

Potsdam-Institut für Klimafolgenforschung

# Originally published as:

Schultz, D., Spiegel, S., Marwan, N., Albayrak, S. (2015): Approximation of diagonal line based measures in recurrence quantification analysis. - Physics Letters A, 379, 14-15, 997-1011

**DOI:** <u>10.1016/j.physleta.2015.01.033</u>

Available at <a href="http://www.sciencedirect.com">http://www.sciencedirect.com</a>

© Elsevier

## Approximation of diagonal line based measures in recurrence quantification analysis

D. Schultz<sup>a,\*</sup>, S. Spiegel<sup>a</sup>, N. Marwan<sup>b</sup>, S. Albayrak<sup>a</sup>

<sup>a</sup>DAI-Lab, Berlin Institute of Technology, Ernst-Reuter-Platz 7, 10587 Berlin, Germany <sup>b</sup>Potsdam Institute for Climate Impact Research, 14412 Potsdam, Germany

## Abstract

Given a trajectory of length N, recurrence quantification analysis (RQA) traditionally operates on the recurrence plot, whose calculation requires quadratic time and space  $(\mathcal{O}(N^2))$ , leading to expensive computations and high memory usage for large N. However, if the similarity threshold  $\varepsilon$  is zero, we show that the recurrence rate (RR) and many diagonal line based RQA-measures, e.g., the determinism (DET), can be obtained algorithmically taking  $\mathcal{O}(N \log(N))$  time and  $\mathcal{O}(N)$  space. Furthermore, for the case of  $\varepsilon > 0$  we propose approximations to the RQA-measures that are computable with same complexity. Experiments with autoregressive systems show that the approximation error is small if the dimension of the trajectory and the minimum diagonal line length are small. When applying the approximate determinism to the problem of detecting dynamical transitions we observe that it performs as well as the exact determinism measure.

*Keywords:* Recurrence quantification analysis, Recurrence plot, Determinism, Approximation, Phase space discretization

## 1 1. Introduction

Recurrence quantification analysis (RQA), i.e., the quantification of struc-2 tures in recurrence plots [1], has established in several fields of research as a 3 powerful tool to investigate recurrence related properties of complex dynamical systems [2]. The popularity of RQA is founded in its simplicity and flexibility to be applied to almost any type of data, including non-stationary processes [3]. In particular the outstanding role of the RQA-measure determinism (DET) 7 has been demonstrated in several applications, including discriminating signals from noise [4], detecting dynamical transitions [5, 6], and the recently proposed ٩ use for pattern mining and classification [7]. A comprehensive overview of re-10 currence plots and its applications is given in [1]. 11

Preprint submitted to Physics Letters A

<sup>\*</sup>Corresponding author

Email address: schultz@dai-lab.de (D. Schultz)

The computation and quantification of recurrence plots generally involves 12 operations with quadratic time and space complexity  $(\mathcal{O}(N^2))$ . This computa-13 tional complexity leads to strongly increasing computation times and memory 14 consumption for long time series (longer than 100,000 data points). Recurrence 15 analysis of long time series, such as audio data [8], epileptic seizures [9], material 16 damage detection [10], or hourly weather variability [11], is, therefore, limited. 17 Another application that can be limited by the high computational complexity 18 is online monitoring of data streams, e.g., for video surveillance [12], monitoring 19 social interactions [13], or assessing driving behavior [7]. Parallel computing 20 approaches (e.g., using GPU calculations [11, 14]) can accelerate computation 21 but do not reduce the computational complexity. 22

In this letter we show the following. If the similarity threshold  $\varepsilon$  is zero, then the recurrence rate and many diagonal line based RQA-measures, e.g., the determinism, are in the computational complexity class  $\mathcal{O}(N \log(N))$ , whereas space complexity is  $\mathcal{O}(N)$ . We use this observation in order to propose approximations to these measures for the case of  $\varepsilon > 0$ . The (approximative) measures are obtained algorithmically, without having to calculate the recurrence plot.

## <sup>29</sup> 2. Motivation

Recent work has introduced recurrence plot-based distance measures, which 30 can be utilized for mining (multi-dimensional) time series with nonlinear dynam-31 ics [15, 16]. However, the quadratic time and space complexity of computation 32 and quantification of recurrence plots makes distance calculations for relatively 33 long time series and online processing of fast time series streams intractable. 34 For these purposes we aim to approximate the proposed recurrence plot-based 35 distance measures in such a way as to reduce the computational complexity 36 while maintaining the classification accuracy. 37

#### **38 3.** Recurrence quantification analysis

For a given *d*-dimensional phase space trajectory  $\vec{x}$  (reconstructed from a time series *x*, e.g., by time-delay embedding [17]) of length *N* and similarity threshold  $\varepsilon \geq 0$  the recurrence plot of  $\vec{x}$  is an illustration of the binary recurrence matrix **R**, given by

 $R_{i,j} = \Theta(\varepsilon - \|\vec{x}_i - \vec{x}_j\|), \quad i, j = 1, \dots, N,$ 

where  $\|\cdot\|$  is a norm in the phase space of  $\vec{x}$  and  $\Theta$  is the Heaviside step function, defined by  $\Theta(y) = 1$  if  $y \ge 0$  and  $\Theta(y) = 0$  if y < 0. Thus  $\Theta$  indicates whether  $\vec{x}_i$  and  $\vec{x}_j$  are in  $\varepsilon$ -proximity (also denoted as similar) or not, i.e.,  $R_{i,j} = 1$ if  $\|\vec{x}_i - \vec{x}_j\| \le \varepsilon$  and  $R_{i,j} = 0$  if  $\|\vec{x}_i - \vec{x}_j\| > \varepsilon$ . This relation is essential for the study of recurrence plots and will be used extensively in this letter. The recurrence plot contains the *line of identity (LOI)*, which means that each entry on the main diagonal of **R** is 1. Structures parallel to the main diagonal, referred to as diagonal lines, are caused by similarly evolving epochs of the phase space trajectory  $\vec{x}$ .

Recurrence quantification analysis was developed in order to quantitatively describe recurrence plots. For this purpose, small scale structures, such as recurrence points or diagonal lines in the recurrence plot are used [18]. The fraction of recurrence points in the recurrence plot is measured by the *recurrence rate*,

58

$$RR = \frac{1}{N^2} \sum_{i,j=1}^{N} R_{i,j},$$
(1)

which is interpreted as the probability to find a recurrence of trajectory  $\vec{x}$ . A more sophisticated RQA-measure is the *determinism*, which is defined for a given minimum diagonal line length  $\mu$  as

$$DET^{(\mu)} = \frac{\sum_{l=\mu}^{N} l \cdot P(l)}{\sum_{i,j=1}^{N} R_{i,j}},$$
(2)

where P(l) is the number of diagonal lines of length l in **R**. *DET* can be interpreted as the probability that a recurrence point belongs to a diagonal line. The parameter  $\mu$  is usually set to 2. This choice is sufficient for most applications. However, in particular cases, larger values of  $\mu$  can be necessary, e.g., reducing effects of tangential motion (oversampling), noise, or embedding effects [1].

As already mentioned, a phase space trajectory of a univariate time series 68 can be reconstructed by time delay embedding [17]. We call this procedure time 69 series embedding, since it is applied to the time series. In the sequel we will 70 apply the method of time delay embedding to the trajectory  $\vec{x}$  (that possibly 71 was created by time series embedding for reconstruction purposes), but with 72 the intention of quantifying diagonal structures in **R**. In order to distinguish 73 that from the time series embedding, we will denote this as *trajectory embedding*. 74 More precisely, for a fixed time delay 1 and embedding dimension  $\nu$ , we consider 75 the trajectory embedding vectors 76

$$\vec{x}_{j}^{\nu} = (\vec{x}_{j}, \vec{x}_{j+1}, \dots, \vec{x}_{j+\nu-1}),$$
(3)

which are of dimension  $d \cdot \nu$ , provided that the trajectory  $\vec{x}$  is d-dimensional. The trajectory embedding of  $\vec{x}$  is then defined to be the sequence  $\vec{x}^{\nu} = (\vec{x}_{j}^{\nu})_{j=1,...,N-\nu+1}$ , which can be imagined as a trajectory in a  $(d \cdot \nu)$ -dimensional phase space. In Sec. 4.2 we show that information about P(l) can be extracted by these repre-

## sentations leading to a surprising identity for the determinism.

## 82 4. RR and DET identities

We deduce identities for RR and  $DET^{(\mu)}$ , which allow fast calculation (without computing the recurrence plot) if the similarity threshold  $\varepsilon$  is zero. The identity for RR does hold for  $\varepsilon = 0$  only. The identity for  $DET^{(\mu)}$  is first shown for arbitrary  $\varepsilon \geq 0$  and the assumption that the phase space norm is the maximum norm  $\|\cdot\|_{\infty}$ . However, in the special case of  $\varepsilon = 0$ , we will argue that the restriction to the  $\|\cdot\|_{\infty}$ -norm becomes redundant. Consequently it follows the important fact that the recurrence rate and the determinism are in  $\mathcal{O}(N \log(N))$ of  $\varepsilon = 0$ , whereas the computational complexity of the classical methods that quantify the recurrence plot is  $\mathcal{O}(N^2)$ .

