Improved multifractal box-counting algorithm, virtual phase transitions, and negative dimensions

Markus Alber and Joachim Peinke
Experimentalphysik II, Universität Bayreuth, D-95440 Bayreuth, Germany

(Received 1 October 1997)

Most algorithms for numerical multifractal analysis rely on some evaluation of related scaling laws. We present a self-consistent way to obtain from a partition sum $S_q(l)$ the spectrum of singularities $f(\alpha)$ and its confidence intervals. With this tool we gain insights into the intricacies of fixed-size algorithms and propose consequent improvements. We give a numerical analysis of the Hénon attractor which displays theoretical predictions of a phase transition. [S1063-651X(98)01005-8]

PACS number(s): 47.53.+n, 05.45.+b, 47.10.+g

Following the seminal paper of Halsey *et al.* [1] on multifractals, a continuing surge of interest in multifractals has arisen. In the course of this development a substantial number of algorithms for the numerical analysis of both physical and artificial multifractal objects have been invented, and partially acquired a widespread popularity despite a number of open questions as to accuracy and reliability.

Most algorithms in use today are based on the thermodynamically inspired formulation of multifractals, and it is for those that the ideas outlined in this paper apply. For the purpose of demonstrating the capabilities of our methods we deliberately pick one class of algorithms which is deemed to be particularly flawed and demonstrate that it can be improved up to, and exceeding, the standard of other algorithms: fixed-size box counting (see Ref. [2]).

Some work has been done to demonstrate that the performance of fixed-size, or box-counting, algorithms (BCAs) is far from perfect [3], several natural limitations have often been pointed out [14,5–7], and many improvements have been proposed [8–13].

In this paper, we demonstrate that correcting the ubiquitous double-logarithmic plots of some sampled quantity for lacunarity effects rids the computations of the dominating source of systematic errors [7], and our self-consistent way of achieving this yields a considerable qualitative improvement of the results. We point out again that in principle similar gains in reliability should be possible also with other sampling procedures (such as correlation integrals [20], box-counting derivates [15], or fixed mass algorithms [16]). On the basis of these findings we can quantify the malperformance of box counting, and subsequently propose amendments.

Let μ be a probability measure defined on a (possibly fractal) support $E\subset\mathbf{R}^d$. We are interested in the spectrum of singularities $f(\alpha)$ of local Hölder exponent α:

$$\alpha(\mathbf{x})=\lim_{l\to 0}\frac{\log\mu(\mathcal{B}(l,\mathbf{x}))}{\log l},\qquad (1)$$

where $\mathcal{B}(l,\mathbf{x})$ is the ball centered at $\mathbf{x}\in E$ with radius l [1,2,17,18]. In many cases, $f(\alpha)$ can be interpreted as the Hausdorff dimension of the set of $\mathbf{x}\in E$ with local Hölder exponent α. To these ends we cover E with a grid of boxes (hypercubes) $B(l)=\Pi_{j=1}^{d}(n_j l,(n_j+1)l)$ of size l, where the n_j are integers. We then calculate the qth moment (or *partition function*) $S_q(l_i)$ of μ for several $l_i\in\mathcal{L}=\{l_1,l_2,\ldots,l_n\}$ and $q\in\mathcal{Q}=\{q_1,q_2,\ldots,q_n\}$ by

$$S_q(l_i)=\sum_{\mu(B)\neq 0}[\mu(B)]^q=\langle\mu^q\rangle.\qquad (2)$$

Brackets $\langle\ \rangle$ indicate sample averages as usual.

The *generalized dimensions* $D(q)$ (for $q\neq 1$) and the *scaling function* $\tau(q)$ are defined by

$$\tau(q)=D(q)(q-1)=\lim_{l\to 0}\frac{\log S_q(l)}{\log l}.\qquad (3)$$

In practice one might hope that S_q scales with l:

$$\log S_q(l_i)=\tau(q)\log(l_i)+c+\epsilon\qquad (4)$$

and so obtain $\tau(q)$ via a least squares line fit to the plot of $\log S_q(l_i)$ against $\log l_i$ for all suitable l_i with the statistical deviation ϵ.

