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LETTER TO THE EDITOR

Are the cusps in the plots of $f(\alpha)$ a real effect?

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Abstract. An explicit example where the cusps in the plots of the $f(\alpha)$ spectrum appear is given. An analysis is provided which gives the support for the claim that these cusps are not a computer artefact and they are a signal of the breakdown of the scaling law.

In recent years progress has been made in describing the strange (fractal) sets occurring in many areas of physics, in particular in the theory of dynamical systems and growth phenomena. It has been recognised that there exist sets which are not strictly self-similar and due to this fact cannot be characterised by the Hausdorff dimension alone. The Renyi dimensions (Renyi 1970) D_q, $q=1,2,\ldots$ were applied to dynamical systems and fractal sets by Grassberger (1983), Hentschel and Procaccia (1983) and Grassberger and Procaccia (1984). This progress culminated in the introduction of the so-called $f(\alpha)$ formalism (Benzi *et al* 1984, Halsey *et al* 1986; for a review see Paladin and Vulpiani 1987, Levi 1986). Since that time the $f(\alpha)$ formalism has been applied to a variety of phenomena; let us mention only diffusion-limited aggregation (Halsey *et al* 1986, Amitrano *et al* 1986, Nittmann *et al* 1987), the Hénon attractor (Arneodo *et al* 1987), and attractors of non-hyperbolic dynamical systems (Politi *et al* 1988).

Quite recently much attention has been paid to the practical limitations imposed on the determination of D_q. In particular the systematic bias and errors caused by the finiteness of the data samples were discussed (Grassberger 1988, Ramsey and Yuan 1989). Smith (1988) derived the necessary bound on the amount of data required for a reliable dimension calculation. Also the problems with the determination of D_q for negative q were studied (Arneodo *et al* 1987, Lee and Stanley 1988, Blumenfeld and Aharony 1989).

In this letter we are going to discuss another phenomenon: we claim that the cusps in the plots of $f(\alpha)$ are a real effect. We know (Livi and Politi, private communication) that the cusps in the plots of $f(\alpha)$ were observed previously but they were dismissed as a computer artefact. We have encountered these cusps in the plots of $f(\alpha)$ for natural numbers (Wolf 1988) and here we will present a more detailed analysis of this phenomenon.

Let us consider a measure ρ with a support A and let $\{A_i\}$ be a covering of A, $A\subseteq\bigcup A_i$, such that all A_i are contained in the ball of radius l. Next, let us form the partition function

$$\chi_q(l)=\sum_{i=1}^{m(l)}\rho^q(A_i) \tag{1}$$

where $m(l)$ is the number of covering sets and depends on l. If the moments $\chi_q(l)$

behave in some regime of l and q like a power of l:

$$\chi_q(l) \sim l^{\tau(q)} \tag{2}$$

then the function $\tau(q)$ characterises the set A. The generalised dimensions are connected to $\tau(q)$ via the definition

$$D_q = \frac{\tau(q)}{q-1} \tag{3}$$

and it can be proved that for self-similar sets D_0 is the usual Hausdorff dimension, D_1 is the information entropy and D_2 is the correlation exponent. Halsey *et al* (1986) proposed using, instead of $\tau(q)$, the Legendre transform of $\tau(q)$:

$$f(\alpha) = \alpha q(\alpha) - \tau(q(\alpha)) \tag{4}$$

where q is expressed by α via the relation

$$\alpha(q) = \frac{\mathrm{d}\tau(q)}{\mathrm{d}q}. \tag{5}$$

A good exposition of the Legendre transformation can be found in Arnold (1978). In order to invert (5) the derivative of $\alpha(q)$ has to be of constant sign: for positive $\alpha'(q)$ the function $\tau(q)$ is termed convex and for negative $a'(q)$ it is termed concave.

