DIFFUSION-LIMITED AGGREGATION DRIVEN BY OPTIMAL TRANSPORTATION

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Abstract. In this article, we combine the DLA model of Witten and Sander with ideas from optimal transportation. We propose a modification of the DLA model in which the probability of sticking is inversely proportional to the additional transport cost from the point to the root. We used a family of cost functions parametrized by a parameter α as studied in ramified optimal transportation. $\alpha < 0$ promotes growth near the root whereas $\alpha > 0$ promotes growth at the tips of the cluster. $\alpha = 0$ is a phase transition point and corresponds to standard DLA. What makes this model interesting is that when α is negative enough (e.g. $\alpha < -2$) the final cluster is an one dimensional curve. On the other hand, when α is positive enough (e.g. $\alpha > 2$) we get a nearly two dimensional disk. Thus our model encompasses the full range of fractal dimension from 1 to 2.

1. Introduction

Diffusion-limited aggregation, or DLA, has been extensively employed since its proposition in 1981 by Witten and Sander [8] to model cluster growth controlled by the random process of diffusion. This leads to structures with very regular fractal properties: for instance, off-lattice DLA in the plane evolves a cluster with fractal dimension 1.71 [7]. While the use of different lattices has an effect on the resulting fractal dimension, yet they fall within a narrow range. This makes it difficult to model processes in which varying a certain parameter affects the shape of the cluster. In particular, electrodeposition experiments use a range of voltages and produce a range of cluster shapes only one of which can correspond to DLA. A number of researchers [9],[1] have proposed a modification of DLA in which the probability of sticking is not always 1. Barlow, Pemantle and Perkins studied the trees produced by a probability function $p = \alpha^{-n}$ where n is the path length to the root [1]. They note that $\alpha > 1$ promotes growth near the root whereas $\alpha < 1$ promotes growth at the tips of the tree. $\alpha = 1$ is a phase transition point and corresponds to the Eden model ($p = 1$ for all n). While this greatly extends the range of possible DLA-like structures, the probability function is not easily related to physical properties because it ignores effects of branching in the tree. In the example of electrodeposition, the amount of current at any point of the cluster depends on the relative resistance of all possible paths to the root electrode. Because current in this model corresponds to the movement, and ultimately aggregation, of ions we should expect that positions of higher current should experience faster

2000 *Mathematics Subject Classification.* Primary 82B24, 49Q20; Secondary 28A80, 74P05.

Key words and phrases. optimal transport path, diffusion-limited aggregation, sticking probability, random walk.

This work is supported by an NSF grant DMS-0710714, and also a VIGRE REU program at UC Davis.

growth. To make DLA accessible to processes relating to physical phenomena which optimize some parameter, commonly energy, we introduce a probability dependent on the cost function used in the study of optimal transport paths [10]. This increases the utility of the d-ary trees studied by Barlow et al while retaining similar growth properties such as the phase transition of the factor α.

This article is organized as follows. We first recall some basic concepts about optimal transport paths between measures of equal total mass as studied in [10] etc. Then we propose a modification of DLA in which the probability of sticking is inversely proportional to the additional transport cost from the point to the root. We use a family of cost functions parametrized by a parameter α as studied in optimal transport paths [10]. Similar to Barlow et al [1], $\alpha < 0$ promotes growth near the root whereas $\alpha > 0$ promotes growth at the tips of the tree. $\alpha = 0$ is a phase transition point and corresponds to DLA. What makes this model interesting is that when α is negative enough (e.g. $\alpha < -2$) the final cluster is an one dimensional curve. On the other hand, when α is positive enough (e.g. $\alpha > 2$) we get a nearly two dimensional disk. Thus our model encompasses the full range of fractal dimension from 1 to 2.

2. Transport paths between positive Radon measures

Recently, optimal transportation systems with branching structures have raised a lot of interest and some attempts have been made to formalize their description [2],[5],[4],[6],[10],[11],[12],[13],[14]. Here, we only recall some basic concepts about optimal transport paths between measures as studied in [10] etc, and then propose a modification of DLA using ideas from optimal transportation.

Let X be a convex compact subset of a Euclidean space $\mathbb{R}^m$. For any $x \in X$, let δ_x be the Dirac measure centered at x. A positive *atomic* measure in X is in the form of

$$\mathbf{a} = \sum_{i=1}^{k} a_i \delta_{x_i}$$

with distinct points $x_i \in X$, and $a_i > 0$ for each $i = 1, \cdots, k$.

For any two positive atomic measures

$$\mathbf{a} = \sum_{i=1}^{k} a_i \delta_{x_i} \text{ and } \mathbf{b} = \sum_{j=1}^{l} b_j \delta_{y_j} \tag{2.1}$$

of equal total mass

$$\sum_{i=1}^{k} a_i = \sum_{j=1}^{l} b_j,$$

a *transport path* from $\mathbf{a}$ to $\mathbf{b}$ is a weighted directed graph G consisting of a vertex set $V(G)$, a directed edge set $E(G)$, and a weight function

$$w : E(G) \to (0, +\infty)$$

such that $\{x_1, x_2, \cdots, x_k\} \cup \{y_1, y_2, \cdots, y_l\} \subset V(G)$ and for any vertex $v \in V(G)$,

$$\sum_{\substack{e \in E(G) \\ e^- = v}} w(e) = \sum_{\substack{e \in E(G) \\ e^+ = v}} w(e) + \begin{cases} a_i, & \text{if } v = x_i \text{ for some } i = 1, \cdots, k \\ -b_j, & \text{if } v = y_j \text{ for some } j = 1, \cdots, l \\ 0, & \text{otherwise} \end{cases} \tag{2.2}$$