Frequently, the Legendre transformation of $\tau(q)$ is considered [1]:

$$\alpha=\frac{\partial\tau}{\partial q},\qquad f=q\alpha-\tau,\qquad (5)$$

which shall not be the main subject here [19].

Apart from obvious questions of how the resolution and finiteness of the sample and the presence of noise affect the algorithm, one finds a number of flaws with the procedure itself. Any fixed-size approach compensates for the lack of knowledge about the fine structure of a fractal or about its generating process by taking the limit of infinitesimal length scales, Eqs. (1),(3). Without any measure for the accuracy or convergence rate of the scaling behavior of a single average on a chosen range of length scales l_i [Eq. (4)], and thus of $\tau(q)$ for a given q, the interpretation of results becomes rather elusive.

In essence, the systematical errors of any fixed-size counting procedure are not quantifiable. Note that these errors are quite distinct from those arising from a lack of statistical resolution of the sample, although both kinds of errors are naturally scale dependent [7] and hence notoriously difficult to disentangle. Although proposals for statistical corrections have been made [4], they have to be based on estimates about the distribution of the measure already obtained by some instance of a sampling procedure, and hence in turn must reflect the deficiencies in resolution of the latter.

One example of these inevitable finite-size problems are the well known lacunarity effects. However, there are less obvious effects, too, equally difficult to treat, and we will demonstrate some on the example of the Hénon attractor.

In practice, much would be gained if error estimates betrayed the presence of hidden systematic errors, and were based on more profound assumptions about the distribution of the statistical error ϵ in Eq. (4). It has been pointed out [3,5] that the (standard Gaussian) error obtained from the least-squares fit grossly underestimates the error present. We propose a robust method based on a Monte Carlo bootstrap approach which helps to overcome this problem.

In order to treat the aforementioned effects, we introduce a scale-dependent intercept into Eq. (4):

$$\log S_q(l_i) = \tau(q)\log l_i + C(l_i,q). \tag{6}$$

The function $C(l_i,q)$ was termed by Cutler [5,6] the *wandering intercept*. Our development depends on two assumptions about the wandering intercept: (i) for fixed l, $C(l,q)$ is a slowly varying function of q; (ii) for "most" q we find

$$C(l,q) = F(l)G(q). \tag{7}$$

These assumptions amount to saying that each moment "knows" about the corresponding deviations from the ideal scaling of moments for nearby q. The idea is to use this information to compensate for the adverse effects of these deviations on the fitting procedure [symmetric scaling-error compensation (SSC)]. Of course, it remains to be shown in each case that these assumptions hold. As we will see, it is often the case that a violation of these assumptions warrants dispensing with the multifractal analysis of a data set by standard means as a whole.

Inspired by a related method introduced by Benzi *et al.* [21] in the statistical description of fully developed turbulence, by using Eqs. (6) and (7) we express $\log S_q$ as a function of $\log S_{q'}$ instead of $\log l$:

$$\log S_q(l_i) = \frac{\tau(q)}{\tau(q')}\log S_{q'}(l_i) + F(l_i)\left(G(q) - \frac{\tau(q)}{\tau(q')}G(q')\right). \tag{8}$$

We can now proceed to fit a line to Eq. (8) to obtain the quotient $\tau(q)/\tau(q')$. Although we still cannot assume that the error distribution is normal, in the absence of at least some of the systematic errors this deserves more credence than the standard procedure. To make best use of the mutual information contained in all moments, it is desirable to plot $\log S_q$ as a function of as many $\log S_{q'}$ as possible. We choose $q_i \in \mathcal{Q}, q_1 < q_2 < \cdots < q_{\max}$ such that $\tau(q_i)/\tau(q_{i+1})$ is approximately constant for all i. We thus arrive at a global linearized $\mathcal{X}^2$ merit function, which in fact is a functional of $\tau(q)$:

$$\mathcal{X}^2 = \sum_{q\in\mathcal{Q}} \sum_{q>q'\in\mathcal{Q}} \sum_{i=1}^{m} \times \left(\frac{[\tau(q')\log S_q(l_i) - \tau(q)\log S_{q'}(l_i) + c_q - c_{q'}]}{(q-q')w(q)w(q')}\right)^2. \tag{9}$$

