) Weighted slope distributions (c) Wasserstein distance

Figure 4: Largest Lyapunov exponent for Lorenz-63. (a) Spreading factor for embeddings for  $\tau = 18$  and  $m \in [2, 9]$ . (b) Weighted slope distributions from panel (a). (c) Convergence of slope distributions.

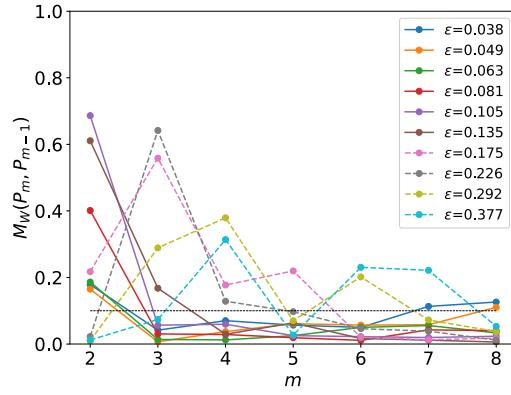


Figure 5: Wasserstein distance for the Lorenz-63 data for a range of  $\epsilon$  in the `lyap_k` algorithm. Figure 4(c) uses  $\epsilon = 0.105$ .

319 results quite sensitive to this scale, however, so choosing a good  $\epsilon$  value—or  
 320 knowing whether a choice is good—can be a challenge. Our method can  
 321 provide some insight in this situation. Figure 5 shows the effect of  $\epsilon$  on  
 322 the Wasserstein distance for the Lorenz-63 data. For the five smallest  $\epsilon$  in  
 323 the figure, the slopes converge by  $m = 3$ . For  $\epsilon = 0.135$ , the slopes still  
 324 converge, but not until  $m = 4$ . Beyond that, the Wasserstein distance is  
 325 non-monotonic, indicating a lack of convergence with increasing dimension.  
 326 This suggests that these larger values of  $\epsilon$  are problematic.

327 **3. Discussion and conclusion**

328 The choice of the embedding dimension is a critical, but challenging,  
329 step in delay reconstruction. As discussed in Section 2.2, a number of good  
330 heuristics have been developed to aid in this process. However these do not  
331 provide confidence intervals, and they involve subjective thresholds that may  
332 or may not be optimal for any particular data set. In the face of this, one  
333 can adopt an iterative approach: use some heuristic to obtain a good first  
334 guess, then compute a dynamical invariant—e.g., the correlation dimension  
335 or Lyapunov exponent—over a range of embedding dimensions, looking for  
336 convergence. This process, too, can be subjective, as these computations  
337 often involve finding, and fitting a slope to, a *scaling region*. Since this is  
338 generally done by eye, it is not immune to confirmation bias.

339 The contribution of this paper is a method that **formalizes** and **automates**  
340 this process. We use the ideas of Deshmukh *et al.* [10] to generate  
341 an ensemble of slopes from prospective scaling regions, creating a slope dis-  
342 tribution that uses interval width and fit quality as weights. Broad, clean  
343 scaling regions manifest as narrow, tall peaks in these distributions. Upon  
344 repeating this calculation for a range of embedding dimensions, this leads  
345 to a good choice of  $m$  values: when the resulting sequence of slope distribu-  
346 tions converges, as signaled by the decrease of a Wasserstein distance below  
347 a threshold that is motivated by the theoretical expectation for samples from  
348 a fixed distribution.

349 We demonstrated the method in Section 2 on four data sets using two  
350 dynamical invariants calculated with the TISEAN package: the correlation  
351 dimension and the largest Lyapunov exponent. Each of these requires com-  
352 puting a slope—of the correlation sum versus the scale parameter, or of the  
353 stretching factor versus time, respectively. The results corroborate known  
354 values, except in one case: a laser data set from [21]. In this case, the  
355 correlation-sum plots, when examined visually, clearly did not contain true  
356 scaling regions.

357 We emphasize that calculations of such dynamical invariants are valid  
358 if, and only if, the plots contain “robust” scaling regions. Robustness is  
359 obviously a subjective term that can lead to real problems in the practice of  
360 nonlinear time-series analysis. To quote Kantz & Schreiber: “Some authors  
361 failed to observe that the curves that they were fitting with straight lines were  
362 actually not quite straight...” [5]. Fitting a line blindly to some arbitrarily  
363 selected portion of a plot is even worse. A strength of our method is that

364 it objectively measures when there is a scaling region—and, if so, indicates  
365 where it is, and what is its slope.

366 Our technique can also be useful in the *invocation* of these algorithms.  
367 Tools like `d2` or `lyap_k` in the TISEAN package attack a difficult problem:  
368 how can one extract dynamical invariants from incomplete samples? Their  
369 implementations involve a number of free parameters such as time scale, the  
370 Theiler window [33], etc. Moreover, the time series must be sufficiently long  
371 for the invariant computation to be valid [34, 35? ]. The best practice for  
372 choosing such parameters mirrors the “asymptotic invariant” approach: vary  
373 the parameter, seeking convergence. One can use our method to accomplish  
374 this—for individual parameters or even for several at once, using a multivariate  
375 sweep. This could include choosing any of the free parameters in delay  
376 reconstruction.

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