

Nonparametric Time Series Analysis 1:

Measures of Complexity from Chaos Theory

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Part I

Reconstructing dynamical systems from time series

- 1 Time series
 - Introduction

- 2 Nonlinear dynamics and chaos
 - Dynamical systems
 - Logistic map
 - Sensitive dependence
 - Hénon
 - Lorenz
 - Rössler

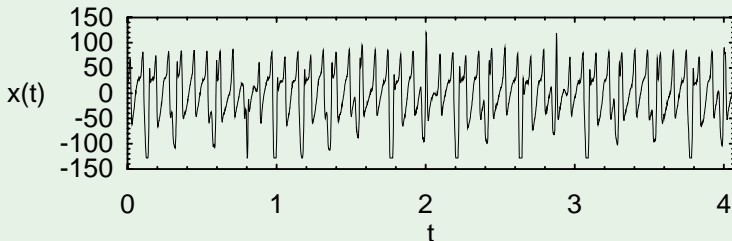
- 3 Attractor reconstruction from time series
 - Takens theorem

Time series

Sequence of measurements over time, for example

- Historic temperature records
- Electrical activity on the heart (ECG)
- Stock prices

Example: Atrial fibrillation (Koefib217)



Time series analysis

Main goals of time series analysis

- Modelling & prediction
- Characterisation & classification

Approaches

- Linear versus nonlinear
- Parametric versus nonparametric

Time series methods from chaos theory

Correlation integrals

- Originally used for estimation of dynamic invariants (deterministic dynamics)
- Measure of complexity (Hoekstra et al.)
- Tests for independence (BDS test, 1987, 1996)
- Distance measures between distributions (Diks et al.)
- Information theoretic dependence measures

Nonlinear dynamics and chaos

Dynamical system

- State space Ω
- Time variable $t \in \mathbb{Z}$ (discrete) or $t \in \mathbb{R}$ (continuous)
- Evolution operator $\phi(\mathbf{x}, t)$, defines a map

$$\phi^t : \Omega \rightarrow \Omega, \quad \phi^t(\mathbf{x}) = \phi(\mathbf{x}, t)$$

(flow over time t)

- (semi-)group properties

$$\phi^0 = \text{Id}, \quad \phi^s \circ \phi^t = \phi^{s+t}$$

$s, t \geq 0$ ($\forall s, t \in \mathbb{Z}$ resp. \mathbb{R} for invertible dynamics)

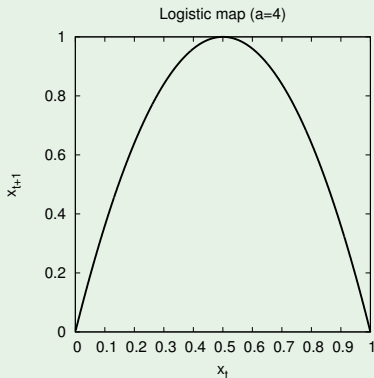


The logistic map

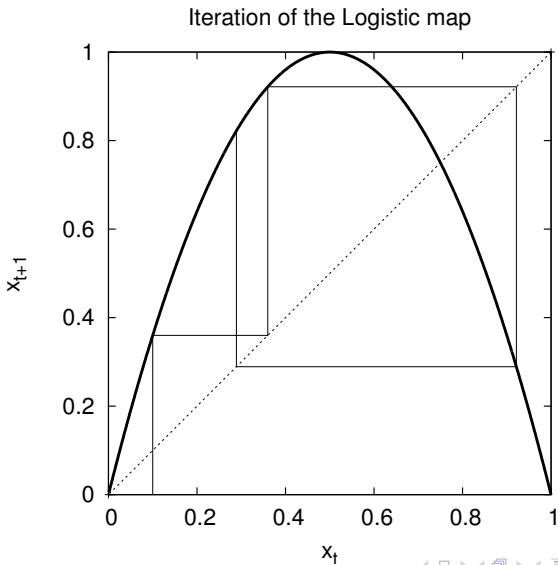
Example: logistic map

Map:

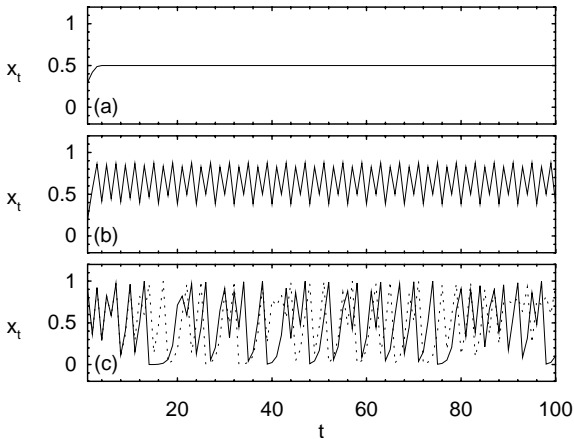
$$x_t = f(x_{t-1}) = ax_{t-1}(1 - x_{t-1}), \quad 0 < a < 4$$