Of course, this functional may be supplied with additional terms assuring compliance with constraints such as the concavity of the $\tau(q)$ function in the manner of maximum entropy methods. Since this method is predominantly intended to be a qualitative means of evaluating an assumed multifractal, with the small number of q this additional term might well be dropped.

We advance by minimizing $\mathcal{X}^2$ with respect to $\tau(q)$, treating the c_q as independent constants. For easier and more stable computation we changed the nonlinear equation (8) to a linear form and introduced an arbitrary weight function $w(q)$, which is intended to amplify the proportion of a moment S_q according to the standard variation of its scaling function $\tau(q)$, thus giving little weight to small $|q|$. Estimates for the confidence intervals of the fitted parameters are obtained by the bootstrap method as described in [23] with the necessary parameters chosen as in [24].

The greatest advantage of this method is that we fit the entire function $\tau(q)$ to all the available information in one step, thereby also reducing lacunarity effects. Also, in estimating the confidence intervals in this comprehensive way, we take into account for all q the systematic errors that stem from the box-counting procedure but become expressed only for larger $|q|$. The increase in confidence intervals for small $|q|$ is a symptom of poor statistical resolution which is completely ignored by the customary least-squares fit. We exploit the interconnection of small and large $|q|$ in the SSC fit to integrate this information into the calculation of the confidence intervals.

Note that the coefficient matrix derived from Eq. (9) is singular with one free constant and requires further information, which can be obtained by taking as reference $\tau(0)$ or the entire $\tau(q)$ as obtained from the standard method. The accuracy of SSC is limited by the systematic and statistical errors of the chosen reference, and thus although SSC is likely to give qualitatively better results, the overall accuracy need not improve.

To demonstrate the potential of SSC, we examine the following seemingly simple example: the sample consists of 2^{10} equally spaced values from a self-similar deterministic "binomial" measure on **R** generated with the transformations w_k and with splitting factors p_k:

$$w_1 = 0.4x, \quad p_1 = 0.7,$$
$$w_2 = 0.5(x+1), \quad p_2 = 1 - p_1 = 0.3. \tag{10}$$

The measure was subsequently "smeared out" by convolution with a Gaussian function with width equal to the resolution of the support of 2^{-10}.

As can be seen from Fig. 1 the standard BCA calculation does not compare well with the analytical solution [1,25]. Note the considerable improvement by SSC for positive q. As a reference, $\tau(0)$ from standard BCA was chosen.

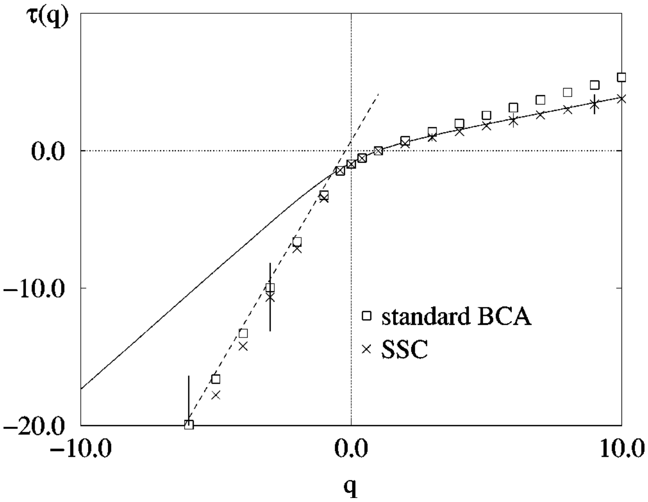

FIG. 1. The $\tau(q)$ curves of the binomial measure (10). The solid line is the analytical solution. Squares were obtained by standard BCA; the error is smaller than the size of the squares. Crosses were obtained by simple box counting followed by SSC. Typical 95% confidence intervals are indicated. The dashed line is the asymptote for $q\rightarrow-\infty$. Notice its positive intercept which relates to negative values of $f(\alpha)$.