#### 92 4.1. Recurrence rate identity

Given the trajectory embedding  $\vec{x}^{\nu}$ , Eq. (3), in analogy to Eq. (1) we define

$$\mathcal{PP}^{(\nu)} := \sum_{i,j=1}^{N-\nu+1} \Theta(\varepsilon - \|\vec{x}_i^{\nu} - \vec{x}_j^{\nu}\|), \tag{4}$$

the number of pairwise proximities of the elements in  $\vec{x}^{\nu}$ . Note that  $RR = \mathcal{PP}^{(1)}/N^2$  is the recurrence rate of  $\vec{x}$  and more general  $\mathcal{PP}^{(\nu)}/(N-\nu+1)^2$  is the recurrence rate of  $\vec{x}^{\nu}$ .

If nominal recurrences [19] are in demand, that is  $\varepsilon = 0$ , then  $\mathcal{PP}^{(\nu)}$  (and

thus the recurrence rate RR) can be determined efficiently, i.e., with algorithmic

complexity of  $\mathcal{O}(N\log(N))$ . In order to achieve this complexity, we employ the

histogram  $h_X$  of the trajectory embedding vectors  $X := \vec{x}^{\nu}$ , which is given by

$$h_X: Y \to \mathbb{N}, \quad \vec{y} \mapsto \sum_{\vec{x} \in X} \Theta(-\|\vec{x} - \vec{y}\|),$$

where Y is the set of unique members of X.

**Theorem 1.** Let  $X = \vec{x}^{\nu}$  be the sequence of trajectory embedding vectors as defined in Eq. (3) and denote by  $h_X$  the histogram of the elements in X. If  $\varepsilon = 0$ , then

$$\mathcal{PP}^{(\nu)} = \sum_{\vec{y} \in Y} \left( h_X(\vec{y}) \right)^2.$$
(5)

PROOF. First note that a similarity (or proximity) corresponds to an equality if  $\varepsilon = 0$ , that is

$$\Theta(-\|\vec{x}_i^{\nu} - \vec{x}_j^{\nu}\|) = 1 \quad \Leftrightarrow \quad \vec{x}_i^{\nu} = \vec{x}_j^{\nu}.$$

The claim follows by simple combinatorial arguments. Assume that for  $\vec{y} \in Y$ there are exactly *n* elements in *X* that are equal to  $\vec{y}$ . Then there are  $n^2$  pairwise equalities of these *n* elements, and hence  $n^2$  pairwise proximities that increase  $\mathcal{PP}^{(\nu)}$  by  $n^2$ . But *n* is exactly determined by  $h_X(\vec{y}) = n$ . Taking the sum over all  $\vec{y} \in Y$  yields the claim.

Based on this observation we can calculate the right hand side of Eq. (5) efficiently. The algorithmic details are discussed in Sec. 5.2.2.

#### 114 4.2. Determinism identity

For the rest of this letter we choose the phase space norm  $\|\cdot\|_{\infty}$ , in particular 115 we assume that **R** and all  $\mathcal{PP}^{(\nu)}$  are obtained for  $\|\cdot\| = \|\cdot\|_{\infty}$ . Then there is a 116 relation between diagonal lines in the recurrence plot and recurrence points of 117 trajectory embeddings. Before we formulate the determinism identity, we will 118 give an intuition for the just mentioned relation: For a trajectory  $\vec{x}$  let **R** be 110 the recurrence plot. Consider the trajectory embedding  $\vec{x}^2$  of  $\vec{x}$  of dimension 120  $\nu = 2$  and the corresponding recurrence plot  ${f R}^{(2)}$ . Now, in the maximum norm, 121 we have that  $R_{i,j}^{(2)} = 1$  is equivalent to  $R_{i,j} = R_{i+1,j+1} = 1$ . In other words, a diagonal line of length 2 in **R** corresponds to a recurrence point in  $\mathbf{R}^{(2)}$ , which 122 123 is quantified by  $\mathcal{PP}^{(2)}$ . 124

**Theorem 2.** Let  $\mu$  be a choice of the minimum diagonal line length. For a trajectory  $\vec{x}$ , let the recurrence plot  $\mathbf{R}$  and the pairwise proximity measures  $\mathcal{PP}^{(1)}, \mathcal{PP}^{(\mu)}, \mathcal{PP}^{(\mu+1)}$  be obtained for  $\|\cdot\| = \|\cdot\|_{\infty}$ . Then for arbitrary  $\varepsilon \ge 0$ it holds

$$DET^{(\mu)} = \frac{\mu \cdot \mathcal{PP}^{(\mu)} - (\mu - 1) \cdot \mathcal{PP}^{(\mu+1)}}{\mathcal{PP}^{(1)}}.$$
(6)

129 PROOF. See Appendix A, Sec. 10.

In some cases the LOI of the recurrence plot should not be included in the histogram P(l), i.e., P(N) is set to zero. Then Theorem 2 holds true with a slight modification:

$$DET^{(\mu)} = \frac{\mu \cdot \mathcal{PP}^{(\mu)} - (\mu - 1) \cdot \mathcal{PP}^{(\mu+1)} - N}{\mathcal{PP}^{(1)}}$$

<sup>133</sup> For further considerations we assume that the *LOI* is included.

It is important to discuss the condition on the underlying phase space norm 134 that compares the elements in  $\vec{x}$ . First of all, the statement from Theorem 2 135 only holds for the  $\|\cdot\|_{\infty}$ -norm. Depending on the application, a specific norm 136 may be selected. Usually, the Euclidean norm  $\|\cdot\|_2$  is considered, but also the 137 maximum norm  $\|\cdot\|_{\infty}$  is often used because it is computationally faster and 138 allows to study recurrence plots analytically [1]. If  $\varepsilon = 0$ , then the statement 139 holds for all norms since each norm  $\|\cdot\|$  only indicates if  $\vec{x}_i$  and  $\vec{x}_j$  are equal, 140 i.e., by definition of a norm we have that  $\Theta(-\|\vec{x}_i - \vec{x}_j\|) = 1$  is equivalent to 141  $\vec{x}_i = \vec{x}_i$ . 142

Two observations from the proof of Theorem 2 describing the relation between P(l) and  $\mathcal{PP}^{(\mu)}$  are worth mentioning here. Firstly,

$$\sum_{l \ge \mu} P(l) = \mathcal{P}\mathcal{P}^{(\mu)} - \mathcal{P}\mathcal{P}^{(\mu+1)},\tag{7}$$

which is the number of diagonal lines in **R** of minimal length  $\mu$ , and secondly

$$\mathcal{PP}^{(\nu)} = \sum_{l \ge \nu} (l - \nu + 1) P(l).$$

By now, the identity in Theorem 2 does not provide a method to compute the determinism efficiently for general  $\varepsilon$ . However, if  $\varepsilon = 0$ , then  $\mathcal{PP}^{(1)}, \mathcal{PP}^{(\mu)}$ and  $\mathcal{PP}^{(\mu+1)}$  can be calculated fast, as argued in Sec. 4.1, and then  $DET^{(\mu)}$  is a simple algebraic computation in terms of these quantities.

It is worth to mention that the relationship between the length of diagonal lines in the recurrence plot and the embedding dimension is of more fundamental nature. For example, the  $K_2$  entropy can be directly estimated from the recurrence plot using the diagonal line lengths [1] instead of the dimension of the embedding dimension [20].

## 155 5. Approximation of RQA

Approximations for RR and  $DET^{(\mu)}$  are presented that are computable in 156  $\mathcal{O}(N \log(N))$ . These approximative measures are obtained algorithmically, that 157 means we do not calculate the recurrence plot. In Sec. 4, we have discussed 158 the simplified case of  $\varepsilon = 0$ , where these measures are in the just mentioned 159 complexity class. In this section we study the case of  $\varepsilon > 0$ , for which we 160 propose a phase space discretization approach in order to approximate  $\mathcal{PP}^{(\nu)}$ . 161 The discretization will generate the situation of a zero threshold, which allows 162 us to apply the results from Sec. 4. 163

#### 164 5.1. Approximation method

We propose to discretize the phase space for a grid size parameter  $\delta > 0$  via

$$\Phi_{\delta} : \mathbb{R}^n \to \mathbb{Z}^n, \quad \vec{y} \mapsto \tilde{\vec{y}} := \left\lfloor \frac{\vec{y}}{\delta} \right\rfloor, \tag{8}$$

where *n* is an arbitrary natural number and  $\lfloor \cdot \rfloor$  is the component-wise round off operation. Applying  $\Phi_{\delta}$  to the trajectory  $\vec{x}$  leads to a partition of the phase space in hypercubes of size  $\delta$ . Then we replace the similarity condition  $\|\vec{x}_i^{\nu} - \vec{x}_j^{\nu}\|_{\infty} \leq \varepsilon$ by affiliation to the same cube, i.e., by the condition  $\tilde{\vec{x}}_i^{\nu} = \tilde{\vec{x}}_j^{\nu}$ . For convenience, we formulate this as a classification problem following the rules,

