

CAN GENERALIZED DIMENSION (D_q) AND $f(\alpha)$ BE USED IN STRUCTURE-MORPHOLOGY ANALYSIS?*

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The family of model (prototype) structures (Sierpiński carpet, Sierpiński gasket, dendrites, *etc.*) have been chosen to test D_q and $f(\alpha)$ as tools for structure-morphology analysis. It turns out that both are very sensitive to deviations from global regularity as well as, to some extent, also to local changes. Based on monotonic increasing property of log function and diffeomorphism of $D_q/f(\alpha)$ the problems of uniqueness and invertibility are formulated and discussed.

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1. Introduction

Structure and morphology are very often used interchangeably [1, 2]. For the sake of clarity we will be using here the term “structure” with an additive “low” or “high resolution” to be able to distinguish cases in which the nature of a generator (structural element) is visible (high resolution) or not (low resolution) within an aggregate of generators (sample). The term “morphology” will be used to describe texture (outlook) of an aggregate of generators forming the sample, no matter the resolution. The intention of this paper is to investigate the self-similar sets, which, in practice, are supposed to be outputs of different sort of microscopies. As a tool for that the generalized dimension (D_q) and its Legendre transform $f(\alpha)$ will be used [3]. To avoid confusion let us briefly recall the notion of a fractal

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dimension, and, in spite of its spectacular success [4], show the reasons for which we should use D_q instead. For the self-similar sets the number of nonempty coverings $N(\varepsilon)$ scales with the current size of covering ε in the following way [5,6]:

$$N(\varepsilon) \propto \varepsilon^{-d_F}, \quad (1)$$

where d_F is a fractal (or box) dimension. Taking the logarithm at the limit $\varepsilon \rightarrow 0$ we get

$$d_F = \lim_{\varepsilon \rightarrow 0} \frac{\ln N(\varepsilon)}{\ln(1/\varepsilon)}. \quad (2)$$

A “weak point” of relation (2) is the nature of a covering set ε . It can cover just one or many points, and if “nonempty” it contributes to $N(\varepsilon)$ with the same “weight”. In some applications, it does not matter [5]. It matters a lot however, when the number of points represents the mass surface density, like in structure-morphology analysis. To get rid of this weak point the generalized dimension D_q was introduced [7]:

$$D_q = \frac{1}{q-1} \lim_{\varepsilon \rightarrow 0} \frac{\ln \sum_{i=1}^{N(\varepsilon)} P_i^q}{\ln \varepsilon}, \quad (3)$$

where P_i equals the number of points in a particular covering (n_i) over the total number of points $\sum_{i=1}^{N(\varepsilon)} n_i$, $q \in \mathbb{R}$. D_q is also called Renyi generalized entropy in information theory [8].

It is easy to see that (3) gives (2) for $q = 0$. For some technical reasons as well as for showing analogies with statistical thermodynamics so called $f(\alpha)$ formalism was introduced which is, essentially, a Legendre transform of D_q [9]. To get a “feeling” for $f(\alpha)$ let us recall its derivation in a few steps:

- (i) from (3) we have to make a concave function of q to fulfill conditions for Legendre transform

$$\tau_q = (q-1)D_q = \lim_{\varepsilon \rightarrow 0} \frac{\ln \sum_{i=1}^{N(\varepsilon)} P_i^q}{\ln \varepsilon}; \quad (4)$$

- (ii) take the family of straight lines αq and construct a function

$$F(\alpha, q) = \alpha q - \tau_q; \quad (5)$$

(iii) take extremum of (5) through

$$\frac{\partial F}{\partial \hat{q}} = 0, \quad (6)$$

and establish one-to-one relation between \hat{q} and $\alpha = \frac{\partial \tau_{\hat{q}}}{\partial \hat{q}}$

$$\alpha(\hat{q}) = \lim_{\varepsilon \rightarrow 0} \frac{1}{\ln \varepsilon} \frac{\sum_{i=1}^{N(\varepsilon)} (P_i^{\hat{q}} \ln P_i)}{\sum_{i=1}^{N(\varepsilon)} P_i^{\hat{q}}}. \quad (7)$$

There is a little chance, if any, to get inverse of (7) analytically so, we have to accept the table form of \hat{q} on α ;

(iv) $f(\alpha)$ spectrum is a function $F(\alpha, \hat{q}(\alpha))$ *i.e.* the Legendre transform of Eq. (4)

$$f(\alpha) = \alpha \hat{q}(\alpha) - \tau_{\hat{q}(\alpha)}. \quad (8)$$

As pointed out elsewhere [10–12] the function $f(\alpha)$ plays a role analogous to the entropy with α being the analog of the energy E (see the plots of $f(\alpha)$ further in the text).