In Wolf (1988) we have looked for the moments (1) for subsets $A(N) = \{1, 2, \ldots, N\}$ of natural numbers. The measure of the interval $A_i(l) = \{i, i+1, \ldots, i+l\} \in A(N)$ of length l we defined as the number of prime numbers contained in it divided by the number of prime numbers in $A(N)$:

$$\rho(A_i(l)) = \frac{\pi(i+l) - \pi(i)}{\pi(N)} \tag{6}$$

where $\pi(x)$ denotes the number of prime numbers smaller than x. The sets $A(N)$ with the measure defined by (6) are very well suited for testing the multifractal formalism because the amount of prime numbers within an interval is precisely determined in contrast to, e.g., the Hénon attractor, where the measure can be obtained only approximately due to the finite number of iterations (Arneodo *et al* 1987, Grassberger 1988).

We have found in appropriate ranges of l and q values the power-like behaviour (2) of the moments $\chi_q(l)$ for natural numbers. We have calculated $f(\alpha)$ numerically and we have obtained the cusps in their plots, see figure 1. These cusps appear in the

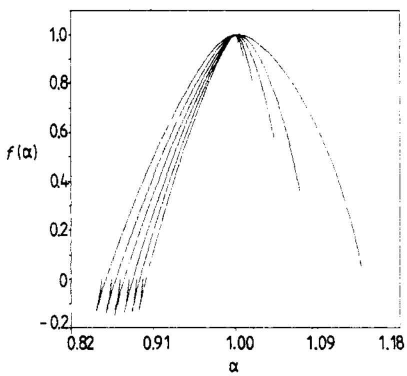

Figure 1. Plots of $f(\alpha)$ for $N = 2^{18}, 2^{19}, \ldots, 2^{23}$. The cusps and right parts of curves shift towards the point $\alpha_{\max} = 1$ for increasing N.

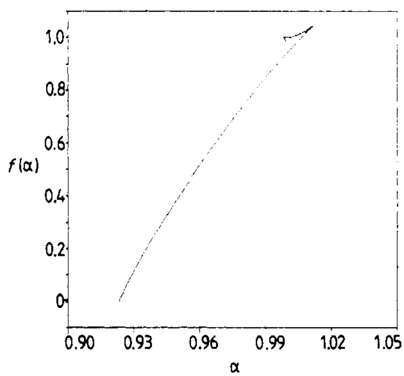

Figure 2. Plot of $f(\alpha)$ obtained from the scaling of the moments with respect to N for $N = 2^{18}, 2^{19}, \ldots, 2^{23}$ and for $l = 2^{12}$.

neighbourhood of $\alpha_{\min}$, so they correspond to positive values of q. As remarked by Coniglio (1986), the sets which are unbounded can display a scaling with respect to the linear sizes of the set. We have checked that this is the case for natural numbers: covering different subsets $A(N)$ by intervals of the same length l we have found the scaling of the moments with respect to N for a fixed l:

$$\chi_q(N) \sim N^{-\tau(q)}. \tag{7}$$

Again we have determined the function $\tau(q)$ numerically by fitting straight lines to the points ($\ln N$, $\ln \chi_q(N)$) by the linear regression procedure, and then plotting the function $f(\alpha)$, see figure 2. Here we see double cusps in the neighbourhood of $\alpha_{\max}$, but as we will see later they are also not linked to negative values q.

At first sight, round-off errors can be a possible explanation of the turnbacks of $\alpha(q)$. The problem of the accuracy of computer calculation is not in general an easy task; see e.g. Björck and Dahlquist (1974). In our case, that part of the calculations linked to the determination of the measure represents an integer-number problem and can be performed exactly by computer. The floating-point operations appear in the determination of χ_q and then in the least-squares fitting and numerical differentiation. We have performed calculations with 20-digit accuracy in the sense that $x+10^{-20}x \neq x$. The sums were calculated in order from the smallest term to largest term—there are two opposite such orderings respectively for $q>0$ and $q<0$. The largest number of terms in the sum (1) was 4096 and the maximal relative error we estimated to be of the order 10^{-16}. It is seen from figure 3 that it is many orders less than the relative changes in the values of $\alpha(q)$. We have also applied improved algorithms (Björck and Dahlquist 1974, § 2.3.5) to calculate the sum, but the difference between the simple summation and the improved algorithm was negligible and did not lead to changes in the shapes of $f(\alpha)$. We have used the following formula (Björck and Dahlquist § 7.5):