- $\vec{x}_i^{\nu}$  and  $\vec{x}_i^{\nu}$  are classified as ...
- 172 (1) similar if  $\Theta(-\|\tilde{\vec{x}}_i^{\nu} \tilde{\vec{x}}_j^{\nu}\|_{\infty}) = 1.$
- (2) dissimilar if  $\Theta(-\|\tilde{\vec{x}}_i^{\nu} \tilde{\vec{x}}_i^{\nu}\|_{\infty}) = 0.$

This point of view leads to the idea of proposing an approximation of  $\mathcal{PP}^{(\nu)}$ for  $\varepsilon > 0$  by replacing  $\Theta(\varepsilon - \|\vec{x}_i^{\nu} - \vec{x}_j^{\nu}\|_{\infty})$  by  $\Theta(-\|\tilde{\vec{x}}_i^{\nu} - \tilde{\vec{x}}_j^{\nu}\|_{\infty})$  in Eq. (4): **Definition 1.** Let  $\varepsilon > 0$ . The approximations  $\widetilde{\mathcal{PP}}^{(\nu)}$  and  $D\widetilde{ET}^{(\mu)}$  of  $\mathcal{PP}^{(\nu)}$ and  $DET^{(\mu)}$  respectively are defined as

$$\widetilde{\mathcal{PP}}^{(\nu)} := \sum_{i,j=1}^{N-\nu+1} \Theta(-\|\tilde{\vec{x}}_i^{\nu} - \tilde{\vec{x}}_j^{\nu}\|_{\infty}),$$
$$D\widetilde{E}T^{(\mu)} := \frac{\mu \cdot \widetilde{\mathcal{PP}}^{(\mu)} - (\mu-1) \cdot \widetilde{\mathcal{PP}}^{(\mu+1)}}{\widetilde{\mathcal{PP}}^{(1)}}$$

The crucial difference between  $\mathcal{PP}^{(\nu)}$  and  $\widetilde{\mathcal{PP}}^{(\nu)}$  is that for the latter the similarity threshold is zero. In this case  $\widetilde{\mathcal{PP}}^{(\nu)}$  can be calculated algorithmically by applying Theorem 1 for  $X = \tilde{x}^{\nu}$  (rather than  $X = \tilde{x}^{\nu}$ ). Then  $D\widetilde{ET}^{(\mu)}$  simply utilizes  $\widetilde{\mathcal{PP}}^{(\nu)}$  for  $\nu = 1, \mu, \mu + 1$  in Theorem 2.

At this point, we emphasize that the approximation method and resulting approximation errors are based on the discretization only. Once we have discretized the data and use a threshold that is zero, we apply the results from Sec. 4 in order to calculate the RQA measures efficiently. Quantifying the discretized data with the use of a recurrence plot will lead to the exact same result. An example of a discretization is illustrated in Fig. 1.



Figure 1: The Lorenz attractor (left) from Eq. (12) and its discretization (right) for grid size parameter  $\delta = 2$ .

#### 188 5.2. Investigation of the approximation method

We explore the phase space discretization from Sec. 5.1 and its impact on the approximation of  $\mathcal{PP}^{(\nu)}$ . Recall that we formulated the approximation procedure as a classification problem.

Denote by  $(x, y) \sim C(S, T)$  the situation that x and y are classified as belonging to class S where they are in fact in class T. Then, if S means 'similar', there are four classification situations (compare with Fig. 2), namely



Figure 2: Classification situations for  $x \in [1.5\delta, 2\delta)$  and  $\delta = 2\varepsilon$ . In this one-dimensional case, the hypercubes are simply intervals in  $\mathbb{R}$ . Here,  $\tilde{x} = 1$  and thus x belongs to the cube no. 1. For  $y \in \mathbb{R}$ , in fact x and y are similar if  $y \in [x - \varepsilon, x + \varepsilon]$ , hence x and y are not classified correctly if  $y \in [\delta, x - \varepsilon)$  or  $y \in [2\delta, x + \varepsilon]$ .

$(x,y) \sim C(S,S)$	$\Leftrightarrow$	$\tilde{x}=\tilde{y}$	and	$\ x - y\ _{\infty} \le \varepsilon.$
$(x,y) \sim C(\neg S, \neg S)$	$\Leftrightarrow$	$\tilde{x} \neq \tilde{y}$	and	$  x - y  _{\infty} > \varepsilon.$
$(x,y) \sim C(S,\neg S)$	$\Leftrightarrow$	$\tilde{x}=\tilde{y}$	and	$  x - y  _{\infty} > \varepsilon.$
$(x,y) \sim C(\neg S,S)$	$\Leftrightarrow$	$\tilde{x} \neq \tilde{y}$	and	$\ x - y\ _{\infty} \le \varepsilon.$

195 For  $\vec{x}^{\nu}$  we conclude the following observations.

- 196 1. If for each pair  $(\vec{x}_i^{\nu}, \vec{x}_j^{\nu}) \sim C(S, S)$  or  $(\vec{x}_i^{\nu}, \vec{x}_j^{\nu}) \sim C(\neg S, \neg S)$ , then clearly 197  $\mathcal{PP}^{(\nu)} = \mathcal{PP}^{(\nu)}$ . However,
- 198 2. if  $(\vec{x}_i^{\nu}, \vec{x}_j^{\nu}) \sim C(\neg S, S)$ , the similarity of  $(\vec{x}_i^{\nu}, \vec{x}_j^{\nu})$  increases  $\mathcal{PP}^{(\nu)}$ , but not 199  $\mathcal{PP}^{(\nu)}$ ; and
- 200 3. if  $(\vec{x}_i^{\nu}, \vec{x}_j^{\nu}) \sim C(S, \neg S)$ , the dissimilarity of  $(\vec{x}_i^{\nu}, \vec{x}_j^{\nu})$  increases  $\widetilde{\mathcal{PP}}^{(\nu)}$ , but 201 not  $\mathcal{PP}^{(\nu)}$ .

Therefore these two types of errors satisfy a mutual cancelling property, and if the number of  $C(\neg S, S)$ -errors equals the number of  $C(S, \neg S)$ -errors, then even  $\widetilde{\mathcal{PP}}^{(\nu)} = \mathcal{PP}^{(\nu)}$  follows.

From these considerations we establish the choice of  $\delta = 2\varepsilon$ .

#### 206 5.2.1. The discretization parameter $\delta$

The grid size  $\delta$  of the discretization determines which elements are classified 207 as similar and thus has to be chosen carefully. If we make no further assumptions 208 to the data, by intuition  $\delta = 2\varepsilon$  is a reasonable choice since the similarity 209 diameter in phase space is  $2\varepsilon$ , and moreover the different error zones have exactly 210 the same measure (see Fig. 2). This also means that  $\delta = 2\varepsilon$  is optimal and 211 leads to nearly zero approximation error if the values of the time series x are 212 independent uniformly distributed (on an appropriate interval). Note that  $\varepsilon > 0$ 213 was supposed implicitly since  $\delta > 0$  is required in Eq. (8). If  $\varepsilon = 0$ , then no 214 discretization is applied, and in fact not necessary since from Theorem 1 follows 215 that the exact quantity  $\mathcal{PP}^{(\nu)}$  can be calculated efficiently. Let us now discuss 216 the algorithmic details. 217

#### 218 5.2.2. Algorithms

The previous findings are used to provide algorithms for the calculation of 219 the approximations from Definition 1; and in case of  $\varepsilon = 0$  for fast calculation of 220 the exact measures  $\mathcal{PP}^{(\nu)}$  and  $DET^{(\mu)}$ . Since the methods for fast processing of 221 the approximations and the exact terms are identical, for  $\varepsilon = 0$  we now denote 222  $\tilde{\vec{x}}^{\nu} := \vec{x}^{\nu}$  and state algorithms for  $\widetilde{\mathcal{PP}}^{(\nu)}$  and  $\widetilde{DET}^{(\mu)}$ , given an arbitrary  $\varepsilon \geq 0$ . 223 As already observed in Sec. 4.1 it is enough to find the histogram  $h_X$  of 224 the (discretized) sequence of trajectory embedding vectors  $X := \tilde{\vec{x}}^{\nu}$ , since then 225  $\mathcal{P}\tilde{\mathcal{P}}^{(\nu)}$  is given by 226

$$\widetilde{\mathcal{PP}}^{(\nu)} = \sum_{\vec{y} \in Y} (h_X(\vec{y}))^2, \tag{9}$$

where Y is again the set of unique members of X. Technically, this may be achieved by assigning unique identifiers to the elements in X, i.e., we are interested in integers  $J_1, \ldots, J_{N-\nu+1}$ , such that

$$\tilde{\vec{x}}_i^{\nu} = \tilde{\vec{x}}_j^{\nu} \Leftrightarrow J_i = J_j \quad \text{for all } i, j,$$

and charge the histogram of these identifiers (compare with Algorithm 1). The calculation of  $D\tilde{E}T^{(\mu)}$  is presented in Algorithm 2. Finally, the efficiency of these procedures is argued in section 5.2.3.