2. Prototype structures

The concept of using a collection of different prototype structures to check the potential of $D_q/f(\alpha)$ formalism can be compared with the “teaching procedure of neuronal nets” [13]. In both cases the system (and its user) is supposed to learn how to detect, firstly, the way in which different structure-morphology features are reflected in $D_q/f(\alpha)$ curves, secondly, what sort of changes are detected and, what is the sensitivity of $D_q/f(\alpha)$ curves to the differences in structure-morphology features. Three groups of the prototypes with different generations have been chosen:

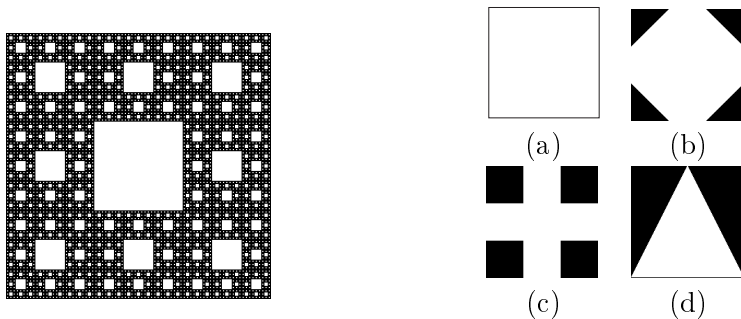


Fig. 1. Sierpiński gasket type set with different generators.

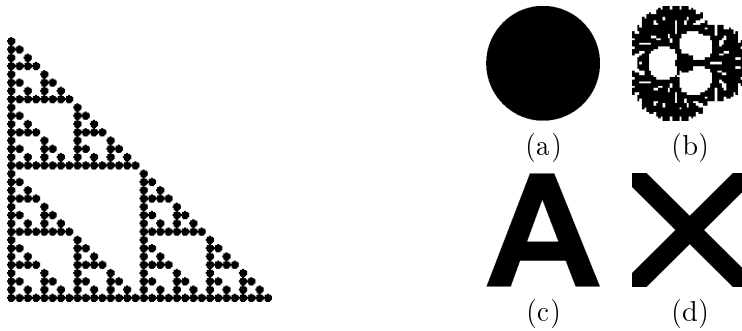


Fig. 2. Sierpiński triangle type set with different generators.

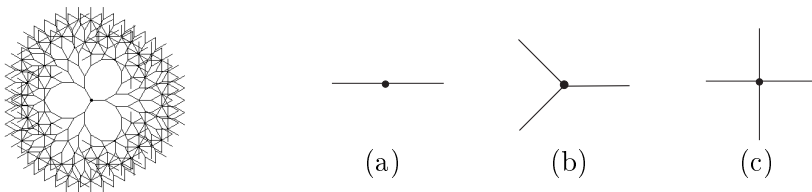


Fig. 3. Dendritic aggregates with cores of different functionality.

Note: Although some of the chosen prototype structures are known to model the real objects, this was not a primary task, at the moment.

3. Results and discussion

A single fractal dimension d_F is not sufficient to describe and discriminate neither all fractal objects nor characterize the particular one in details. In fact, there are about ten distinct fractal dimensions of different origin introduced to describe various properties and features of fractal sets [3]. Not all of them are independent quantities like the critical point exponents, which are related by the scaling laws. But unlike the scaling laws the relation between different fractal dimensions is rather heuristic [11]. An alternative, in some sense, is a generalized fractal dimension D_q which provides infinitely many dimensions, strictly related but still with a “weak physics” behind. Before referring to results obtained from the prototype structure studies let us point out several useful properties of $D_q/f(\alpha)$ functions emerging just from their definitions. First observation leads to the conclusion that uniform distribution gives a straight line for $D_q \rightarrow q$, and a single point in first quarter of $f(\alpha) \rightarrow \alpha$ plane, what can be easily derived from Eq. (3) *i.e.*:

$$\begin{aligned}
 D_q &= \frac{1}{q-1} \lim_{\varepsilon \rightarrow 0} \frac{\ln \sum_{i=1}^{N(\varepsilon)} \left(\frac{1}{N(\varepsilon)} \right)^q}{\ln \varepsilon} = \frac{1}{1-q} \lim_{\varepsilon \rightarrow 0} \frac{\ln \left(N(\varepsilon) \left(\frac{1}{N(\varepsilon)} \right)^q \right)}{\ln \frac{1}{\varepsilon}} \\
 &= \frac{1}{1-q} \lim_{\varepsilon \rightarrow 0} \frac{(1-q) \ln N(\varepsilon)}{\ln \frac{1}{\varepsilon}} = \lim_{\varepsilon \rightarrow 0} \frac{\ln N(\varepsilon)}{\ln \frac{1}{\varepsilon}} = d_F = D_0. \quad (9)
 \end{aligned}$$

From Eqs. (4) and (7) it follows that

$$\alpha = \frac{d\tau_{\hat{q}}}{d\hat{q}} = \frac{d(\hat{q}-1)D_q}{d\hat{q}} = \frac{d(\hat{q}-1)d_F}{d\hat{q}} = d_F, \quad (10)$$

and

$$f(\alpha) = \alpha\hat{q} - (\hat{q}-1)D_q = d_F\hat{q} - (\hat{q}-1)d_F = d_F. \quad (11)$$

Note: This only confirms an obvious fact that “nonempty box” requirement, in a simple box counting, is equivalent to the uniform P_i distribution in a generalized dimension approach. The second observation concerns the roots of $f(\alpha)$ function. As can be seen from Eq. (8) with the help of Eqs. (4) and (7) the condition for that reads:

$$\sum_{i=1}^{N(\varepsilon)} P_i^q \ln P_i^q \cong \sum_{i=1}^{N(\varepsilon)} P_i^q \ln \sum_{i=1}^{N(\varepsilon)} P_i^q, \quad (12)$$

and holds if:

(i)

$$\exists_j \forall_{i \neq j} P_j \ll P_i \Rightarrow \lim_{q \rightarrow -\infty} \ln \sum_{i=1}^{N(\varepsilon)} P_i^q = \ln P_j^q, \quad (13)$$

for the right root, and

(ii)

$$\exists_j \forall_{i \neq j} P_j \gg P_i \Rightarrow \lim_{q \rightarrow +\infty} \ln \sum_{i=1}^{N(\varepsilon)} P_i^q = \ln P_j^q, \quad (14)$$

for the left root of $f(\alpha)$.

Note: In case there is no root of $f(\alpha)$ present the wings of $f(\alpha)$ spectrum are lifted proportionally to the multiplicity of extremum values of P_i . The third, and the last observation, at the moment, binds the width of $f(\alpha)$ spectrum with $(P_{\max} - P_{\min})$, value (this is an indication, characteristics, of heterogeneity of a set in question). Being aware of the above let us see

what new can we learn from the systematic studies of the prototype structures. Different prototype structures are supposed to deliver, a clear though partial, answer to the question posed as a title of this work. Namely, in Sec. 3.1, we would like to investigate the sensitivity of $D_q/f(\alpha)$ on the kind of perturbation done with respect to original set, in Sec. 3.2, we intent to check the influence of generators as well as effect of resolution, and lastly, in Sec. 3.3, we try to visualize the influence of “more realistic” generators (structural elements) on value and shape of $D_q/f(\alpha)$ *i.e.* we try to show the correspondence between morphology of $D_q/f(\alpha)$, and morphology of 2D sets in question.

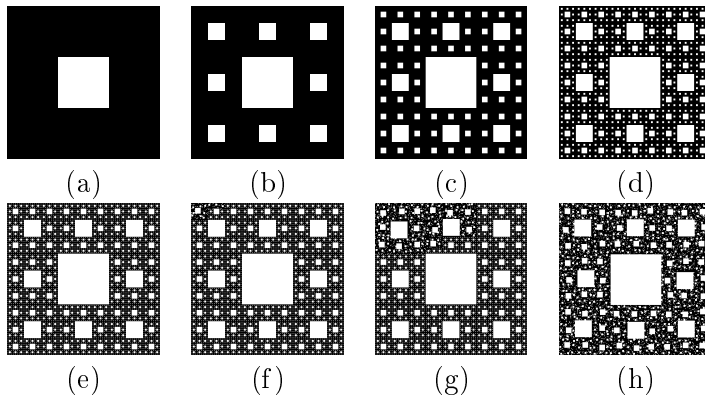


Fig. 4. Generator (a), subsequent generations (b)–(e), distorted fourth generation with 100 (f), 1000 (g) distortions, and fully distorted (h) Sierpiński carpet.

3.1. Sierpiński carpet

As we stated before this set of prototype structures has been used to demonstrate the sensitivity of $D_q/f(\alpha)$ for deviations from the original regularity (self-similarity). The most spectacular behaviour was shown for the case of the set generated by 1(a) (see Fig. 5).

As can be learned from Figs. 5 and 6 $D_q/f(\alpha)$ spectra are very sensitive to record displacement of even one structural element (see Fig. 5). Our “experiment” of destroying original regularity consists of shifting some of elements (pores). It is interesting that this operation changes $D_q/f(\alpha)$ a lot leaving however the range of self-similarity scaling almost on the same level (see the subfigure 5). Please, note that increasing number of disturbances can be measured “almost” quantitatively as $(D_{-\infty} - D_{+\infty})$ difference (see Fig. 5). Please observe, however, that the distortions affect almost only negative part of D_q spectrum, which corresponds to low values of P_i s. It takes at least a few hundred distortions to affect the positive (including D_0) part of the spectrum.

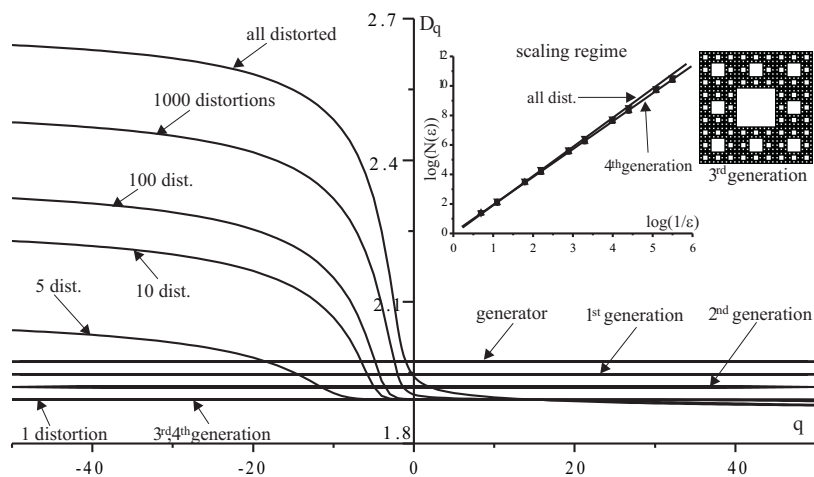


Fig. 5. Subsequent generations of Sierpiński carpet and the influence of distortions imposed on initially strictly regular set shown on generalized dimension graphs.