The devastating failure of standard box counting for negative q stems from a set of boxes with spuriously small mass which we will call clipping errors. When raised to a negative power in the partition sum, these boxes become dominating and hence obliterate all information about the original measure [3,14,13].

Selecting the appropriate scaling interval $l\in[l_{\min},l_{\max}]$ is greatly facilitated by using correlation plots of wandering intercepts $C(l_i,q)$ against $C(l_i,q')$. These plots often show single points off the line which signals correlation in the $C(l_i,q)$ [such as in Fig. 2(a)]. These points correspond to length scales l_i affected by transitory behavior at large length scales, and noise or statistical resolution problems at small scales. Quite frequently we find that, especially for larger $q>0$, the range of suitable length scales becomes smaller. We interpret this effect as a sign of depletion of the data set, and conclude that the corresponding $S_q(l)$ and $\tau(q)$ no longer take into account the rare events in the sample. In the example (10), this happens for q at around 5. Interestingly, we find a sharp increase in the confidence intervals for $\tau(q)$ for $q>5$.

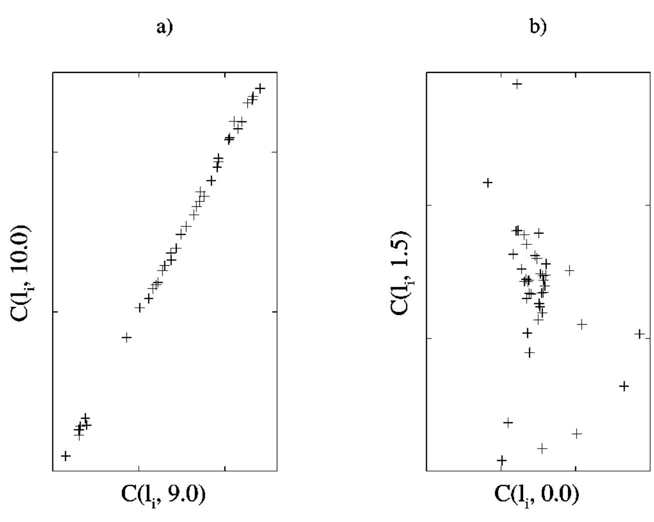

FIG. 2. Wandering intercepts for the Hénon attractor plotted against each other. (a) Good coherence for $C(l_i,10.0)$ against $C(l_i,9.0)$, (b) no coherence at the ''plateau'' for $C(l_i,1.5)$ against $C(l_i,0.0)$.

Although SSC cannot serve to eliminate a lack of statistics, it clearly reveals its influence on the analysis and is a valuable aid in assessing the outcome. The question may be raised if information which fails to be resolved at the stage of computing the partition function can possibly be retrieved at a later stage at all.

At first sight, the situation is hopeless with negative q. However, the sharp kink in $\tau(q)$ at $q=q_c$ and its abnormal behavior for $q<0$ can both serve as a model case for a phase transition between measures and give some information about the structure of the original measure. From the correlation plots of $C(l_i,q)$ against $C(l_i,q')$ we find that all coherence is lost for q only a little smaller than 0, see Fig. 2(b) and reestablished for even smaller $q<q_c$. We interpret these incoherent fluctuations as a ''phase transition'' between the genuine measure μ and a *virtual measure* ν generated by clipping errors at ''temperature'' q_c. Although it is impossible to define neither the measure ν nor its support in the limit $l\rightarrow 0$, there are clearly more almost empty boxes at a finite length scale than there ought to be. In the limit of infinite resolution this measure vanishes, hence the term ''virtual.'' We support this view with the following findings.