Recall the designations. For more clarity, we eliminate the vector arrows in the algorithms, i.e.,  $x := \vec{x}$  is the trajectory of length  $N, \varepsilon \ge 0$  is the similarity threshold,  $\mu$  the minimum diagonal line length,  $\nu$  is the trajectory embedding dimension and  $x^{\nu} := \vec{x}^{\nu}$  is the matrix that consists of the rows  $x_j^{\nu} := \vec{x}_j^{\nu}$ ,  $j = 1, \ldots, N - \nu + 1$ . We emphasize that the algorithm is not restricted to one-dimensional trajectories x, provided appropriate implementation. In Sec. 6 we provide MATLAB<sup>®</sup> code that handles multi-dimensional data.

Algorithm 1 Fast calculation of  $\tilde{\mathcal{PP}}^{(\nu)}$  (or  $\mathcal{PP}^{(\nu)}$  if  $\varepsilon = 0$ )

1: procedure PPAPPROX $(x, \varepsilon, \nu)$ 2: if  $\varepsilon = 0$  then ▷ No discretization, method is exact. 3:  $\tilde{x} \leftarrow x$ 4: else $\triangleright$  Discretization of phase space, Eq. (8). 5:  $\delta \leftarrow 2\varepsilon$  $\tilde{x} \leftarrow \Phi_{\delta}(x)$ 6: end if 7:  $\begin{aligned} &\tilde{x}^{\nu} \leftarrow \text{apply\_trajectory\_embedding}(\tilde{x},\nu) \\ &J = (J_1,\ldots,J_{N-\nu+1}) \leftarrow \text{find\_unique\_row\_IDs}(\tilde{x}^{\nu}) \\ &h \leftarrow \text{histogram}(J) \end{aligned}$ 8: 9 10: $\tilde{\mathcal{PP}}^{(\nu)} \leftarrow \sum_i h_i^2$ 11: 12: end procedure

240 5.2.3. Complexity analysis

Denote by  $\mathcal{O}_c$  and  $\mathcal{O}_s$  the computational and space complexity respectively.

**Theorem 3.** Let  $\nu$  and  $\mu \in \mathbb{N}$  be fixed choices of the trajectory embedding dimension and the minimum diagonal line length, respectively.

Algorithm 2 Fast calc. of  $D\tilde{E}T^{(\mu)}$  (or  $DET^{(\mu)}$  if  $\varepsilon = 0$ )

1: procedure DETAPPROX $(x, \varepsilon, \mu)$ 

2:  $\mathcal{PP}^{(1)} \leftarrow \operatorname{PPapprox}(x,\varepsilon,1)$ 

3:  $\mathcal{PP}^{(\mu)} \leftarrow \mathrm{PPapprox}(x, \varepsilon, \mu)$ 

4:  $\mathcal{PP}^{(\mu+1)} \leftarrow \mathrm{PPapprox}(x,\varepsilon,\mu+1)$ 

5:  $D\widetilde{E}T^{(\mu)} \leftarrow (\mu \cdot \mathcal{PP}^{(\mu)} + (\mu - 1) \cdot \mathcal{PP}^{(\mu+1)})/\mathcal{PP}^{(1)}$ 

6: end procedure

247

- (i) The complexity classes of the approximations  $\widetilde{\mathcal{PP}}^{(\nu)}$  and  $D\widetilde{E}T^{(\mu)}$  are  $\mathcal{O}_c(N\log(N))$ and  $\mathcal{O}_s(N)$ .
- (ii) If  $\varepsilon = 0$ , then the exact terms  $\mathcal{PP}^{(\nu)}$  and thus the exact RQA-measures
  - $\mathcal{R}R$  and  $DET^{(\mu)}$  are in the complexity classes  $\mathcal{O}_c(N\log(N))$  and  $\mathcal{O}_s(N)$ ,

given an arbitrary phase space norm  $|| \cdot ||$ .

PROOF. We investigate the complexity of Algorithm 1. The complexity class ofAlgorithm 2 is clearly identical.

(i) It is easy to verify that the operations in lines 2-8 are in  $\mathcal{O}_c(N)$  and 251  $\mathcal{O}_{s}(N)$ . The main cost is taken by line 9. One way to find unique identifiers for 252 the rows of  $\tilde{\vec{x}}^{\nu}$  is based on sorting the rows lexicographically. Provided a one 253 dimensional sorting algorithm that operates in  $\mathcal{O}_c(N\log(N))$  and  $\mathcal{O}_s(N)$ , e.g., 254 QuickSort, the computational complexity of sorting the rows lexicographically 255 is in  $\mathcal{O}_c(N\nu\log(N))$  [21]. Then incrementally each row  $\vec{x}_i^{\nu}$  is assigned to an ID 256  $J_i$  in  $\mathcal{O}_c(1)$ , leading to a complexity of  $\mathcal{O}_c(N)$  for the assignment step. Since 257  $\nu$  is constant, the overall complexity in line 9 is  $\mathcal{O}_c(N\log(N))$ . In line 10 it 258 is enough to incrementally count equal entries in J, giving  $\mathcal{O}_c(N)$ . Finally the 259 complexity in line 11 is  $\mathcal{O}_c(N)$  since  $n \leq N$ , where n is the length of the vector 260 h. Altogether the dominating complexity classes are  $\mathcal{O}_c(N\log(N))$  and  $\mathcal{O}_s(N)$ . 261 (ii) Let  $\varepsilon = 0$ . Determine  $\mathcal{PP}^{(1)}$  using Algorithm 1 and set  $RR = \mathcal{PP}^{(1)}/N^2$ . 262 Compute  $DET^{(\mu)}$  using Algorithm 2. By Theorem 1 and 2 these expressions 263 coincide with the exact RQA-measures. As already mentioned in Sec. 4.2, if 264 = 0, then the identities hold for an arbitrary phase space norm since each 265 norm only indicates whether two elements in phase space are equal. The claim 266 on the complexity classes is proven in the first part. 267

We remark that sorting the rows lexicographically is not the only possibility. One could, for instance, use a hash function that maps the embedding vectors to  $\mathbb{R}$  in order to get the identifiers for the embedding vectors and then apply a simple one-dimensional sorting algorithm to find the histogram incrementally. However, such hash functions do not guarantee unique identifiers since they are not injective in general.

274 5.2.4. Worst case error

As shown in Theorem 3, if  $\varepsilon = 0$ , then  $\mathcal{PP}^{(\nu)}$  can be calculated exactly and efficiently. If  $\varepsilon > 0$ , the approximation  $\mathcal{PP}^{(\nu)}$  of  $\mathcal{PP}^{(\nu)}$  satisfies the following estimates. **Theorem 4.** Let  $\varepsilon > 0$  and  $\delta = 2\varepsilon$ . In d-dimensional phase space it holds

$$\frac{1}{2^{d\nu}}\mathcal{PP}^{(\nu)} \le \mathcal{\widetilde{PP}}^{(\nu)} \le 2^{d\nu}\mathcal{PP}^{(\nu)}.$$

**PROOF.** Denote  $m = d\nu$ . The lower bound is reached if the number of  $C(\neg S, S)$ -279 errors is maximal. Let  $\vec{y}$  be a vertex of the discretization lattice. In m-280 dimensional space there are  $2^m$  adjoint hypercubes surrounding  $\vec{y}$ . Hence it is 281 possible to place  $2^m$  points  $\vec{x}_i$ , each in another cube, such that  $\|\vec{y} - \vec{x}_i\|_{\infty} \leq \varepsilon/2$ 282 for all *i*. It follows that  $\|\vec{x}_i - \vec{x}_j\|_{\infty} \leq \varepsilon$  for all *i*, *j*. Hence each pair  $(\vec{x}_i, \vec{x}_j)$ 283 is similar, but by construction classified as dissimilar if  $i \neq j$ . In this case we 284 have  $\mathcal{PP}^{(\nu)} = (2^m)^2$  and  $\mathcal{PP}^{(\nu)} = 2^m$ . The argument is finished since placing 285 additional points only leads to a reduction of the number of  $C(\neg S, S)$ -errors. 286

The upper bound follows in a similar manner by producing errors of type  $C(S, \neg S)$ .

By now the bounds are shown to be existent (hence the theorem is true) 289 but not that they are sharp. One would have to show that there is a trajectory 290 whose embedding vectors are constructed as above. For  $\nu = 2$  and d = 1 an 291 appropriate trajectory is given by  $\vec{x} = (\eta, \eta, -\eta, -\eta, \eta)$ , where  $\eta < \varepsilon/2$ . The four 292 resulting trajectory embedding vectors of  $\vec{x}$  satisfy the above construction. For 293 general  $\nu$  and d this becomes more technical, but we think that this investigation 294 is unnecessary at this point. It is more interesting how the approximation error 295 behaves empirically. 296

#### 297 5.2.5. Empirical approximation error

As seen in Sec. 5.2.4 the bounds of the approximation error of  $\widetilde{\mathcal{PP}}^{(\nu)}$  are rather large and monotonic in  $\nu$ . However, the constructions given in the proof of Theorem 4 to reach these bounds are very specific.