Iterating the logistic map

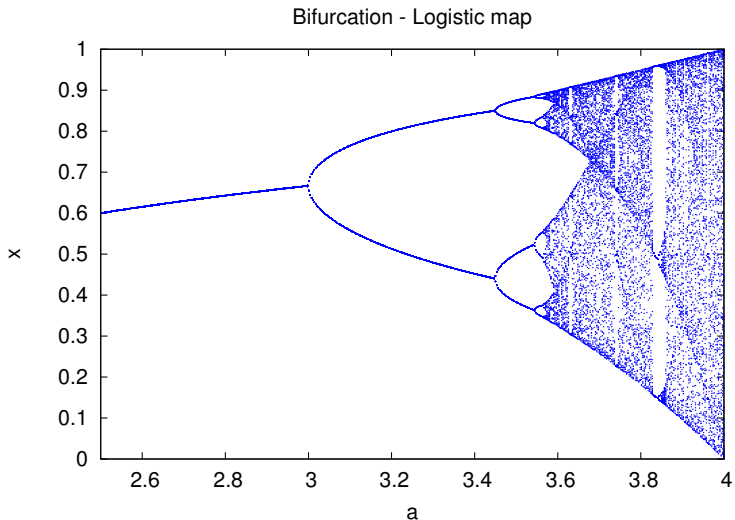


Qualitative behaviour depends on a



(a) $a = 2$, (b) $a = 3.5$, (c) $a = 4$

Bifurcation diagram for logistic map



Sensitive dependence on initial conditions

Near states may either diverge or converge in the long-run

Average growth rate of near trajectories characterized by the Lyapunov exponent

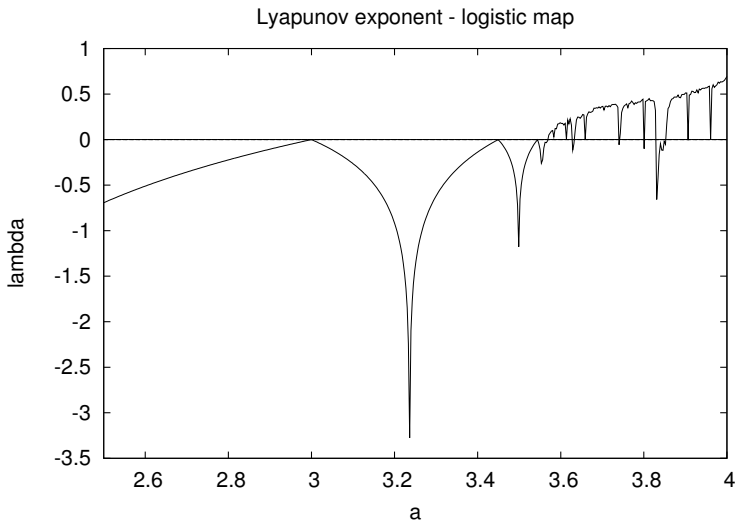
Lyapunov exponent (for 1-dimensional maps)

$$\lambda = \lim_{T \rightarrow \infty} \frac{1}{T} \sum_{t=1}^T \log |f'(x_t)|, \quad \text{with } f'(x) = \frac{df(x)}{dx}$$

If the system has a unique invariant measure, μ say, λ is the same for μ -almost all initial states $x_0 \sim \mu$



Lyapunov exponents



The Hénon map

Example: The Hénon map

$$\begin{aligned}x_{t+1} &= 1 - ax_t^2 + y_t \\ y_{t+1} &= bx_t\end{aligned}$$

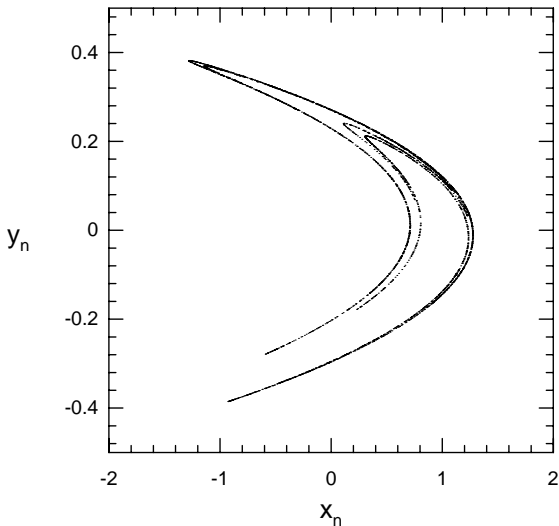
Default values: $a = 1.4$, $b = 0.3$

Jacobian

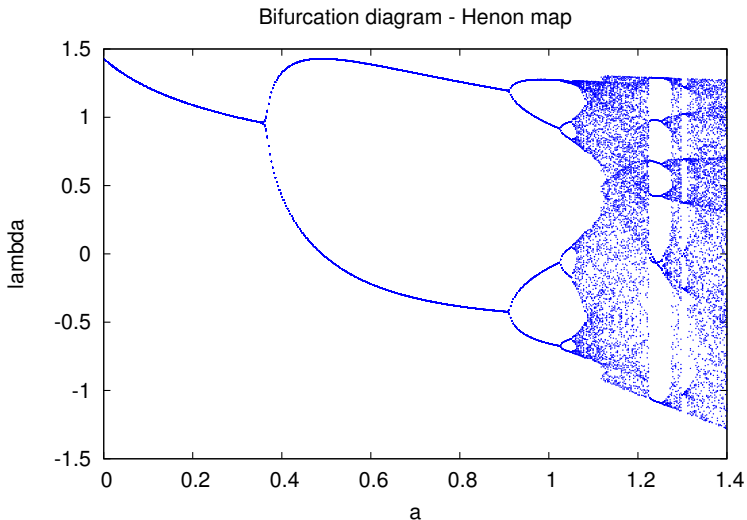
$$J = \begin{pmatrix} -2ax_n & 1 \\ b & 0 \end{pmatrix} \quad \det J = -b$$