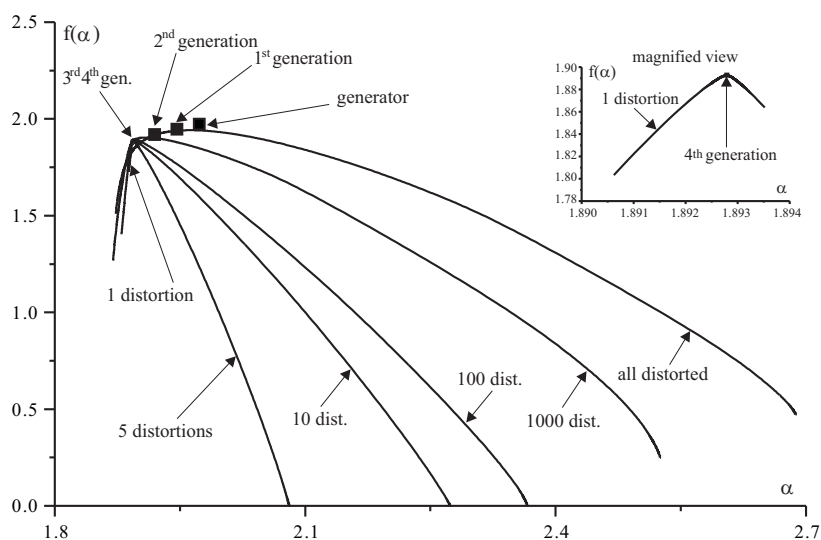


Fig. 6. Subsequent generations of Sierpiński carpet and the influence of distortions imposed on initially strictly regular set shown on $f(\alpha)$ graphs.

One more observation is worthy to be discussed. Namely, the character of $D_q/f(\alpha)$ spectra for the sets generated by three other generators (Figs. 1(b), 1(c), 1(d)) — give no straight lines in general, *i.e.* not for a full range of covering (Fig. 8). Without going into details we can say that this is due to geometry of covering (in our case it was a square). If the

shape of covering (ε) matches the geometry of elements the set consists of, the “regularity” of a set is recorded by $D_q/f(\alpha)$ as “ideal” (straight line or/and a point), if this is not the case, then the $D_q/f(\alpha)$ registers some deviations from ideal self-similarity (Fig. 7). For such cases the $D_q/f(\alpha)$ are less sensitive to small number of distortions. Their larger numbers, however, still cause dramatic changes in the spectra. This means that we do not need to adjust a coverage (squares, triangles, hexagonals) to the investigated (possibly experimental) objects and still expect valid results. It seems unreasonable to expect real objects, like pores, to follow a strictly regular pattern which we can easily impose on prototype structures.