In this section we study the approximation errors of  $\mathcal{PP}^{(\nu)}$  and  $\widetilde{DET}^{(\mu)}$ empirically. For this sake the relative mean errors of 100 realizations, designed as follows, are determined. For each experiment the autoregressive process  $\vec{x} = (x_1, \ldots, x_N)$ , with

$$x_i = ax_{i-1} + b\eta_i, \quad i = 2, \dots, N$$
 (10)

is generated for N = 1000 time steps, where  $x_1 = 0$ , a, b are fixed values 305 that are chosen randomly independent uniformly distributed on [0, 1] and  $\eta$  is 306 a vector of Gaussian white noise. Then the approximations are determined by 307 the algorithms from section 5.2.2 and the exact quantities  $\mathcal{PP}^{(\nu)}$  and  $DET^{(\mu)}$ 308 are calculated by the classical method in order to specify the accuracy of the 309 approximations. The results are illustrated in Fig. 3 for several combinations 310 of  $\nu$  (resp.  $\mu$ ) and  $\varepsilon$ , where the height of the bars corresponds to the mean 311 error and the color of the bars corresponds to the value  $\mathcal{PP}^{(\nu)}$  and  $DET^{(\mu)}$ . 312 respectively. It is customary to select  $\varepsilon$  as a few percent of the phase space 313 diameter [1, 22], which in this case is given by range( $\vec{x}$ ) = max( $\vec{x}$ ) – min( $\vec{x}$ ). 314

We observe that the approximation errors are basically increasing in  $\nu$  (resp. 315  $\mu$ ) and  $\varepsilon$ . However, most of the combinations of  $\nu$  (resp.  $\mu$ ) and  $\varepsilon$  have little 316 relevance. First, if  $\varepsilon$  is small and  $\nu$  (resp.  $\mu$ ) is large, the probability to find 317 recurrences is low. Consequently the bars in Fig. 3 (a) are of deep blue color. 318 Therefore the low error in this area is an artefact. Conversely, if  $\nu$  (resp.  $\mu$ ) 319 is small and  $\varepsilon$  is large, too many recurrences are found, resulting in red colors. 320 Reasonable choices of  $\nu$  (resp.  $\mu$ ) and  $\varepsilon$  are indicated by colors in the range 321 from blue-green to orange-red in Fig. 3 (a). 322

As an example, assume that we want to determine the recurrence rate and the determinism of the trajectory  $\vec{x}$ . For the calculation of the determinism, a minimal line length of  $\mu = 2$  is sufficient, because for the autoregressive process we do not expect much effect of tangential motion or sampling [1]. Then for all sensible values of  $\varepsilon$ , i.e., from 0 to 8 percent of the range, we obtain mean approximation errors below 1.4% for the recurrence rate and below 2.7% for the determinism.

It should be noticed that we have investigated one-dimensional trajectories 330  $\vec{x}$  that are not reconstructed by time series embedding. However, the trajectory 331 embedding of dimension  $\nu$  can also be imagined as time series embedding if we 332 postulate that  $\vec{x}$  is the time series and  $\vec{x}^{\nu}$  is the trajectory, which is obtained 333 from  $\vec{x}$  by time series embedding with time delay 1 and embedding dimension 334  $\nu$ . Then Fig. 3 (a) reflects the approximation errors of the recurrence rate 335 of  $\vec{x}^{\nu}$ , which is given by  $\mathcal{PP}^{(\nu)}/(N-\nu+1)^2$ . The essence of this technical 336 point of view is that the approximation errors increase if the dimension of the 337 trajectory increases. We also observe this in the experiment from Sec. 6 for the 338 3-dimensional Lorenz attractor, see Tab. 2. 339

#### <sup>340</sup> 6. Execution Time of Algorithm 1

We compare the execution times of  $\mathcal{PP}$  and its approximation  $\mathcal{PP}$  on a consumer computer (2.3 GHz Intel Core i7 quad core processor, 16 GB 1600 MHz DDR3 RAM). Since execution times do not only depend on the algorithm, but also on the implementation, we provide MATLAB<sup>®</sup> code. Note that, however, this code uses standard MATLAB<sup>®</sup> routines and may be strongly optimized by the MATLAB<sup>®</sup> compiler.

We evaluate two systems, the autoregressive process

 $x_1 = 0, \quad x_i = 0.57x_{i-1} + 0.24\eta_i, \quad i = 2, \dots, 100.000.000$  (11)

and the well known 3-dimensional Lorenz system (see Fig. 1)

$$\dot{x} = a(y - x), \quad \dot{y} = x(b - z) - y, \quad \dot{z} = xy - cz$$
 (12)

for the parameters a = 10, b = 28, c = 8/3. Then these systems are truncated according to the values of N as listed in the tables of results, Tab. 1 and 2, and processed by the routines. The threshold  $\varepsilon$  was choosen for each N separately as 7% of the phase space diameter and no embedding is applied, i.e. m = 1 in the following MATLAB<sup>®</sup> function.



(a) Approximation error of  $\tilde{RR}^{(\nu)}$ 



(b) Approximation error of  $\tilde{DET}^{(\mu)}$ 

Figure 3: Relative mean errors obtained from 100 autoregressive process realizations. The bar color in Figure (a) indicates the value of the exact recurrence rate  $RR^{(\nu)} = \mathcal{PP}^{(\nu)}/(N-\nu+1)^2$  of the embedded trajectory  $\vec{x}^{\nu}$ . The bar color in Figure (b) reflects the exact determinism  $DET^{(\mu)}$  of the trajectory  $\vec{x}$ , given a minimum diagonal line length  $\mu$ .



Figure 4: Example from the transition experiment. The system of the upper plot is generated as described in Sec. 7.2. The lower graphic shows the window-wise determinism sequence  $\mathcal{D}$  (red) and its approximation  $\tilde{\mathcal{D}}$  (blue). The dashed lines are the confidence levels.

```
352 MATLAB<sup>®</sup> code for \tilde{\mathcal{PP}}.
```

```
function pp = PPapprox( x, eps, m)
353
    [N,d] = size(x);
354
    if eps > 0
                                               % discretize if eps > 0
355
         x = floor(x/(2*eps));
356
    end
357
                                               % apply trajectory embedding
    X = zeros(N-m+1,d*m);
358
    for i = 1:m
359
        X(:,d*(i-1)+1:d*i) = x(i:N-(m-i),:);
360
    end
361
    [u,~,iu] = unique(X,'rows');
                                               % find row ID's iu
362
    h = hist(iu,size(u,1));
                                               % find histogram of row ID's
363
    pp = sum(h.^2);
364
    % end of function PPapprox
365
    MATLAB^{\mathbb{R}} code for \mathcal{PP}.
366
    function pp = PP(x, eps)
367
    R = pdist2(x,x,'chebychev') <= eps;</pre>
                                               % calculate recurrence plot
368
    pp = nnz(R);
                                               % count non zeros
369
    \% end of function PP
370
```

Since the available memory on the computer was 12 GB, we limited the data size for the exact measure  $\mathcal{PP}$ . Indeed a single recurrence plot for N = 40.000consumes about 12 GB of RAM, provided double precision and no storage optimization. For N = 100.000 even about 75 GB of memory would be required.

Ν	Execution Time $\mathcal{PP}$ (sec.)	Execution Time $\widetilde{\mathcal{PP}}$ (sec.)	Approximation Error
100	0.0552	0.0005	0.0275
1.000	0.0078	0.0005	0.0104
10.000	0.9058	0.0018	0.0098
20.000	3.7314	0.0158	0.0098
30.000	8.3865	0.0233	0.0096
35.000	13.7078	0.0131	0.0092
100.000	-	0.0169	-
1.000.000	-	0.1912	-
10.000.000	-	2.2587	-
100.000.000	-	28.5899	-

Table 1: Mean execution times obtained from 10 realizations of the Autoregressive processs (11). The approximation error is again the mean over the relative errors  $|\mathcal{PP} - \tilde{\mathcal{PP}}|/\mathcal{PP}$ .

Ν	Execution Time $\mathcal{PP}$ (sec.)	Execution Time $\widetilde{\mathcal{PP}}$ (sec.)	Approximation Error
100	0.0513	0.0009	0.0471
1.000	0.0077	0.0006	0.3655
10.000	0.9071	0.0052	0.2885
20.000	3.7200	0.0074	0.2646
30.000	8.2962	0.0117	0.2746
100.000	-	0.0396	-
1.000.000	-	0.3645	-

Table 2: Mean execution times obtained from 10 realizations of the Lorenz system (12). The approximation error is again the mean over the relative errors  $|\mathcal{PP} - \tilde{\mathcal{PP}}|/\mathcal{PP}$ .