\Rightarrow volume contracting for $|b| \leq 1$

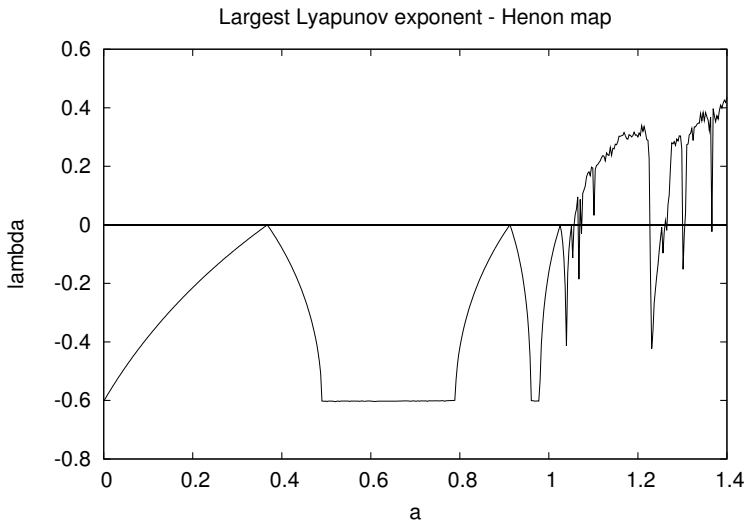
Phase plot – Hénon attractor



Bifurcation plot – Hénon map



Largest Lyapunov exponent – Hénon map



The Lorenz attractor

Lorenz system

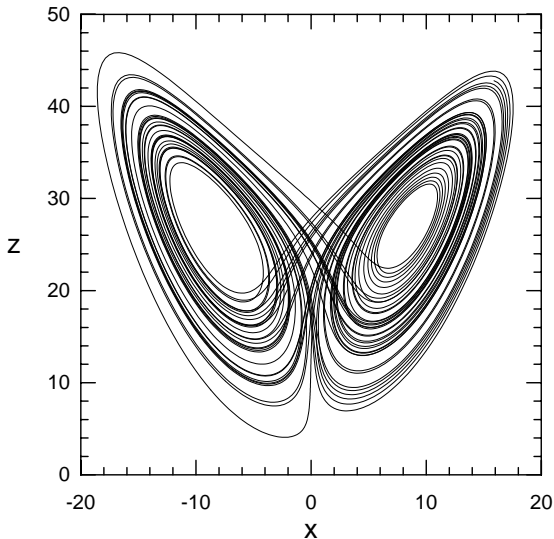
$$\begin{aligned}\dot{x} &= \sigma(y - x) \\ \dot{y} &= (r - z)x - y \\ \dot{z} &= xy - bz\end{aligned}$$

Default parameter values

$$\begin{aligned}b &= 8/3, \\ \sigma &= 10, && \text{(Prandtl number)} \\ r &= 28 && \text{(Rayleigh number)}\end{aligned}$$



Lorenz butterfly



The Rössler dynamical system

Rössler system

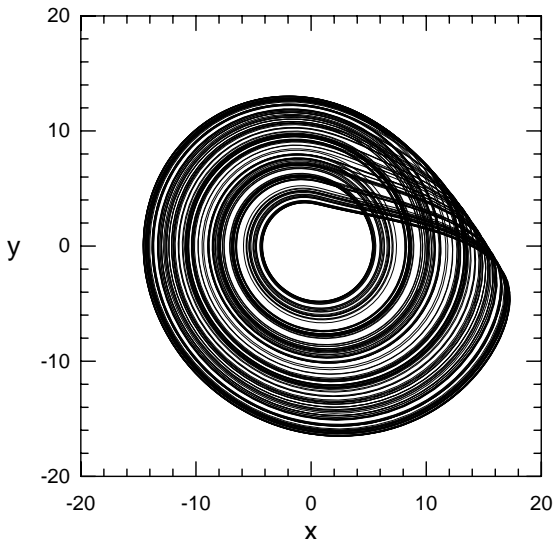
$$\begin{aligned}\dot{x} &= -y - z \\ \dot{y} &= x + ay \\ \dot{z} &= b + z(x - c)\end{aligned}$$

Standard parameter values

$$\begin{aligned}a &= 0.15, \\ b &= 0.2, \\ c &= 10\end{aligned}$$



Rössler attractor



Takens reconstruction theorem

The state space can be reconstructed from an observed scalar time series.

Main idea: starting from a given state, a unique time series pattern arises

Use consecutive data $(X_t, X_{t+\tau}, \dots, X_{t+(m-1)\tau})$ to fix the state at time t

Under which conditions does this work? If it does, how should m and τ be chosen?

Takens reconstruction theorem

Assumptions (continuous time case):

- Unknown dynamical system

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}_t), \quad \mathbf{y} \in \Omega$$

- Dynamics confined to finite dimensional compact subspace $M \subset \Omega$
- Observations are generated as $x_t = h(\mathbf{y}_t)$, at regularly spaced times $t = t_0 + k\tau$, (k integer) where h is a continuous **measurement function**

$$h : M \rightarrow \mathbb{R}, \quad \mathbf{y} \mapsto h(\mathbf{y})$$

- For flows: some requirements on the time interval τ (e.g. no periodic orbits with period $k\tau$)



Takens reconstruction theorem

Continuous time: flow over time interval τ is described by map

$$\phi^\tau : \Omega \rightarrow \Omega, \quad \phi^t(\mathbf{y}) = \phi(\mathbf{y}, t)$$

From now, use same notation for discrete and continuous time, with map $F : \Omega \rightarrow \Omega$ describing the flow over a time lag τ

Note:

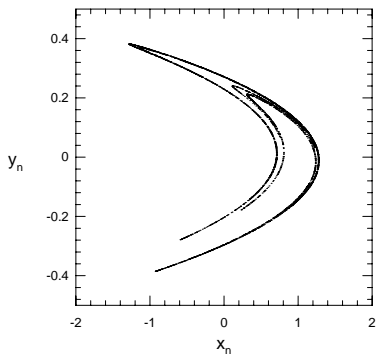
$$\Phi_2 : \mathbf{y} \mapsto (h(\mathbf{y}), h(F(\mathbf{y})))$$

is a map from $M \subset \Omega$ to the plane, \mathbb{R}^2

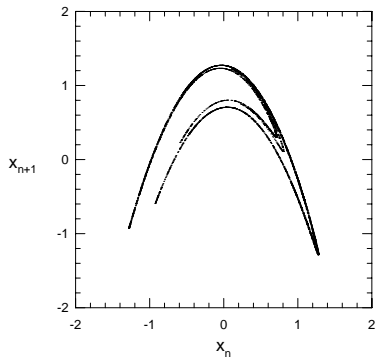


Reconstruction of the Hénon attractor

Original



Reconstruction



Takens reconstruction theorem

Generalisation:

$$\Phi_m : \mathbf{y} \mapsto (h(\mathbf{y}), h(F(\mathbf{y})), \dots, h(F^{m-1}(\mathbf{y})))$$

is a map from $M \subset \Omega$ to \mathbb{R}^m

Takens reconstruction theorem

For smooth measurement functions h , and for m sufficiently large, Φ_m generically is a smooth invertible map from M to \mathbb{R}^m with a smooth inverse (diffeomorphism)