$$f'(x) = \frac{f(x+2h) - 8f(x+f) + 8f(x-h) - f(x-2h)}{12h}$$

for the numerical differentiation of $\tau(q)$. We have changed the step h from 1.0 to 0.025 without any changes in the shapes of $f(\alpha)$.

As is well known, the subtraction of nearly equal numbers and division by the very small numbers can lead to significant loss of accuracy. We have looked for the operations appearing in the least-squares method and we have not found such cases.

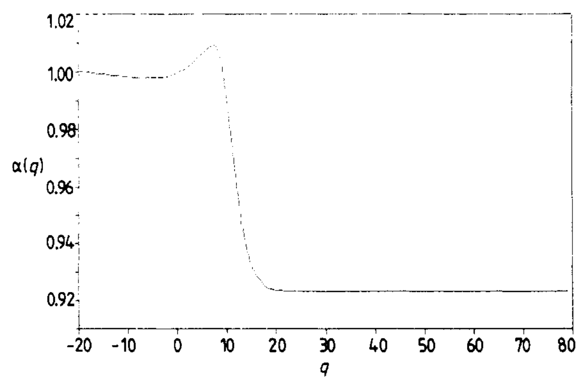

Figure 3. Plot of $\alpha(q)$ for the example presented in figure 2.

After this analysis we come to the conclusion that the cusps in the plots of $f(\alpha)$ are not due to the round-off errors. What is the explanation for them? The cusps are caused by the turnbacks of $\alpha(q)$—in figure 3 we have plotted an example of $\alpha(q)$ for the case of scaling of moments with respect to N for $N = 2^{18}, 2^{19}, \ldots, 2^{23}$ and for $l = 2^{12}$. Let us stress that the turnbacks appear for positive q. We see that, contrary to the general feature of the partition function (see the appendix), $\alpha(q)$ is not a decreasing function for all q. To explain this contradiction let us recall the formula for the least-squares method. If we have a set of points (x_i, y_i), $i = 1, 2, \ldots, m$, then the slope b of the straight line $a + bx$ best fitting these points is given by the formula

$$b = \frac{m\Sigma x_i y_i - \Sigma x_j \Sigma y_k}{m\Sigma x_i^2 - (\Sigma x_i)^2}. \tag{8}$$

In our case $y_i \sim \ln \chi_q(N_i)$ and $b \sim \tau(q)$. Although each $\ln \chi_q$ is a convex function of q, the function $\tau(q)$ calculated by means of (8) need not be convex because of the minus sign between the two terms in the numerator of (8). (Let us remark that the y_i do not appear in the denominator.) We link these changes of the sign of the derivative of $\alpha(q)$ to oscillations in the plots of $\ln \chi_q$ against $\ln l$. These oscillations were observed by Badii and Politi (1984) and Smith *et al* (1986) and they are inherent to lacunar fractals. The non-concavity of $\tau(q)$ is evidence of departures from the scaling law (2).

By the way, let us remark that usually the points x_i are equally spaced, $x_i \sim i$, and the numerator possesses the property that it depends always on an even number of y_i—for an odd number of y_i the middle y_i cancels out.