Despite its artificial nature, the virtual measure shares some of the features which are commonly held to be peculiar to fractal measures: it displays a scaling behavior and can thus be assigned a dimensionlike quantity, and it lives (tentatively) on a support which is the subset of a fractal. In fact, the slope of $\tau(q<q_c)$ corresponds to the density of the measure on the clipping boxes and is thus directly related not only to the multifractal measure itself, but also to issues such as noise and statistical and spatial resolution of the data. Secondly, the intercept of the asymptote shows how the boundary of the l-parallel body of $E=\text{supp}(\mu)$ scales with l. Quite obviously this interpretation is only meaningful if we bear in mind that we do not treat a multifractal in its mathematical sense, but only a very limited approximation of it. In these terms, $f(\alpha(q=-\infty))$ is a measure of how much the experimental μ is concentrated on its apparent support, and hence the degree of apparent fractality of the sample. The smaller $f(\alpha(q=-\infty))$, the smaller the resemblance of the experimental fractal to its idealized image.

We find increased and incoherent fluctuations in $C(l_i,q)$ for q in a small interval around q_c as well as a kink in $\tau(q)$ at q_c. The assumptions for SSC do not hold. These signs are usually read as the signature of a phase transition. It is impossible to distinguish this virtual phase transition from a real one by the mere information provided by the algorithm.

As Mandelbrot [26] pointed out, for measures such as the virtual measure in this case negative values of $f(\alpha)$ can occur naturally as a consequence of their randomness. This can be attributed to the fact that for a virtual measure the limit $l\rightarrow 0$ of the expected values $S_q(l)=\langle\mu^q\rangle$ need not converge to the expected value of the limit, which in this case is zero. In example (10) there are indeed negative values for $f(\alpha)$, as can be read from the positive intercept with the vertical axis

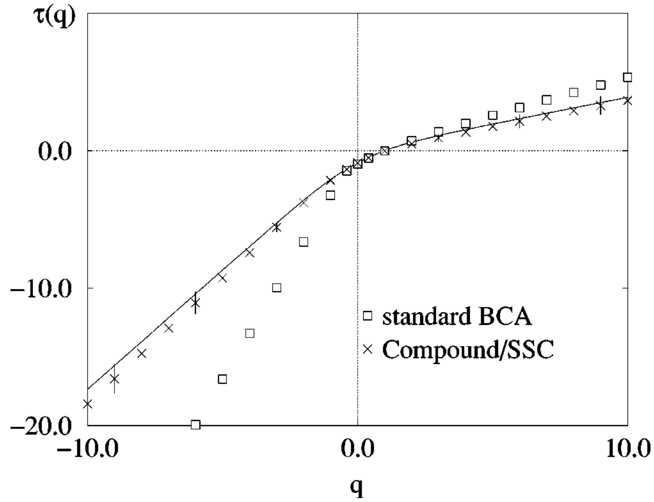

FIG. 3. The $\tau(q)$ curves of example (10). The solid line and opaque squares are as in Fig. 1. Crosses indicate results obtained by fuzzy disc counting followed by SSC. Typical error bars are given.

of the asymptote to $\tau(q)$ for negative q, as well as, to much greater accuracy, from the ratios of $\tau(q_1)/\tau(q_2)$ obtained from SSC. (Note that there exist $q_1<q_2<0$ with $\tau(q_1)/\tau(q_2)>q_1/q_2$ if and only if the intercept of the asymptote is positive.)

The final check is to cross check the standard BCA with one of the algorithms specially devised to eliminate clipping errors as introduced in [8,13] and in the following. Although the adverse effects of the virtual measure are diminished, SSC nevertheless reveals a phase transition, but typically shifted to smaller q_c.

The best results might be obtained by combining SSC with the compound algorithm discussed in detail below, see Fig. 3.