Reconstructed attractor

Corollary of the reconstruction theorem

Delay vectors $(x_t, x_{t+\tau}, \dots, x_{t+(m-1)\tau}) \in \mathbb{R}^m$ lie on a faithful image of the attractor (for m large enough)

In case there is a finite dimensional attractor, the delay vectors also lie on a finite dimensional set, the **reconstructed attractor**

Takens: $m \geq 2 \dim M + 1$ suffices

This bound can be improved further (Sauer et al., 1991):
 $m > 2 \text{boxdim } A$ (box-counting dimension of the attractor)

For estimation of $\dim A$, only $m \geq \dim A$ is required



Perspective

- Control theory: Takens' theorem is an observability result (Aeyels)
- Generalisation of Whitney's embedding theorem (to a restricted set of maps from M to \mathbb{R}^m)



Part II

Correlation integrals



- 4 Correlation integrals
 - Correlation integrals

- 5 Dynamic invariants
 - GP algorithm

- 6 Correlation integrals for noisy data
 - Observational vs dynamic noise
 - Gaussian kernel correlation integrals

Characterising the reconstructed attractor

- Delay vectors $(X_t, X_{t+\tau}, \dots, X_{t+(m-1)\tau})$ for stationary time series have a well-defined long-run distribution
- Reconstruction has an associated measure $\mu_{m,\tau}$, called **reconstruction measure**
- The dynamics has some properties that don't depend on the representation of the dynamics (dynamic invariants)
- For instance, correlation dimension and correlation entropy are independent on the representation



Correlation integrals

Definition of the correlation integral

The correlation integral of the reconstruction measure for embedding dimension m is

$$C_m(r) = \int_{\mathbb{R}^m} \int_{\mathbb{R}^m} \Theta(r - \|\mathbf{x} - \mathbf{y}\|) \mu(d\mathbf{y}) \mu(d\mathbf{x})$$

with

$$\Theta(s) = \begin{cases} 0, & s < 0, \\ 1, & s \geq 0. \end{cases}$$

(Heaviside function)

Compact notation

$$C_m(r) = \int_{\mathbb{R}^m} \int_{\mathcal{B}_r(\mathbf{x})} \mu(d\mathbf{y}) \mu(d\mathbf{x}) := \int_{\mathbb{R}^m} \mu(\mathcal{B}_r(\mathbf{x})) \mu(d\mathbf{x})$$

Scaling law

For finite dimensional attractors: scaling relation

$$C_m(r) \sim e^{-mrK_2} r^{D_2}$$

- D_2 is called the **correlation dimension**. Geometric measure of complexity
- K_2 is known as the **correlation entropy**. Dynamical measure of complexity

Renyi spectrum

Renyi family of correlation integrals indexed by order q

$$\begin{aligned} C_{q,m}(r) &= \left(\int_{\mathbb{R}^m} \left(\int_{\mathbb{R}^m} \Theta(r - \|\mathbf{x} - \mathbf{y}\|) \mu(d\mathbf{y}) \right)^{q-1} \mu(d\mathbf{x}) \right)^{\frac{1}{q-1}} \\ &= \left(\int_{\mathbb{R}^m} (\mu(B_r(\mathbf{x})))^{q-1} \mu(d\mathbf{x}) \right)^{\frac{1}{q-1}} \end{aligned}$$

Scaling law

$$C_{q,m}(r) \propto e^{-mrK_q} r^{D_q}$$

Directly generalises D_2 and K_2



Sufficient condition for chaos

Definition of chaos: $K_1 > 0$

Estimation of inner integral

$$\left(\int_{\mathbb{R}^m} \Theta(r - \|\mathbf{x} - \mathbf{y}\|) \mu(d\mathbf{y}) \right)^{q-1}$$

problematic for $q = 1$. For $q \rightarrow 1$, one finds (l'Hopital)

$$C_{1,m}(r) := \lim_{q \rightarrow 1} C_{q,m}(r) = \int \ln \left(\int_{B_r(\mathbf{x})} \mu(d\mathbf{y}) \right) \mu(d\mathbf{x})$$

$K_2 > 0$ implies K_1 , hence chaos



Estimating correlation integrals

empirical reconstruction measure

The set of delay vectors with equal mass $\frac{1}{n}$ associated to each point (also called **empirical delay vector distribution**)

Empirical correlation integral

$$\frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n \Theta(r - \|\mathbf{x}_i - \mathbf{x}_j\|)$$

(V-statistic)

$$\frac{2}{n(n-1)} \sum_{i=2}^n \sum_{j=1}^{i-1} \Theta(r - \|\mathbf{x}_i - \mathbf{x}_j\|)$$

(U-statistic)

Theiler correction

In practice we use

$$\frac{2}{(n-T)(n-T+1)} \sum_{i=T+1}^n \sum_{j=1}^{i-1} \Theta(r - \|\mathbf{x}_i - \mathbf{x}_j\|)$$

T is called the Theiler correction. $T = 1$ corresponds to a U-statistic (no Theiler correction)