The results give numerical evidence for the complexity we have proved in The-375 orem 3 and reflect the large difference between  $\mathcal{O}(N^2)$  and  $\mathcal{O}(N\log(N))$  for 376 increasing N. For example the ratio of execution times for the autoregressive 377 process with N = 35.000 is about 1.046. Moreover, the algorithm is very fast for 378 extreme large data and the approximation error decreases slightly with growing 379 N. In Tab. 2 the small approximation error for N = 100 is due to the short 380 and hence almost linear attractor. As expected, the other errors of the Lorenz 381 experiment are higher since the attractor is 3-dimensional. 382

## 383 7. Application to transition detection

## 384 7.1. Introduction to the problem

Assume that we are given a time series or a stream  $x = (x_1, x_2, x_3, ...)$  which changes its dynamics at unknown time segments. It has been shown that the determinism  $DET^{(\mu)}$  is able to find these periods [5, 6, 23]. For this, the time series is analyzed window-wise for a window size w and step size s, leading to a

sequence  $\mathcal{D}$  of determinism-values. More precisely,  $\mathcal{D}(j)$  contains the determin-389 ism of the sub-sequence  $(x_{s \cdot j}, \ldots, x_{s \cdot j+w-1}), j = 1, 2, 3, \ldots$  A transition in the 390 dynamics is indicated when the system leaves its typical dynamical behaviour, 391 in this case its typical range of the window-wise determinism values [6]. The 392 bounds of this range are referred to as confidence levels. An example of a graph 393 of  $\mathcal{D}$  is illustrated as red line in Fig. 4. In the gray marked area the system 394 from the upper plot changes its dynamics (details in Sec. 7.2) and consequently 395  $\mathcal{D}$  exceeds its upper confidence bound, which is represented by the dashed red 396 line. 397

In this section we compare our proposed approximation  $D\tilde{E}T^{(\mu)}$  to the exact measure  $DET^{(\mu)}$  for the problem of identifying transition times. Again, we consider a minimal line length of  $\mu = 2$ . It remains to select  $\varepsilon$ . For each window is determined separately such that the recurrence rate is a small fraction, e.g., 0.1 [6]. This leads to a constant (in time index *i*) denominator in Eq. (2) accentuating the behaviour of the changes in P(l).

#### 404 7.2. Design of the experiment with autoregressive data

<sup>405</sup> The experiment is inspired by [6]. We evaluate 100 realizations employing <sup>406</sup> autoregressive processes of order 2,

$$x_i = ax_{i-1} - bx_{i-2} + c\eta_i.$$

The test time series is initially generated for  $x_1 = x_2 = 0$  and a = 1.8, b = 0.972, c = 0.64 for 1300 time steps. Then the parameters change for a period of 500 time steps to a = 1.85, b = 0.917, c = 0.76. Finally the system returns to the initial parameters and stops at time step 3500. The resulting time series x is then analysed for a window size w = 400 and step size s = 25.

In the exact case  $\mathcal{D}$  contains the values of  $DET^{(2)}$ , where  $\varepsilon$  is chosen such that the recurrence rate  $\mathcal{PP}^{(1)}/w^2$  is 0.1. In the approximative case  $\widetilde{\mathcal{D}}$  contains the values of  $D\widetilde{E}T^{(2)}$ , where  $\varepsilon$  is chosen such that the approximate recurrence rate  $\widetilde{\mathcal{PP}}^{(1)}/w^2$  is 0.1.

In order to find the upper confidence level, we assume that the system with 416 initial parameters is observed for  $N = 100\,000$  time steps and the distribution 417 of the (approximate) determinism values for the windows is charged. We choose 418 as transition level the 99.95%-quantile of those distributions, leading to a con-419 fidence level of 0.4425 for  $DET^{(2)}$  and 0.4523 for  $DET^{(2)}$ . For the evaluation 420 the time points of exceeding and falling below these levels are compared to 421 the actual transition time at 1300 and 1800. The results reveal that our fast 422 approximation performs as well as the slow exact method (Tab. 3). 423

## 424 7.3. Transitions in the logistic map

We briefly illustrate that the approximate determinism  $D\widetilde{E}T$  is also able to find transitions in the logistic map

$$x_1 = 0.7, \quad x_{i+1} = ax_i(1 - x_i),$$

Measure	Left transition error	Right transition error
$DET^{(2)}$	61.25	64.75
$D\widetilde{E}T^{(2)}$	85.00	45.50

Table 3: Mean transition errors obtained from 100 realizations as described in Sec. 7.2. The left/right transition error is defined as the absolute deviation from time index 1300/1800.



Figure 5: Bifurcation diagram of the logistic map and its dynamics. We observe multiple chaos-period transitions that are found by both measures, DET (red) and  $D\tilde{E}T$  (blue).

with control parameter a in the range [3.6, 3.8]. In the experiment we observed that the quality of the approximation is sensitive to  $\varepsilon$ . We found that a rather small threshold is beneficial. More precisely, we selected  $\epsilon$  for each a separately such that the recurrence rate resp. the approximate recurrence rate is 0.01. Fig. 5 confirms that  $D\tilde{E}T$  has the capability to find dynamical transitions.

#### 430 8. Other RQA measures

Using  $\mathcal{PP}^{(\nu)}$  it is possible to specify identities for other diagonal line based RQA-measures. Detailed analysis of those is out of the scope of this work, but we briefly state the formulas in this section. In the following equations the left hand side is the classical definition and the right hand side is the identity in terms of  $\mathcal{PP}^{(\nu)}$ . As before,  $\mu$  denotes the minimum diagonal line length, the phase space norm is  $\|\cdot\|_{\infty}$  and the *LOI* is included unless otherwise stated. For the ratio  $RATIO^{(\mu)}$  between  $DET^{(\mu)}$  and RR, we get

$$N^{2} \frac{\sum_{l \ge \mu} lP(l)}{\left(\sum_{l \ge 1} lP(l)\right)^{2}} = N^{2} \frac{\mu \mathcal{P} \mathcal{P}^{(\mu)} - (\mu - 1) \mathcal{P} \mathcal{P}^{(\mu+1)}}{\left(\mathcal{P} \mathcal{P}^{(1)}\right)^{2}}.$$

<sup>438</sup> Due to Eq. (7), the averaged diagonal line length  $L^{(\mu)}$  is given by

$$\frac{\sum_{l \ge \mu} lP(l)}{\sum_{l > \mu} P(l)} = \frac{\mu \mathcal{P} \mathcal{P}^{(\mu)} - (\mu - 1) \mathcal{P} \mathcal{P}^{(\mu+1)}}{\mathcal{P} \mathcal{P}^{(\mu)} - \mathcal{P} \mathcal{P}^{(\mu+1)}}$$

and the length of the longest diagonal line  $L_{\text{max}}$  (excluding the *LOI*, i.e., P(N) := 0), determined by

$$\max\{l \mid P(l) \neq 0\} = \min\{\nu \mid \mathcal{PP}^{(\nu)} = N - \nu + 1\} - 1,$$

can be found by binary search in  $\mathcal{O}(\log(N))$  iterations since  $\nu \mapsto \mathcal{PP}^{(\nu)}$  is monotonically decreasing.

Finally we should remember that these expressions can be calculated exactly and efficiently if  $\varepsilon = 0$ ; and in case of  $\varepsilon > 0$  the measures can be approximated efficiently by replacing  $\mathcal{PP}$  by  $\mathcal{PP}$ . In both cases Algorithm 1 determines the pairwise proximity measures efficiently. For  $\tilde{L}_{max}$  the resulting computational complexity is  $\mathcal{O}(N \log^2(N))$ . All other approximative measures are in  $\mathcal{O}(N \log(N))$ , whereas the complexity of the classical measures is  $\mathcal{O}(N^2)$ [11].

## 450 9. Conclusions

We have shown that the recurrence rate and many diagonal line based RQA-451 measures can be calculated efficiently, i.e., in  $\mathcal{O}(N\log(N))$  if the similarity 452 threshold  $\varepsilon$  is zero. For the case  $\varepsilon > 0$  we have introduced approximations 453 to these measures that are based on phase space discretization and a relation 454 between the histogram of the diagonal line lengths P(l) and the introduced 455 pairwise proximity measures of trajectory embeddings. For small embedding 456 dimension  $\nu$  or minimum diagonal line length  $\mu$  the proposed approximations 457 are very close to the exact quantities in our experiments with one-dimensional 458 data, while execution times and memory consumption are significantly lower. 459 However, we recommend to compare the approximations to the exact measures 460 on the data of interest before doing serious RQA with it. In particular, if the 461 trajectory is multi-dimensional the approximation error may increase. We also 462 recommend to keep  $\varepsilon$  as small as possible since it determines the grid size of the 463 discretization. Of course a small grid size leads to a gentle discretization and 464 hence to low approximation errors. 465

In future work it should be investigated whether data-adopted discretization lattices are able to improve the approximation accuracy. It is also interesting if there are conditions under which the ratio  $D\tilde{E}T(\vec{x})/DET(\vec{x})$  stays stable (nearly constant) in changing  $\vec{x}$ . Of course, if the approximation error is small this stability is present, but if the error is large, this stability would still allow us to compare dynamics rather than determine dynamics, which is sufficient formany applications, e.g. transition detection.

#### 473 References

[1] N. Marwan, M. C. Romano, M. Thiel, J. Kurths, Recurrence Plots for the
Analysis of Complex Systems, Physics Reports 438 (5–6) (2007) 237–329.
doi:10.1016/j.physrep.2006.11.001.

[2] C. L. Webber, Jr., N. Marwan, Recurrence Quantification Analysis –
Theory and Best Practices, Springer, Heidelberg, 2015. doi:10.1007/
978-3-319-07155-8.

[3] C. L. Webber, Jr., N. Marwan, A. Facchini, A. Giuliani, Simpler methods
do it better: Success of Recurrence Quantification Analysis as a general
purpose data analysis tool, Physics Letters A 373 (2009) 3753-3756. doi:
10.1016/j.physleta.2009.08.052.