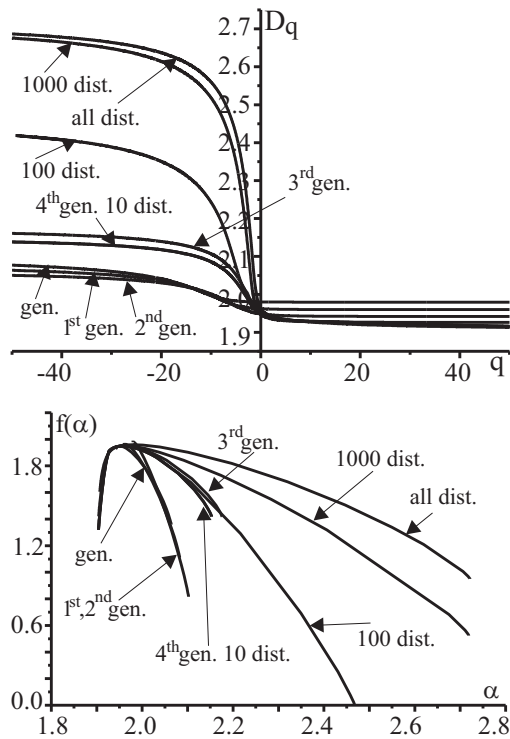


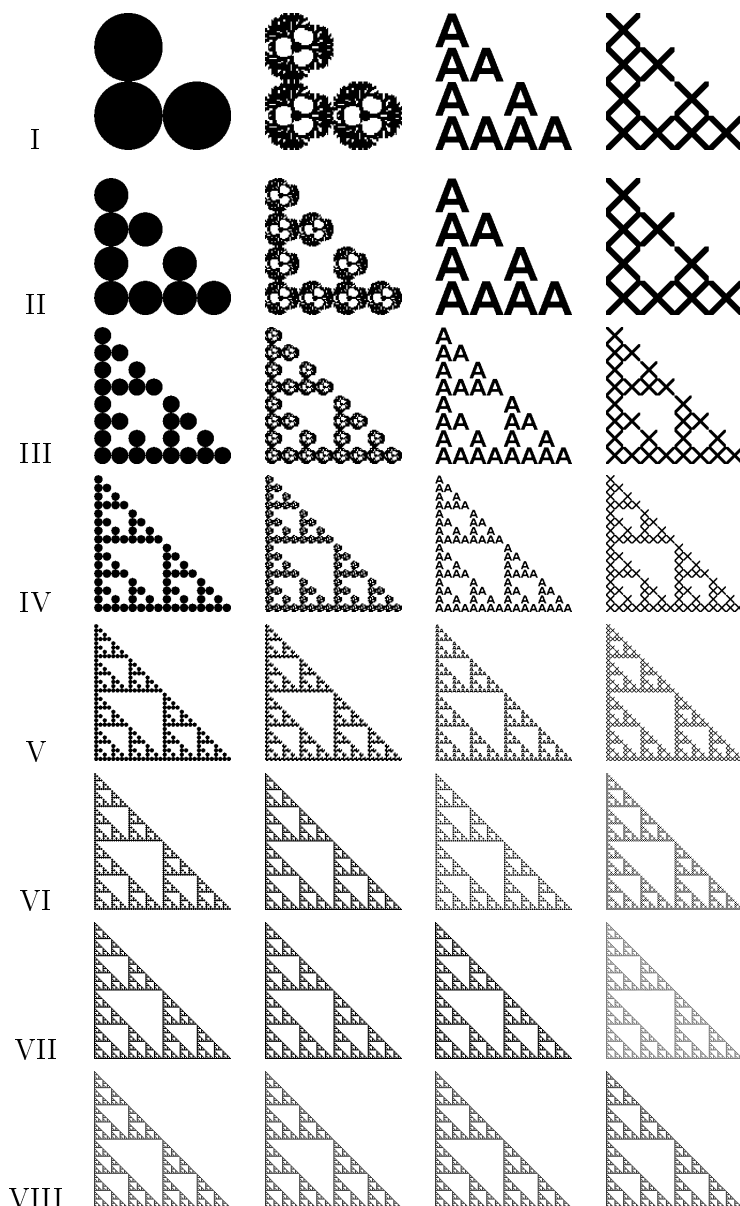
Fig. 7. Spectra of Sierpiński carpet for hexagonal generator (see Fig. 1(b)).

3.2. Sierpiński gasket

As we have seen from the previous section the kind of a generator, even of such a simple structure, plays an important role in gathering knowledge on structure-morphology analysis. In this section we would like to demonstrate more about an importance of a generator but, first of all, about a resolution with which the outputs are presented. The idea of this concept is clearly seen from Table I.

TABLE I

Different structural elements (see Fig. 2) seen with decreasing resolution converge to ideally self-similar structure of Sierpiński gasket.



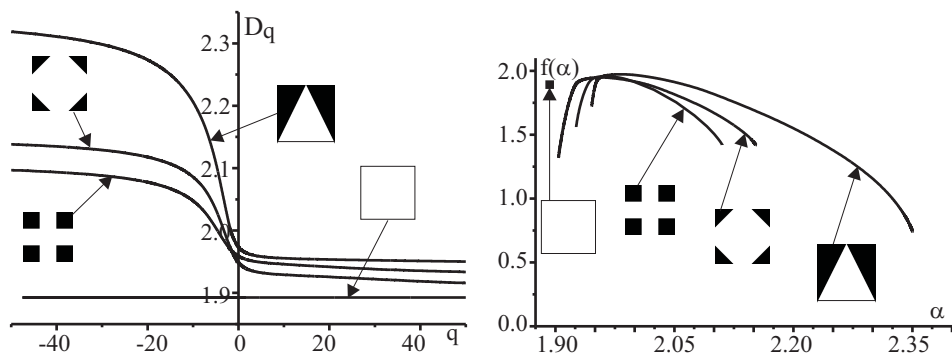


Fig. 8. Comparison of $D_q/f(\alpha)$ spectra of Sierpiński carpet for four different generators.

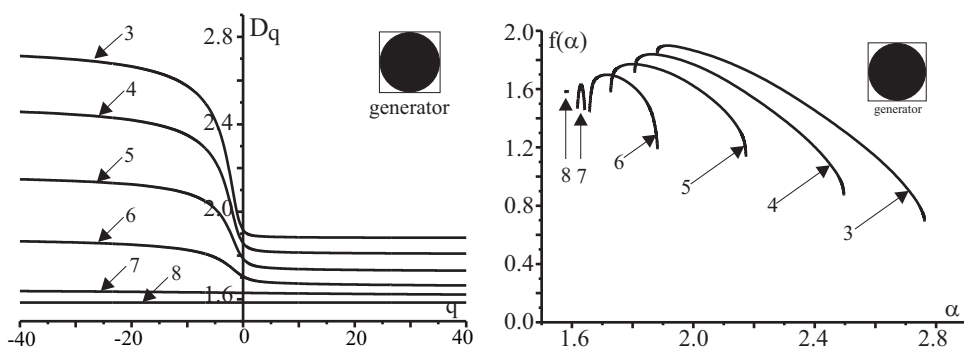


Fig. 9. Convergence of $D_q/f(\alpha)$ spectra of Sierpiński gasket for generator presented on Fig. 2(a).