Statistically, the Theiler correction is a finite sample size correction



Grassberger-Procaccia method for estimating D_2 and K_2

- 1 Estimate the correlation integral for $m = 1, \dots, m_{\max}$

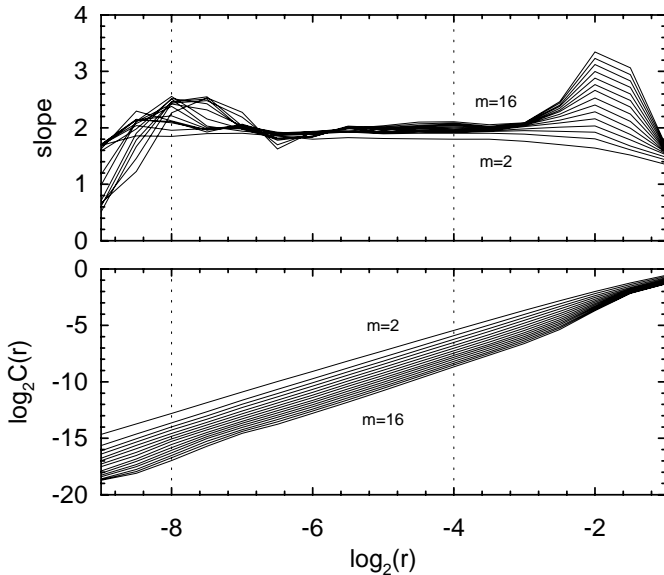
$$\hat{C}_m(r) = \frac{2}{(n-T)(n-T+1)} \sum_{i=T+1}^n \sum_{j=1}^{i-1} \Theta(r - \|\mathbf{x}_i - \mathbf{x}_j\|)$$

for a range of r -values, typically $r = ca^k$ for integer k

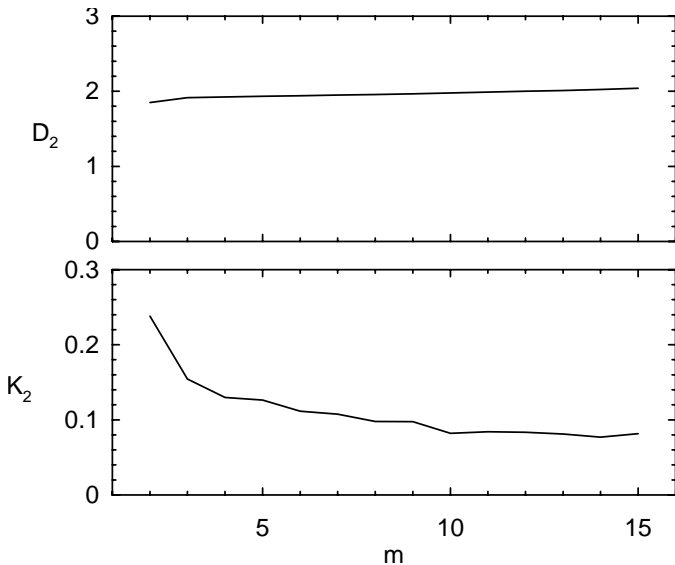
- 2 Look for a 'scaling region' of r -values
- 3 Estimate D_2 and K_2 using the estimated correlation integrals from the scaling region
- 4 Check for convergence with m



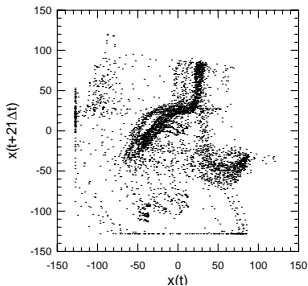
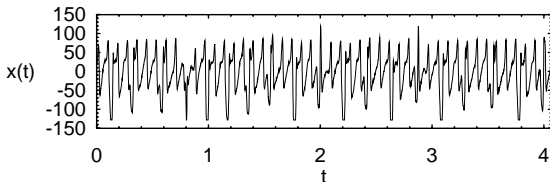
Correlation integrals for the Rössler



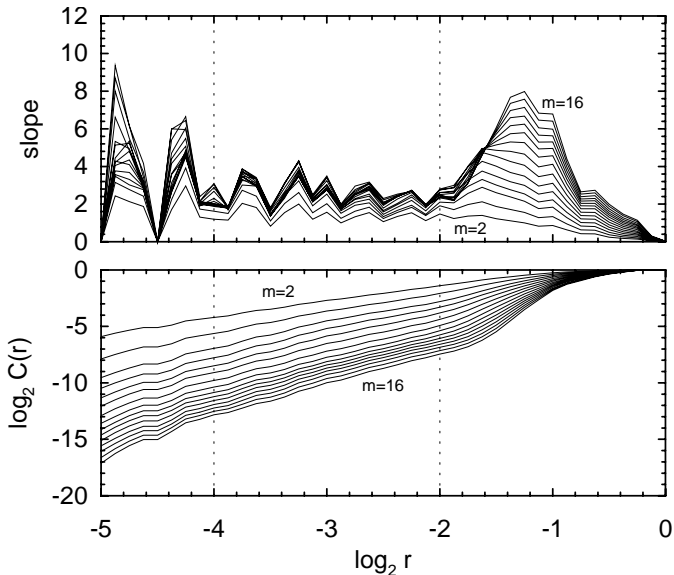
Estimated correlation dimension and entropy