Recently Lee and Stanley (1988) (see also Lee *et al* 1989) reported on the phase transition in the multifractal spectrum of diffusion-limited aggregation. By phase transition these authors mean the existence of such a critical value q_c that on the one side of it there is a scaling law fulfilled and for q on the other side of q_c the moments do not scale with l. Lee and Stanley have plotted (figure 5(b) in their paper) the derivative $\alpha'(q)$, which in the framework of the thermodynamical formalism (Feigenbaum 1987) can be interpreted as a specific heat, and they found the sharp peak characteristic of the usual phase transitions. In figure 4 the 'specific heat' corresponding to $\alpha(q)$ from figure 3 is plotted and the points of phase transition are marked by arrows. Let us recall that in the usual statistical physics cusps in the plots of some thermodynamical quantities are evidence of phase transitions. Lee and Stanley did

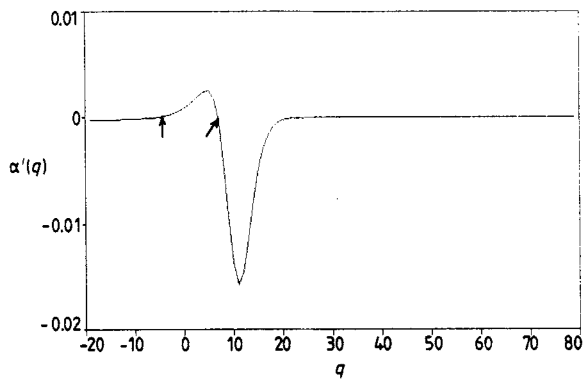

Figure 4. Plot of the derivative of $\alpha(q)$ from figure 3. The arrows indicate critical points where $\alpha'(q) = 0$.

not propose any equation for the determination of the critical point. From our analysis it follows that the cusps in the plots of $f(\alpha)$ are evidence of the breakdown of power-law scaling and q_c can be determined as the point where the turnbacks in $f(\alpha)$ appear:

$$\left.\frac{d\alpha(q)}{dq}\right|_{q=q_c}=0 \qquad \left.\frac{d^2\alpha(q)}{dq^2}\right|_{q=q_c}\neq 0.$$

The second equation picks up the true points of phase transition because it rules out the domains of q where $\alpha(q)$ reaches its asymptotic constant values.

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Appendix

From the definition (1) we get:

$$\frac{d}{dq}\ln\chi_q=\frac{1}{\chi_q}\sum_i \rho_i^q\ln\rho_i\leqslant 0$$

since $\ln\rho_i\leqslant 0$ for a probabilistic measure. We now obtain

$$\frac{d^2}{dq^2}\ln\chi_q=\chi_q^{-2}\left[\sum_i\rho_i^q\sum_j\rho_j^q\ln^2\rho_j-\left(\sum_i\rho_i^q\ln\rho_i\right)^2\right].$$

Let us apply the Cauchy-Schwarz inequality:

$$\left(\sum_i a_ib_i\right)^2\leqslant\sum_i a_i^2\sum_j b_j^2.$$

Putting here $a_i=\rho_i^{q/2}$, $b_i=\rho_i^{q/2}\ln\rho_i$, we obtain

$$\frac{d^2}{dq^2}\ln\chi_q\geqslant 0. \tag{A1}$$

To perform the Legendre transformation, $\tau''(q)$ should also be of constant sign. Let us rewrite the scaling law (2) in the form

$$\chi_q(l)=A(q)l^{\tau(q)}$$

from which we get:

$$\tau(q)=\frac{\ln\chi_q(l)}{\ln l}-\frac{\ln A(q)}{\ln l}.$$

Because of the prefactor $A(q)$, it follows that (A1) is not sufficient alone to ensure the concavity of $\tau(q)$—only in the limit $l\to 0$ or $l\to\infty$ do we obtain that $\tau''(q)$ is of constant sign. Practically it is not possible to reach the asymptotes, and in some cases even if the scaling law is fulfilled the bad behaviour of $A(q)$ can lead to cusps in $f(\alpha)$. Let us add that because the Legendre transformation is involutive (Arnold 1978), i.e. its square is equal to the identity, it follows that the information supplied by $f(\alpha)$ is the same as supplied by $\tau(q)$: the Legendre transformation of $f(\alpha)$ reproduces $\tau(q)$.

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