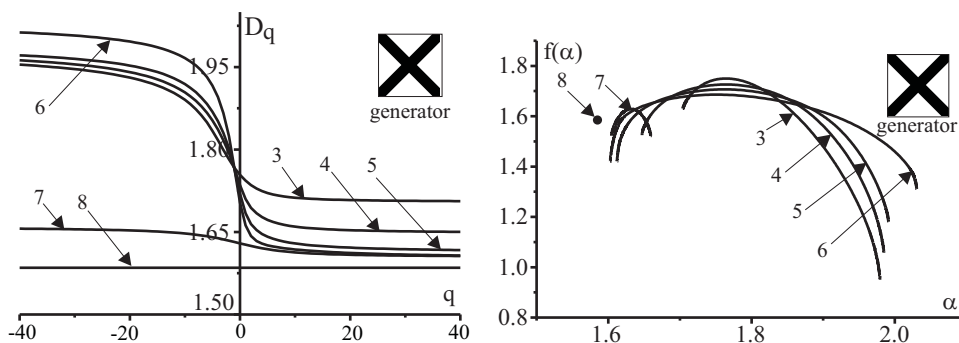


Fig. 10. Convergence of $D_q/f(\alpha)$ spectra of Sierpiński gasket for generator presented on Fig. 2(d).

It is rather obvious that high resolution output shows more different details, and consequently, its $D_q/f(\alpha)$ spectra are more complicated. We can see the way of changing $D_q/f(\alpha)$ spectra from high resolution (the first few generations) where structure of generators is significant, to low resolution outputs (the higher generations *cf.* Table I), by looking at the patterns in Figs. 9, 10. For the sake of clarity we omitted the results for generators 2(b) and 2(c) as they exhibit similar behaviour to those already presented.

This is quite obvious expectation to see a sort of convergence between gaskets, built up (aggregated) from different generators, to the standard, ideally self-similar one. Please note that we can build up a sort of “diagnostic” system for structure-morphology analysis based on:

- characteristic values of D_q (like D_0 , D_1);
- the width of $f(\alpha)$ spectrum ($D_{-\infty} - D_{+\infty}$);
- symmetry of $f(\alpha)$ branches;
- altitude of $f(\alpha)$ maximum;
- placements of ends of the $f(\alpha)$ graph;
- presence of $f(\alpha)$ roots.

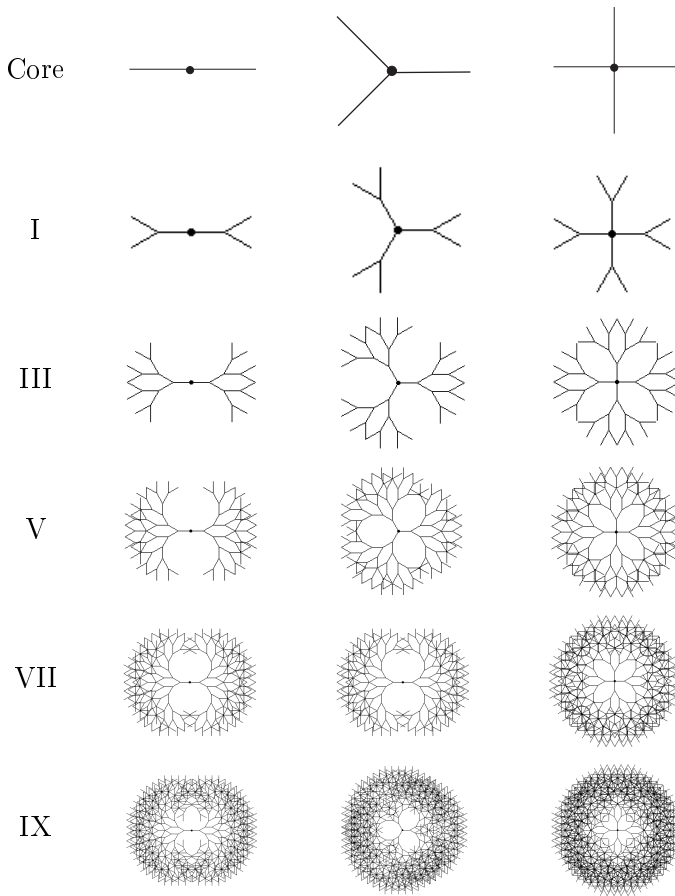
More regular structural elements (which scale better and preserve their symmetries) produce more regular D_q and $f(\alpha)$ graphs (compare Figs. 9 and 10). Note that in both cases the positive parts of D_q show similar output. Still the graphs differ in their negative parts, which are much more sensitive to small deviations from regularity.

3.3. Dendritic polymers

Trees, nervous system, some synthetic polymers show a fascinating architectures of fractal construction that is not only beautiful and complex but also very useful, and still far from being well understood [15]. In this section we would like to check whether the properties detected by $D_q/f(\alpha)$ can be of any help in contribution to the understanding of their complicated nature. Evolving around a core atoms or molecule, they possess repeating “generations” of branches that branch again and again until an almost globular shape with a dense surface is reached. To emulate various dendritic growth we have chosen three different functionalities (see Table II), and ranged the number of generations from 1 to 10.