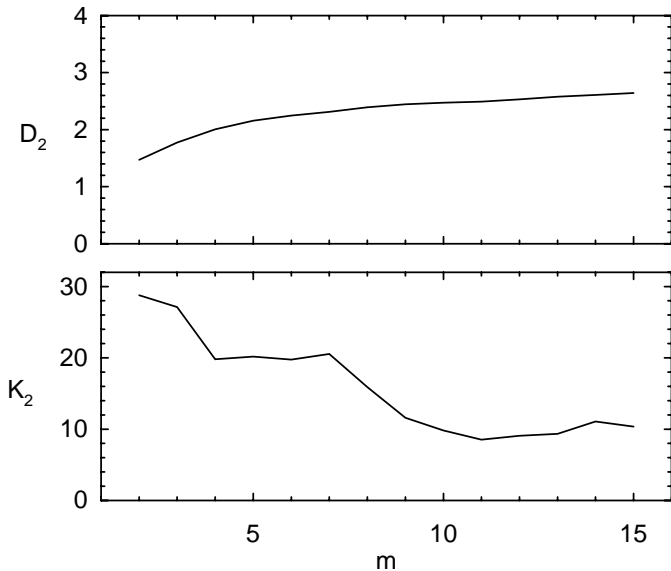
Application to atrial fibrillation



Atrial fibrillation: correlation integrals



Atrial fibrillation: estimated D_2 and K_2



Observational vs dynamic noise

Observational noise

$$\mathbf{Y}_t = F(\mathbf{Y}_{t-1})$$
$$X_t = h(\mathbf{Y}_t) + \varepsilon_t,$$

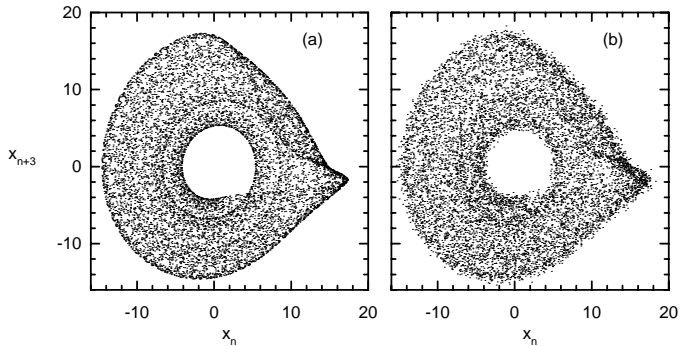
Dynamic noise

$$\mathbf{Y}_t = F(\mathbf{Y}_{t-1}, \varepsilon_t),$$

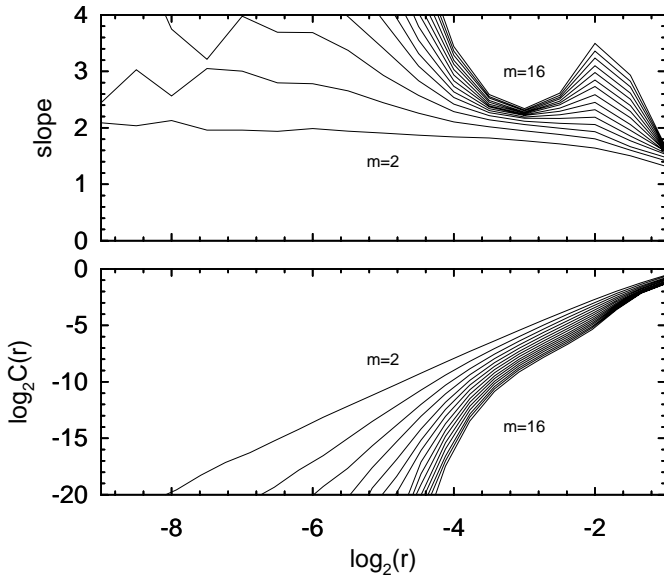
For example:

$$\mathbf{Y}_t = F(\mathbf{Y}_{t-1}) + \varepsilon_t,$$
$$X_t = h(\mathbf{Y}_t)$$

Phase plots from clean and noisy (5%, normal) Rössler data



Correlation integrals for noisy Rössler data



Effect of observational noise on reconstruction measure

Delay vector (m -dimensional)

$$\mathbf{X}_t^m := (X_{t-m+1}, \dots, X_t)$$

is replaced by

$$\mathbf{X}_t^m := (X_{t-m+1} + \varepsilon_{t-m+1}, \dots, X_t + \varepsilon_t)$$

⇒ The ‘clean’ reconstruction measure μ_m^0 is replaced by $\mu_m = \mu_m^0 \circ \nu_m$ (convolution) where ν_m denotes the noise reconstruction measure



Correlation integrals under observational noise

Correlation integral

$$\begin{aligned}C_m(r) &= \int_{\mathbb{R}^m} \int_{\mathbb{R}^m} I_{[0,r]}(\|\mathbf{x} - \mathbf{y}\|) \mu(d\mathbf{x}) \mu(d\mathbf{y}) \\ &= \int_{\mathbb{R}^m} \cdots \int_{\mathbb{R}^m} I_{[0,r]}(\|\mathbf{x} + \mathbf{v} - \mathbf{y} - \mathbf{w}\|) \nu(d\mathbf{v}) \nu(d\mathbf{w}) \mu^0(d\mathbf{x}) \mu^0(d\mathbf{y}) \\ &= \int_{\mathbb{R}^m} \int_{\mathbb{R}^m} I_{[0,r]}(\|\mathbf{z} + \mathbf{s}\|) \nu(d\mathbf{s}) \xi(d\mathbf{z})\end{aligned}$$

with

$$\eta(A) = \mathbb{P}[\mathbf{V} - \mathbf{W} \in A], \quad (\mathbf{V}, \mathbf{W} \sim \nu \text{ independent})$$

and

$$\xi(A) = \mathbb{P}[\mathbf{X} - \mathbf{Y} \in A], \quad (\mathbf{X}, \mathbf{Y} \sim \mu^0 \text{ independent})$$



Correlation integrals under observational noise (ctd)

Clean correlation integral:

$$C_m^0(r) = \int_{\mathbb{R}^m} I_{[0,r]}(\|\mathbf{z}\|) \xi(d\mathbf{z}) = \int_0^r dC_m^0(s)$$

Correlation integral in presence of observational noise

$$C_m(r) = \int_{\mathbb{R}^m} \int_{\mathbb{R}^m} I_{[0,r]}(\|\mathbf{z} + \mathbf{s}\|) \nu(d\mathbf{s}) \xi(d\mathbf{z})$$