To ameliorate the effect of ill-adapted, i.e., clipping covers we propose an algorithm based on balls with a ‘‘fuzzy’’ center location. For every length scale l_k we define a set of displacements $|\delta(l_k)_j|<l_k$ $j=1,2,\ldots,n$ and define the ‘‘mass’’ of the ball $\mathcal{B}(\mathbf{x}_i)$ with radius l_k belonging to the l_k-grid point $\mathbf{x}_i$ as

$$\overline{\mu}(\mathbf{x}_i)=\mu(\mathcal{B}(\mathbf{x}_i))\prod_j \Theta(\mu(\mathcal{B}(\mathbf{x}_i+\delta_j))), \tag{11}$$

for $q>0$, where $\Theta(x)$ denotes the Heaviside function. For $q<0$ this is modified by taking the geometric mean over all displaced balls:

$$\overline{\mu}(\mathbf{x}_i)=\left(\prod_{j=1}^{n}\mu(\mathcal{B}(\mathbf{x}_i+\delta_j))\right)^{1/n}, \tag{12}$$

which effectively amounts to taking the average Hoelder exponent of μ over all balls considered. For these algorithms $S_q(l_i)$ in Eq. (2) has to be replaced by a normalized version:

$$S_q^*(l_i)=S_q(l_i)/(S_1(l_i))^q, \tag{13}$$

since $S_1(l)$ is no longer constant.

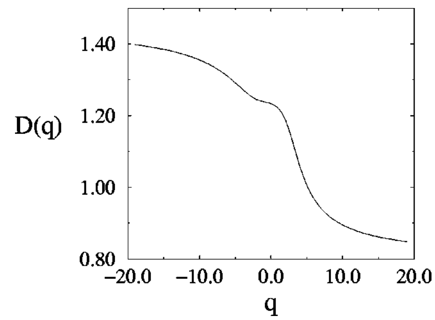

FIG. 4. The generalized dimensions $D(q)$ for the Hénon attractor as obtained with fuzzy disc counting.

With this compound algorithm we also made an analysis of the attractor of the standard Hénon mapping [27] with parameters $a=1.4$ and $b=0.3$. The Hénon attractor puts any algorithm to a serious test because of its nonhyperbolicity, which was elaborated on from a theoretical point of view in [14,29,30]. With respect to the numerics, the algorithm should resolve the transition from the ‘‘hyperbolic phase’’ to the ‘‘nonhyperbolic phase’’ at $q_c\approx 2.24$ [29], which constitutes a problem in itself far from the limit of infinitesimal length scales. Furthermore, the distribution of the residence measure on the attractor is far from even: while the ‘‘turning points’’ (i.e., the vicinity of the homoclinic tangency points) attract the bulk of the iterations and are statistically highly resolved, very little mass is spread out along the stratified parts of the attractor [7]. In effect, the algorithm has to deal with poor statistical and spatial resolution even if many iterations are taken into account.

To demonstrate the performance of our algorithm for an experimental setup, we restrict the calculation to 250 000 iterations, using 32 displacements for fuzzy disc counting up to 1/4 l. Figure 4 shows the spectrum of generalized dimensions which is in excellent agreement with theoretical predictions given in [29] and numerical findings in [14,28,16]. Remarkably, SSC does not only show signs of a phase transition for $q\approx 2.24$, but also, if the l_i are chosen small enough, for the whole hyperbolic phase from -1 to 2. We interpret this as a sign of the onset of data depletion, and the competing measure in this case as a number of isolated points on the attractor without statistical significance. For even smaller l_i this may even lead to a nondecreasing function of generalized dimensions. In our analysis, the range of length scales was chosen from 1/16 to 1/2048 of the diameter of the attractor.

We should point out that in some cases SSC becomes numerically unstable if too many q are used in the calculation, i.e., $\tau(q_i)/\tau(q_{i+1})$ becomes too small. However, our main objective was to provide a reliable qualitative tool, and we have been led to believe that SSC extracts much of the information contained in the set of S_q, and quite frequently reveals deficiencies; e.g., the virtual measures which would otherwise be overlooked by standard methods. Together with powerful counting algorithms, the long standing limitations of BCAs could be overcome.