TABLE II

Subsequent generations for varying cores and Y-shaped generator.



The corresponding $D_q/f(\alpha)$ spectra are collected in Fig. 11. It can be seen in Fig. 11 that as the dendrite grows, all D_q moment grow proportionally, independent of the core functionality. Moreover, the functionality affects selectively the mass scaling, thus it changes only the fractal dimension d_F , and not the shape of $D_q/f(\alpha)$ spectra.

The size of the core is also “detectable” by the $D_q/f(\alpha)$ formalism (see Fig. 13). It may be observed that the larger the core the wider the $f(\alpha)$ spectrum. Finer analysis shows that the presence of the left root on the $f(\alpha)$ graph indicates that the size of the dendrite core is larger than the width of its branches, still being smaller than coverage size. For larger cores their sizes correspond to the value $f(\alpha)$ for $\alpha = D_{+\infty}$ (the left ending of the graph), see Fig. 13.

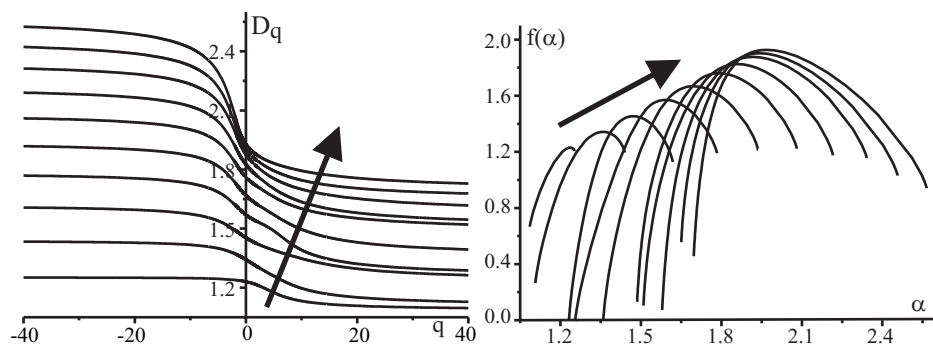


Fig. 11. $D_q/f(\alpha)$ spectra for dendrites with 3-valent core for generations 1–10. Arrows show increasing number of generations.

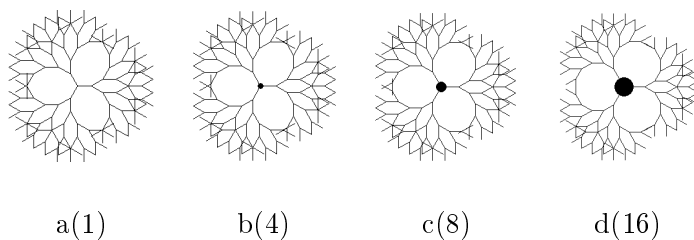


Fig. 12. Dendrites with varying core size (given in parentheses).

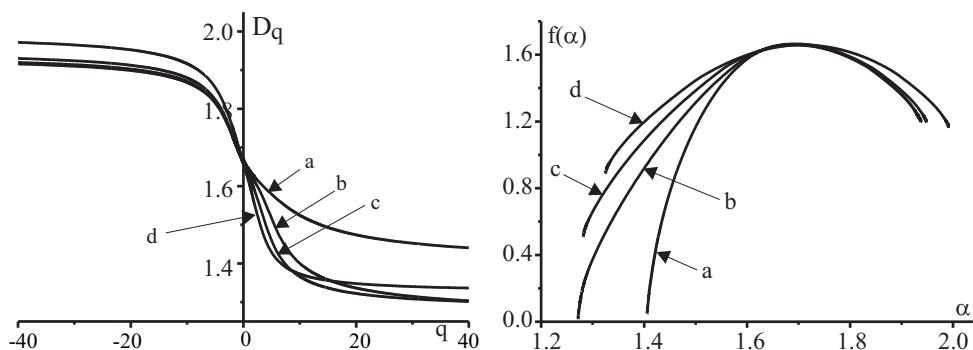


Fig. 13. Spectra for dendrites with varying core size (shown on Fig. 12).

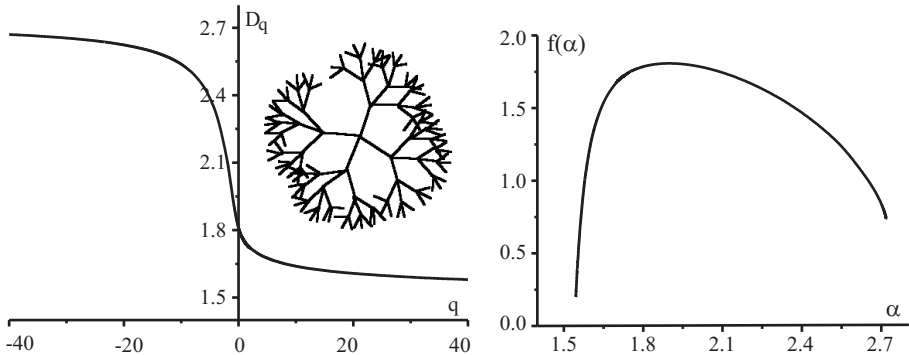


Fig. 14. Any image produces only one D_q and $f(\alpha)$ spectra.