Gaussian observational noise already difficult analytically

- Inner integral difficult to evaluate
- Generally, noisy CI is not a functional of the 'clean' CI



Gaussian kernel correlation integral

Although the CI generally is not a functional of the ‘clean’ CI, it is if $\|\cdot\|$ is the Euclidean norm. In that case we can define:

$$\int_{\mathbb{R}^m} I_{[0,r]}(\|\mathbf{z} + \mathbf{s}\|) \nu_m(d\mathbf{s}) := g_r(\|\mathbf{z}\|),$$

and hence

$$C_m(r) = \int_{\mathbb{R}^m} g_r(\|\mathbf{z}\|) \xi(d\mathbf{z}) = \int_0^\infty g_r(s) f_{\|\mathbf{z}\|}^0(s) ds = \int_0^\infty g_r(s) dC_m^0(s)$$

More generally, whenever the kernel function used for calculating the CI depends on the Euclidean distance, the noisy CI is a functional of the noise-free CI



Relations between 'noisy' and 'clean' correlation integrals

The 'classical' correlation integral is of the general form

$$T_m^0(h) = \int_0^\infty K_{m,h}(s) f_{\|\mathbf{z}\|}^0(s) ds$$

with $K_{m,h}(s) = I_{[0,h]}(s)$.

$$T_m(r) = \int_0^\infty g_r(s) f_{\|\mathbf{z}\|}^0(s) ds$$

If $g_r(s)$ is of the same form as the kernel function used for calculating the correlation integral, the noisy and clean CI's then will be automatically simply related.



The Gaussian kernel

For

$$K_{m,h}(s) = e^{-\frac{1}{2} \frac{s^2}{h^2}}$$

$$\begin{aligned} g_r(\|\mathbf{z}\|) &= \int_{\mathbb{R}^m} e^{-\frac{1}{2h^2} \|\mathbf{z}+\mathbf{s}\|^2} \nu_m(d\mathbf{s}) \\ &= (2\pi\sigma)^{\frac{m}{2}} \int_{\mathbb{R}^m} e^{-\frac{1}{2h^2} \|\mathbf{z}+\mathbf{s}\|^2 - \frac{1}{2\sigma^2} (s_1^2 + \dots + s_m^2)} d\mathbf{s}_1 \dots d\mathbf{s}_m \\ &= \prod_{i=1}^m \int_{\mathbb{R}} e^{-\frac{1}{2h^2} (z_i+s_i)^2 - \frac{1}{2\sigma^2} s_i^2} ds_1 \dots ds_m \end{aligned}$$

Since

$$\int_{\mathbb{R}} e^{-\frac{1}{2h^2} (z+s)^2 - \frac{1}{2\sigma^2} s^2} ds = \left(\frac{h^2}{h^2 + \sigma^2} \right)^{\frac{1}{2}} e^{-\frac{1}{2(h^2 + \sigma^2)} z^2}$$

one finds

$$g_r(\|\mathbf{z}\|) = \left(\frac{h^2}{h^2 + \sigma^2} \right)^{\frac{m}{2}} e^{-\frac{\|\mathbf{z}\|^2}{2(h^2 + \sigma^2)}}$$



Modified scaling law in the presence of noise

Gaussian kernel correlation integral in the presence of noise

$$T_m(h) = \left(\frac{h^2}{h^2 + \sigma^2} \right)^{\frac{m}{2}} T_m^0(h^2 + \sigma^2)$$

The noise-free gaussian kernel behaves similar to the usual

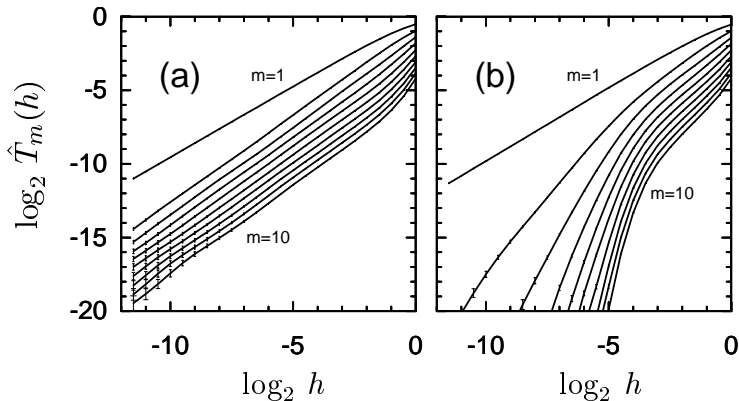
$$T_m^0(h) \simeq \text{cnst} \times m^{-\frac{D}{2}} e^{-Km} h^D.$$

Modified scaling law

$$T_m(h) \simeq \text{cnst} \times m^{-\frac{D}{2}} \times \left(\frac{h^2}{h^2 + \sigma^2} \right)^{\frac{m}{2}} e^{-Km} (h^2 + \sigma^2)^{\frac{D}{2}}$$



Noisy and noise-free Hénon CI



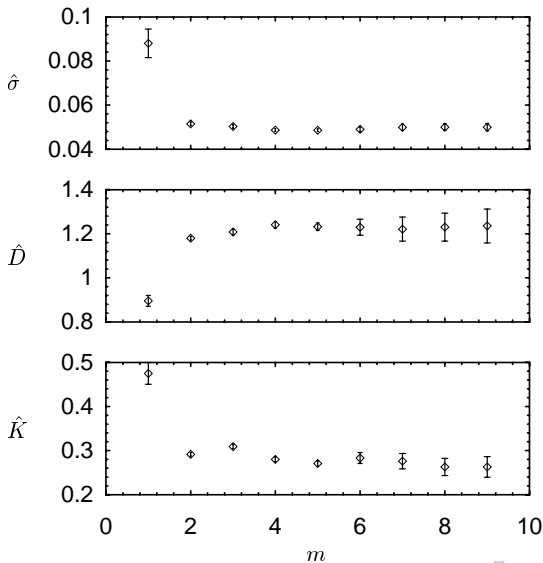
Estimation of D_2 and K_2 in presence of noise