M.A. gratefully acknowledges the outstanding support he enjoyed at St. Andrews, and acknowledges useful discussions with K. Falconer and L. Olsen.

[1] T. Halsey, M. Jensen, L. Kadanoff, I. Procaccia, and B. Shraiman, Phys. Rev. A **33**, 1141 (1986).
[2] K. J. Falconer, *Fractal Geometry, Mathematical Foundations and Applications* (Wiley, Chichester, 1990).
[3] S. Borgani, G. Murante, A. Provenzale, and R. Valdarinini, Phys. Rev. E **47**, 3879 (1993).
[4] P. Grassberger, Phys. Lett. A **128**, 369 (1989).
[5] C. D. Cutler, in *Nonlinear Time Series and Chaos: Dimension Estimation and Models*, edited by H. Tong (World Scientific, Singapore, 1993), Vol. I.
[6] C. D. Cutler, J. Stat. Phys. **62**, 651 (1991).
[7] A. Arneodo, G. Grasseau, and E. J. Kostelich, Phys. Lett. A **124**, 426 (1987).
[8] W. E. Caswell and J. A. Yorke, in *Dimensions and Entropies in Chaotic Systems*, edited by G. Mayer-Kress (Springer, Berlin, 1986).
[9] A. Gorgilli, D. Casati, L. Sironi, and L. Galgani, Phys. Lett. A **115**, 202 (1986).
[10] L. S. Liebovitch and T. Toth, Phys. Lett. A **141**, 386 (1989).
[11] X. Hou, R. Gilmore, G. B. Mindlin, and H. G. Solari, Phys. Lett. A **151**, 43 (1990).
[12] A. Block, W. von Bloh, and H. J. Schellnhuber, Phys. Rev. A **42**, 1869 (1990).
[13] R. Pastor-Satorras and R. H. Riedi, J. Phys. A **29**, L391 (1996).
[14] P. Grassberger, R. Badii, and A. Politi, J. Stat. Phys. **51**, 135 (1988).
[15] A. Chhabra and R. V. Jensen, Phys. Rev. Lett. **62**, 1327 (1989).
[16] R. Badii and G. Broggi, Phys. Lett. A **131**, 339 (1988).
[17] B. B. Mandelbrot, H. Peitgen, H. Jürgens, and D. Saupe, *Chaos and Fractals* (Springer, New York, 1992).
[18] G. Paladin and A. Vulpiani, Phys. Rep. **156**, 147 (1987).
[19] Due to the great leverage of q in the Legendre transform, it is not always numerically stable. In those cases where $f(\alpha)$ is sought directly, an alternative evaluation of the box counts [15] appears preferable. We note, that the basic ideas of this paper pertain to this variety of box counting also.
[20] P. Grassberger, Phys. Lett. **97A**, 224 (1983).
[21] R. Benzi, L. Biferale, S. Ciliberto, M. V. Struglia, and R. Tripiccione, Physica D **96**, 162 (1996).
[22] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes in C* (Cambridge University Press, Cambridge, England, 1994).
[23] B. Efron, Ann. Stat. **7**, 1 (1979).
[24] S. T. Buckland, Biometrics **40**, 811 (1984).
[25] R. Cawley and R. D. Mauldin, Adv. Math. **92**, 196 (1992).
[26] B. B. Mandelbrot, Proc. R. Soc. London, Ser. A **434**, 79 (1991).
[27] M. Hénon, Commun. Math. Phys. **50**, 69 (1976).
[28] R. Badii and A. Politi, Phys. Rev. A **35**, 1288 (1987).
[29] A. Politi, R. Badii, and P. Grassberger, J. Phys. A **21**, L763 (1988).
[30] C. Beck, Physica D **41**, 67 (1990).