4. Uniqueness

Last but not least we would like to make a few remarks on uniqueness of $D_q/f(\alpha)$ characterization of 2D sets as well as comment on “an inverse” problem. By the uniqueness here we mean the fact that one set gives one, and only one, $D_q \rightarrow q$ and $f(\alpha) \rightarrow \alpha$ spectrum.

This is not very difficult to demonstrate, especially when the principle property of log function *i.e.* monotonicity is recalled. Namely, from Eq. (3) one can see that for a fixed P_i the expression $\sum_{i=1}^{N(\varepsilon)} P_i^q$ generates the distinct numbers which, in turn, gives a distinct (and unique) values of D_q the case of $q = 1$ is trivial to handle (so well known that we would not comment on it!). Altogether, it leads to a conclusion that the $D_q/f(\alpha)$ coding is unique. Quite a different situation is connected to, so called, “inverse problem” [16] *i.e.* the situation, in which we try to point out conditions under which the determination of original set is possible from $D_q/f(\alpha)$ spectra. In a way of doing this, we have to notice that $D_q/f(\alpha)$ is invariant under the diffeomorphism [17] *i.e.* is the same for a set of images obtained one from another by piecewise translation, rotation, shifting and other differentiable operations. It simply means that it is obvious to expect quite a few differently looking sets to share the same $D_q/f(\alpha)$. In conclusion then, we have to state that an inverse problem is not unique! Now, the question is; is this a real drawback or rather a feature of the method? The images (sets) may be differently looking but they need to be piecewise similar and, consequently, produce the same distribution of P_i values. We tend to think that especially for natural objects (like microscopy outputs) the collection of coverages, the object is subjected to, forms a representation of the properties of the whole analyzed object. Hence we could rotate the sample or perhaps pick the image

in slightly different location yet still get the same distribution of P_i values — and $D_q/f(\alpha)$ spectra. Apparently the method fails to recover from the spectra any specific placement information but it provides important information about structural elements (like pores) size distribution and scaling or about deviations from any regular placement patterns (*i.e.* defects).

5. Concluding remarks

We have presented generalized dimension and $f(\alpha)$ spectra for three classes of prototype structures, with the hope that the results would be extendable to analysis of other structures, especially experimental ones. Indeed they seem to confirm the applicability of the suggested approach to structure and morphology analysis. It turned out, however, that it was difficult to get the comprehensive information from solely one of these tools. Even though both share actually the same features (because both are transforms of each other), some aspects are easier to read from one of them. $f(\alpha)$ spectrum, thanks to its clearer output, seems to provide deeper insight into the analysis.

Both tools appear to be very sensitive to changes in the analyzed set, especially to regularity breaking changes (defects). For strictly regular prototype structures (see Fig. 4) the defects are reflected in almost quantitative manner. Even one distortion can be detected. However, the less regular the original image the worse sensitivity of the method appears (compare Figs. 5 and 7). The shape of the structural elements also plays an important role. Figs. 9 and 10 show that it may be the loss of internal symmetries that severely affects the spectra (compare almost ideal changes on Figs. 9 and 10).

Some properties of $D_q/f(\alpha)$ spectra proved to be the most useful ones. Such list contains: characteristic values of D_q (some of them have a putative physical meaning, like D_0 , D_1 or D_2), the width of $f(\alpha)$ spectrum (equal to $D_{-\infty} - D_{+\infty}$), symmetry of $f(\alpha)$ branches, altitude of $f(\alpha)$ maximum, position of ends of the $f(\alpha)$ graph and presense of $f(\alpha)$ roots.

There is a common understanding that regular structures have a very simple spectra (flat D_q , short $f(\alpha)$). While generally true, it should be noted that D_q is reduced to a straight line (and $f(\alpha)$ to a point) only in rather rare cases when the shape of the structural element matches its covering. In more realistic circumstances the method is less sensitive, though the general tendency of enriching the spectra for more internally varied structures still holds.

Even though the inverse problem is non-unique, still we can recover some of the properties of the original set. Merged with the knowledge about the class of analyzed objects $D_q/f(\alpha)$ significantly help in the analysis. For

example both methods make a clear distinction between elements of coverage (ε) and subcoverage (*i.e.* size of the structural element is smaller than ε) size. The former correspond to positive part of the D_q and left branch of $f(\alpha)$ and can be bound with features like core (kernel) size, number of main branches, scaling of the structural elements. The latter reflects (corresponding to the negative part of the D_q and right branch of $f(\alpha)$) small scale features like minor irregularities, minor branches, shape and symmetries of the structural element *etc.* Perhaps the most important is the effect of various distortions and defects which is much more pronounced on this part of the spectra.

This paper deals exclusively with 2D (black & white) images which lack the depth information. There is however a collection of methods (like [18,19]) which can be successfully applied to 3D images to calculate both D_q and $f(\alpha)$. Hence this analysis should be fairly extendable to handle such data like microscopy outputs (which usually comes as a 3D image and where the depth information is crucial), as the properties visualized by these tools remain the same.

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