[4] N. Marwan, J. Kurths, Comment on "stochastic analysis of recurrence plots
with applications to the detection of deterministic signals" by rohde et
al. [physica d 237 (2008) 619–629], Physica D 238 (16) (2009) 1711–1715.
doi:10.1016/j.physd.2009.04.018.

[5] A. Facchini, C. Mocenni, N. Marwan, A. Vicino, E. B. P. Tiezzi, Nonlinear time series analysis of dissolved oxygen in the Orbetello Lagoon (Italy), Ecological Modelling 203 (3-4) (2007) 339-348. doi:10.1016/j.
ecolmodel.2006.12.001.

[6] N. Marwan, S. Schinkel, J. Kurths, Recurrence plots 25 years later – gaining
confidence in dynamical transitions, Europhysics Letters 101 (2013) 20007.
doi:10.1209/0295-5075/101/20007.

[7] S. Spiegel, J.-B. Jain, S. Albayrak, A Recurrence Plot-Based Distance Measure, Springer, Cham, 2014, pp. 1–15.

[8] Serrà, M. Müller, P. Grosche, J. L. Arcos, Unsupervised Music Structure Annotation by Time Series Structure Features and Segment Similarity, IEEE Transactions on Multimedia 16 (5) (2014) 1229–1240. doi:10.1109/ TMM.2014.2310701.

[9] S. Raiesdana, S. M. R. H. Golpayegani, S. M. P. Firoozabadi, J. M. Habibabadi, On the discrimination of patho-physiological states in epilepsy by means of dynamical measures, Computers in Biology and Medicine 39 (12) (2009) 1073–1082. doi:10.1016/j.compbiomed.2009.09.001.

 J. M. Nichols, S. T. Trickey, M. Seaver, Damage detection using multivariate recurrence quantification analysis, Mechanical Systems and Signal Processing 20 (2) (2006) 421–437. doi:10.1016/j.ymssp.2004.08.007.

- T. Rawald, M. Sips, N. Marwan, D. Dransch, Fast Computation of Recurrences in Long Time Series, Springer, Cham, 2014, pp. 17–29.
- [12] K. Kulkarni, P. Turaga, Recurrence textures for human activity recognition
  from compressive cameras, 2012, pp. 1417–1420. doi:10.1109/ICIP.2012.
  6467135.
- [13] G. Varni, G. Dubus, S. Oksanen, G. Volpe, M. Fabiani, R. Bresin,
  J. Kleimola, V. Välimäki, A. Camurri, Interactive sonification of synchronisation of motoric behaviour in social active listening to music with mobile
  devices, Journal on Multimodal User Interfaces 5 (3-4) (2012) 157-173.
  doi:10.1007/s12193-011-0079-z.
- [14] T. Rybak, Using GPU to improve performance of calculating recurrence
  plot, Zeszyty Naukowe Politechniki Białostockiej. Informatyka 6 (2010)
  77–94.
- 521 URL http://www.bogomips.w.tkb.pl/publications/zn-2010-cuda. 522 pdf
- [15] S. Spiegel, S. Albayrak, An order-invariant time series distance measure
  position on recent developments in time series analysis, in: Proceedings
  of 4th International Conference on Knowledge Discovery and Information
  Retrieval (KDIR), SciTePress, 2012, pp. 264–268.
- 527 [16] S. Spiegel, B.-J. Jain, S. Albayrak, A recurrence plot-based distance mea528 sure, Springer Proceedings in Mathematics Translational Recurrences:
  529 From Mathematical Theory to Real-World ApplicationsTO APPEAR.
- [17] N. H. Packard, J. P. Crutchfield, J. D. Farmer, R. S. Shaw, Geometry
  from a Time Series, Physical Review Letters 45 (9) (1980) 712-716. doi:
  10.1103/PhysRevLett.45.712.
- [18] N. Marwan, A Historical Review of Recurrence Plots, European Physical Journal Special Topics 164 (1) (2008) 3–12. doi:10.1140/epjst/
  e2008-00829-1.
- [19] C. Bandt, A. Groth, N. Marwan, M. C. Romano, M. Thiel, M. Rosenblum, J. Kurths, Analysis of Bivariate Coupling by Means of Recurrence, Understanding Complex Systems, Springer, Berlin, Heidelberg, 2008, pp. 153–182. doi:10.1007/978-3-540-75632-3\\_5.
- [20] I. P. P. Grassberger, Estimation of the kolmogorov entropy from a chaotic signal, Phys. Rev. A 9 (1-2) (1983) 2591–2593.
- J. Wiedermann, The complexity of lexicographic sorting and searching,
  in: J. Bečvář (Ed.), Mathematical Foundations of Computer Science 1979,
  Vol. 74 of Lecture Notes in Computer Science, Springer Berlin Heidelberg,
- <sup>545</sup> 1979, pp. 517–522. doi:10.1007/3-540-09526-8\_52.
- <sup>546</sup> URL http://dx.doi.org/10.1007/3-540-09526-8\_52

[22] S. Schinkel, O. Dimigen, N. Marwan, Selection of recurrence threshold for signal detection, European Physical Journal – Special Topics 164 (1) (2008) 45–53. doi:10.1140/epjst/e2008-00833-5.
[23] L. L. Trulla, A. Giuliani, J. P. Zbilut, C. L. Webber, Jr., Recurrence quantification analysis of the logistic equation with transients, Physics Letters A 223 (4) (1996) 255–260. doi:10.1016/S0375-9601(96)00741-4.

#### <sup>553</sup> 10. Appendix A - Proof of the Determinism Identity

PROOF OF THEOREM 2. Let  $\vec{x} = (\vec{x}_1, \ldots, \vec{x}_N)$  be a *d*-dimensional phase space trajectory  $(d \in \mathbb{N})$  of length N and the similarity threshold  $\varepsilon \geq 0$  as well as the minimum diagonal line length  $\mu \in \mathbb{N}$  be given. Assume that  $\|\cdot\|_{\infty}$  is the underlying phase space norm, i.e., the recurrence plot of  $\vec{x}$  is given by

$$R_{i,j} = \Theta(\varepsilon - \|\vec{x}_i - \vec{x}_j\|_{\infty}), \quad i, j = 1, \dots, N_j$$

and for all  $\nu \in \mathbb{N}$  the pairwise proximity measures  $\mathcal{PP}^{(\nu)}$  are defined as

$$\mathcal{PP}^{(\nu)} = \sum_{i,j=1}^{N-\nu+1} \Theta(\varepsilon - \|\vec{x}_i^{\nu} - \vec{x}_j^{\nu}\|_{\infty}).$$

By definition it holds  $\sum_{i,j=1}^{N} R_{i,j} = \mathcal{PP}^{(1)}$ , thus we have to show that the numerators in Eq. (6) are equal. We show

$$\sum_{l=\mu}^{N} l \cdot P(l) = \mathcal{P}\mathcal{P}^{(\mu)} + (\mu - 1) \cdot (\mathcal{P}\mathcal{P}^{(\mu)} - \mathcal{P}\mathcal{P}^{(\mu+1)}),$$

which gives additional insights into the relation between P(l) and  $\mathcal{PP}$  (7). For this, we define the following index sets.

$$I^{\mu} = \{(i,j) \mid \Theta(\varepsilon - \|\vec{x}_{i}^{\mu} - \vec{x}_{j}^{\mu}\|_{\infty}) = 1\}$$

$$I_{l} = \{(i,j) \mid \sum_{k=0}^{l-1} \Theta(\varepsilon - \|x_{i+k} - x_{j+k}\|_{\infty}) = \sum_{k=-1}^{l} \Theta(\varepsilon - \|x_{i+k} - x_{j+k}\|_{\infty}) = l\}$$

$$J_{l} = \{(i+k,j+k) \mid (i,j) \in I_{l}, k = 0, \dots, l-1\}$$

$$I_{l}^{\mu} = I^{\mu} \cap J_{l}$$

<sup>563</sup>  $I^{\mu}$  contains exactly the index pairs (i, j) such that  $\vec{x}_{i}^{\mu}$  and  $\vec{x}_{j}^{\mu}$  are similar, <sup>564</sup> thus  $\mathcal{PP}^{(\mu)}$  is already determined by  $\mathcal{PP}^{(\mu)} = \sum_{(i,j)\in I^{\mu}} \Theta(\varepsilon - \|\vec{x}_{i}^{\mu} - \vec{x}_{j}^{\mu}\|_{\infty})$ . <sup>565</sup>  $I_{l}$  is the set of index pairs (i, j) such that there is a diagonal line of exactly

<sup>505</sup>  $I_l$  is the set of index pairs (i, j) such that there is a diagonal line of exactly <sup>506</sup> length l in **R** starting at (i, j), thus  $P(l) = |I_l|$ .

J<sub>l</sub> is the set of index pairs (i, j) that exactly cover all diagonal lines of length l in **R**, i.e.,  $l \cdot P(l) = |J_l|$ .