Nonlinear least squares (Levenberg-Marquardt), either

- Weighted least squares. Requires standard errors and possibly covariances of $\hat{T}_m(h)$.
- We used $\text{Var} \hat{T}_m(h) \propto \hat{T}_m(h)(2 - \hat{T}_m(h))$.
- Unweighted
- Implicitly also imposes weights (log-log scale, lin-lin scale)



Estimated invariants from noisy Hénon CI



Course-grained quantities

Even if assumptions made so far (determinism + gaussian observational noise) are violated, one may use correlation integrals

Idea is to use behavior of correlation integrals as a measure of complexity:

- Large slope of $\ln C_m(r)$ indicates large number of relevant state variables
- Difference $\ln C_m(r) - \ln C_{m+1}(r)$ is a measure of unpredictability at scale r

Motivates examining course-grained quantities



Definition of course-grained quantities

Course-grained correlation dimension and entropy

Coarse-grained correlation dimension

$$D_2(m, r) = \frac{d \ln C_m(r)}{d \ln r}$$

Course-grained correlation entropy

$$K_2(m, r) = \ln C_m(r) - \ln C_{m+1}(r)$$

Part III

Local linear prediction

7 Prediction by analogy

8 Casdagli method

Prediction by analogy, nearest neighbour method

Reconstruct state space, state vectors \mathbf{X}_s^m , $1 \leq s \leq n$

Idea is to exploit

$$\mathbf{X}_{t+l} = g(\mathbf{X}_t^m)$$

To make ℓ -step-ahead forecast from \mathbf{X}_t^m we need an approximation (estimate) of g

- find k nearest neighbours $\mathbf{X}_{s_i}^m$ among \mathbf{X}_s^m , $s < t$ or $s \neq t$
- locally constant model leads to prediction by averaging

$$\hat{\mathbf{X}}_{t+l} = \sum_{i=1}^k \mathbf{X}_{s_i+l}$$

- alternatively, construct local linear map through linear regression (requires $k > m$). Model:

$$\mathbf{X}_{t+l} = \mathbf{a}_0 + \sum_{j=1}^m \mathbf{a}_j \mathbf{X}_{s_i+1-j} + \varepsilon_{t+l}, \quad i = 1, \dots, k$$

Prediction by analogy, kernel methods

Comparable to k -nearest neighbour method, only using all points with weights determined by distance

Prediction

$$\hat{\mathbf{X}}_{t+l} = \sum_s w_{s,t} \mathbf{X}_{s+l}$$

weights w_i determined by distance in state space

$$w_{s,t} = \frac{K_h(\mathbf{X}_s^m - \mathbf{X}_t^m)}{\sum_s K_h(\mathbf{X}_s^m - \mathbf{X}_t^m)}$$



Prediction by analogy, other methods

- Polynomials (global nonlinear model)
- Neural networks (global nonlinear)
- Radial basis functions (local, linear in coefficients)

$$F(\mathbf{x}) = \alpha_0 + \sum_i \alpha_i \Phi(\|\mathbf{x} - \mathbf{x}_i\|)$$

e.g. $\Phi(\mathbf{s}) = 1/(1 + e^{\mathbf{b}\mathbf{x}-c})$

Parameter estimation by error backpropagation (gradient descent)



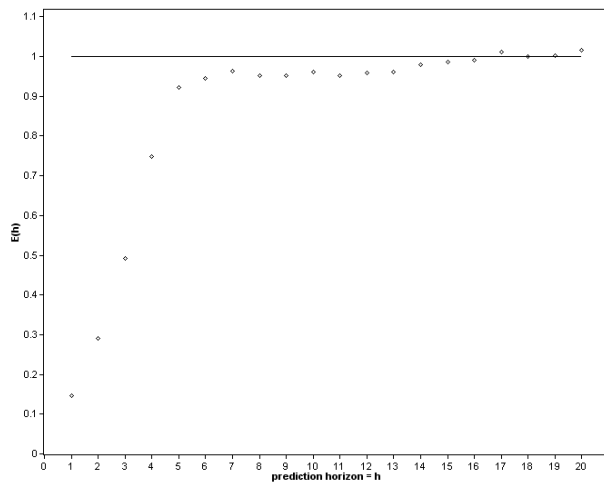
Casdagli method

- Divide the data in a fitting set x_1, \dots, x_{N_f} and a testing set $x_{N_f+1}, \dots, x_{N_f+N_t}$
- Vary k in the nearest neighbour method, for each k :
- Choose a number of random reference points to predict from
- Determine prediction error $e_i(k) = |\hat{x}_{i+l}(k) - x_{i+l}|$
- Repeat to determine RMSE

$$E_m(k) = \left(\frac{1}{n} \sum_i e_i^2(k) \right)^{\frac{1}{2}} / \sigma$$



Example Casdagli method (Hénon data)



$m = 3, \varepsilon = 0.1, 200$ predictions

- Takens' reconstruction theorem, correlation integrals, fractal dimensions, correlation entropy, estimation of dynamic invariants, local linear prediction
- *Nonparametric tests based on correlation integrals:* Divergences between reconstruction measures, U-statistics estimators, tests for symmetry of multivariate distributions, attractor comparison, testing for reversibility, tests for serial independence and linearity
- *Statistical aspects of nonparametric tests:* asymptotic results for U-statistics in time series context, bootstrap and Monte Carlo tests, consistency, bandwidth selection problem, diagnostic model checking, nuisance parameters, tests based on empirical copulas
- *Granger causality tests:* conditional independence, linear versus nonlinear Granger causality, nonparametric Granger causality tests, testing for Granger causality using correlation integrals, consistency, local measures of conditional dependence