Denote  $\theta_k = \Theta(\varepsilon - ||x_{i+k} - x_{j+k}||_{\infty})$ , then the relation between  $I_l^{\mu}$  and  $I_l$  is described by

$$(i,j) \in I_l \quad \Leftrightarrow \quad \theta_{-1} = \theta_l = 0 \quad \text{and} \quad \Theta(\varepsilon - \|\vec{x}_{i+k} - \vec{x}_{j+k}\|_{\infty}) = 1 \quad \text{for all } k = 0, \dots, l-1$$

$$\Leftrightarrow \quad \theta_{-1} = \theta_l = 0 \quad \text{and} \quad \Theta(\varepsilon - \|\vec{x}_{i+k}^{\mu} - \vec{x}_{j+k}^{\mu}\|_{\infty}) = 1 \quad \text{for all } k = 0, \dots, l-\mu$$

$$\Leftrightarrow \quad \theta_{-1} = \theta_l = 0 \quad \text{and} \quad \sum_{k=0}^{l-\mu} \Theta(\varepsilon - \|\vec{x}_{i+k}^{\mu} - \vec{x}_{j+k}^{\mu}\|_{\infty}) = l - \mu + 1$$

$$(13)$$

$$\Leftrightarrow \quad (i+k,j+k) \in I_l^{\mu} \quad \text{for all } k = 0, \dots, l-\mu.$$

$$(14)$$

Moreover, note that by construction  $I_{l_1}^{\mu} \cap I_{l_2}^{\mu} = \emptyset$  for  $l_1 \neq l_2$  and  $\bigcup_{l \geq \mu} I_l^{\mu} = I_l^{\mu}$  $I^{\mu}$ :

$$I_{l_1}^{\mu} \cap I_{l_2}^{\mu} = (I^{\mu} \cap J_{l_1}) \cap (I^{\mu} \cap J_{l_2}) \subset (J_{l_1} \cap J_{l_2}) = \emptyset \text{ for } l_1 \neq l_2, \qquad (15)$$

$$\bigcup_{l \ge \mu} I_l^{\mu} = \bigcup_{l \ge \mu} I^{\mu} \cap J_l = I^{\mu} \cap \bigcup_{l \ge \mu} J_l = I^{\mu}.$$
(16)

 $_{573}$   $\,$  Now we have collected all relations to begin the actual proof. Since

$$P(l) = |I_l| = \sum_{(i,j)\in I_l} 1 \stackrel{(13)}{=} \sum_{(i,j)\in I_l} \frac{\sum_{k=0}^{l-\mu} \Theta(\varepsilon - \|\vec{x}_{i+k}^{\mu} - \vec{x}_{j+k}^{\mu}\|_{\infty})}{l-\mu+1},$$

574 we get

$$(l - \mu + 1)P(l) = \sum_{(i,j)\in I_l} \sum_{k=0}^{l-\mu} \Theta(\varepsilon - \|\vec{x}_{i+k}^{\mu} - \vec{x}_{j+k}^{\mu}\|_{\infty})$$

575 and therefore

$$\sum_{l \ge \mu} (l - \mu + 1) P(l) = \sum_{l \ge \mu} \sum_{(i,j) \in I_l} \sum_{k=0}^{l-\mu} \Theta(\varepsilon - \|\vec{x}_{i+k}^{\mu} - \vec{x}_{j+k}^{\mu}\|_{\infty})$$

$$\stackrel{(14)}{=} \sum_{l \ge \mu} \sum_{(i,j) \in I_l^{\mu}} \Theta(\varepsilon - \|\vec{x}_i^{\mu} - \vec{x}_j^{\mu}\|_{\infty})$$

$$\stackrel{(15)}{=} \sum_{(i,j) \in \bigcup_{l \ge \mu} I_l^{\mu}} \Theta(\varepsilon - \|\vec{x}_i^{\mu} - \vec{x}_j^{\mu}\|_{\infty})$$

$$\stackrel{(16)}{=} \sum_{(i,j) \in I^{\mu}} \Theta(\varepsilon - \|\vec{x}_i^{\mu} - \vec{x}_j^{\mu}\|_{\infty})$$

$$= \mathcal{PP}^{(\mu)}.$$

**576** Rearranging this equation leads to

$$\sum_{l \ge \mu} lP(l) = \mathcal{P}\mathcal{P}^{(\mu)} + (\mu - 1) \sum_{l \ge \mu} P(l),$$
(17)

 $_{\tt 577}$   $\,$  and it remains to show that

$$\mathcal{PP}^{(\mu)} - \mathcal{PP}^{(\mu+1)} = \sum_{l \ge \mu} P(l).$$

**578** But this already follows by applying (17) for  $\mu$  and  $\mu + 1$ :

$$\begin{aligned} \mathcal{PP}^{(\mu)} - \mathcal{PP}^{(\mu+1)} &= \sum_{l \ge \mu} lP(l) - (\mu - 1) \sum_{l \ge \mu} P(l) - \left( \sum_{l \ge \mu + 1} lP(l) - \mu \sum_{l \ge \mu + 1} P(l) \right) \\ &= \sum_{l \ge \mu} lP(l) - (\mu - 1) \sum_{l \ge \mu} P(l) - \left( \sum_{l \ge \mu} lP(l) - \mu P(\mu) - \mu \sum_{l \ge \mu} P(l) + \mu P(\mu) \right) \\ &= \sum_{l \ge \mu} P(l). \end{aligned}$$

579

г	-	-	٦.
L			н
L			н
÷			

## 580 11. Appendix B - Example

584

598

607

Assume that we want to compute the determinism of the sample trajectory  $\vec{x} = (0.5, 0.8, 0.4, 0.6, 0.8, 0.4, 0.9)$ , given a similarity threshold  $\varepsilon = 0.1$ . First we consider the recurrence plots

$$R_{i,j}^{(\nu)} := \Theta(\varepsilon - \|\vec{x}_i^{\nu} - \vec{x}_j^{\nu}\|_{\infty}), \quad \widetilde{R}_{i,j}^{(\nu)} := \Theta(-\|\tilde{\vec{x}}_i^{\nu} - \tilde{\vec{x}}_j^{\nu}\|_{\infty})$$
(18)

of the embedded (3) trajectory  $\vec{x}^{\nu}$  and its discretization  $\tilde{\vec{x}}^{\nu} = \Phi_{\delta}(\vec{x}^{\nu})$ , where  $\delta = 0.2$  (see (8) and Sec. 5.2.1). The embedded trajectories and the corresponding recurrence plots are illustrated in Fig. 6 for several embedding dimensions  $\nu = 1, 2, 3$  in black, blue, and orange color, respectively. For example the recurrence plots for  $\nu = 2$  comprise the recurrences marked by blue color, the black only highlighted entries are no recurrences for  $\nu = 2$ .

For  $\nu = 1$  (write  $\mathbf{R} = \mathbf{R}^{(1)}$ ) we observe that  $R_{1,4} = 1$ , but  $\tilde{R}_{1,4} = 0$ . That means the pair (0.5, 0.6) is similar, i.e.,

$$|0.5 - 0.6| = 0.1 \le \varepsilon,$$

but classified as dissimilar:

$$\Phi_{\delta}(0.5) = \left\lfloor \frac{0.5}{0.2} \right\rfloor = 2 \neq 3 = \left\lfloor \frac{0.6}{0.2} \right\rfloor = \Phi_{\delta}(0.6).$$

<sup>501</sup> Due to symmetry the pairs (0.5, 0.6) and (0.6, 0.5) lead to  $C(S, \neg S)$ -errors (see <sup>502</sup> section 5.2). For all other pairs the classified and actual similarity statements <sup>503</sup> coincide.

Recall that the determinism is the ratio between the number of points on diagonal lines and all points in the recurrence plot. For the non-embedded trajectories  $\vec{x} = \vec{x}^1$  and  $\tilde{\vec{x}} = \tilde{\vec{x}}^1$  we obtain by counting the structures in the recurrence plots:

$$DET^{(2)} = \frac{17}{21} \approx 0.81, \qquad D\tilde{E}T^{(2)} = \frac{15}{19} \approx 0.79.$$
 (19)

<sup>599</sup> Of course we have calculated the approximation inefficiently by employing <sup>600</sup> the recurrence plot  $\tilde{\mathbf{R}}$ . Using Theorem 2 and Algorithm 1 we may compute <sup>601</sup>  $D\tilde{E}T^{(2)}$  algorithmically:

Following Algorithm 1 we assign unique identifyers to the rows of  $\tilde{\vec{x}}^{\nu}$ . Note that in Fig. 7 the  $\vec{x}^{\nu}$  are transposed, hence in this case we are interested in unique columns. The histograms of the identifyers (col\_ID) are charged and due to Theorem 1 we calculate (compare with Fig. 7)

606 • 
$$\widetilde{\mathcal{PP}}^{(1)} = 3^2 + 3^2 + 1^2 = 19$$

• 
$$\mathcal{PP}^{(2)} = 2^2 + 2^2 + 1^2 + 1^2 = 10$$

**608** • 
$$\widetilde{\mathcal{PP}}^{(3)} = 1^2 + 1^2 + 1^2 + 1^2 + 1^2 = 5$$

Finally, using Definition 1 (which is based on Theorem 2) we get the same resultas before in Eq. (19):

Figure 6: Recurrence Plots (RPs) of the recurrence matrices from Eq. (18) for  $\nu = 1, 2, 3$ , illustrated in black, blue, orange, respectively.



Figure 7: Histograms of trajectory embedding vectors.

611