where e^- and e^+denotes the starting and ending endpoints of each directed edge $e \in E(G)$. Here, the balanced equation (2.2) simply means that the total mass flowing into v equals the total mass flowing out of v. When G is viewed as a polyhedral chain, (2.2) can be simply expressed as

$$\partial G = \mathbf{b} - \mathbf{a}.$$

Let

$$Path\,(\mathbf{a}, \mathbf{b})$$

be the space of all transport paths from $\mathbf{a}$ to $\mathbf{b}$. Among all paths in $Path\,(\mathbf{a}, \mathbf{b})$ we want to find an optimal path which allows for the possibility that some parts overlap in a cost efficient fashion. For this reason we introduce the following cost function on transport paths in [10].

For each transport path $G \in Path\,(\mathbf{a}, \mathbf{b})$ as above and any $\alpha \in (-\infty, +\infty)$, the $\mathbf{M}_\alpha$ cost of G is defined by

$$\mathbf{M}_\alpha\,(G) := \sum_{e \in E(G)} [w\,(e)]^\alpha\, length\,(e)\,.$$

When $\alpha < 1$, a "Y-shaped" path from two points to one point is usually more preferable than a "V-shaped" path. In general, a ramifying structure is more efficient than a "linear" structure. An $\mathbf{M}_\alpha$ minimizer in $Path(\mathbf{a}, \mathbf{b})$ is called an *optimal transport path* from $\mathbf{a}$ to $\mathbf{b}$.

3. Modification of DLA using ideas of optimal transportation

Now, we want to use the idea of optimal transportation to propose a modification of the standard diffusion-limited aggregation (DLA). Here the key idea is that the probability of sticking is inversely proportional to the additional cost of transporting the new particle to the root via the existing transport system in the current aggregate.

The model of diffusion-limited aggregation begins with any number of seeds in a space. A particle is released at a radius slightly larger than the maximum radius of the current aggregate and undergoes a random walk (Brownian motion). Once it comes within some critical distance of the existing aggregate it sticks and the process starts over. We may represent the current aggregate by a weighted directed tree G. When a new particle arrives at a position x which is adjacent to a vertex v of G, then we get a new aggregate represented by another weighted directed tree $\tilde{G}$. Suppose Γ_v is the unique path on the weighted directed tree G from the vertex v to the root. Then the additional transport cost for transporting a mass ϵ at x through Γ_v to the root is

$$\begin{aligned} & \mathbf{M}_\alpha\left(\tilde{G}\right) - \mathbf{M}_\alpha\,(G) \\ = & \sum_{e \in \Gamma_v} \left([w\,(e) + \epsilon]^\alpha - [w\,(e)]^\alpha \right) length\,(e) + \epsilon^\alpha L \\ = & \epsilon^\alpha L \left(\sum_{e \in \Gamma_v} \left(\left[\frac{w\,(e)}{\epsilon} + 1 \right]^\alpha - \left[\frac{w\,(e)}{\epsilon} \right]^\alpha \right) \frac{length\,(e)}{L} + 1 \right), \end{aligned}$$

where L is the distance from x to v. Now we take a unit mass $\epsilon = 1$, and also take the length of each edge of the path to be a constant (e.g. the diameter of the particle). DLA is often done on a square, triangular or hexagonal lattice in which case the edge length would be the lattice size. Then we may assume the additional cost is

$$c(v) = \sum_{e \in \Gamma_v} \left([w(e)+1]^\alpha - [w(e)]^\alpha \right) + 1,$$

and set the probability $p(v)$ of a new particle sticking at vertex v to be inversely proportional to $c(v)$, e.g. $p(v) = \frac{1}{c(v)}$.

Note that when $\alpha = 0$ we always have $c(v) = 1$ and $p(v) = \frac{1}{c(v)} = 1$. Thus we get the standard DLA structure. When $\alpha > 0$, $c(v) \geq 1$ and $p(v) = \frac{1}{c(v)} \leq 1$. However, when $\alpha < 0$ we have that $c(v) \leq 1$ and $\frac{1}{c(v)} \geq 1$. To get a probability we normalize $\frac{1}{c(v)}$ and set

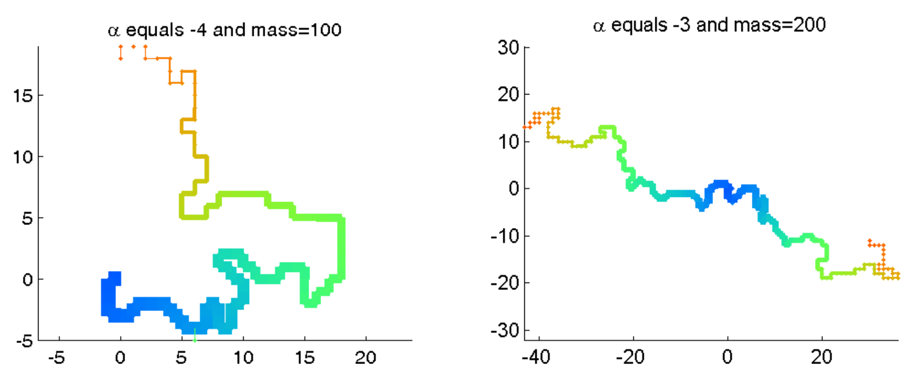
$$p(v) = \frac{c_G}{c(v)}$$

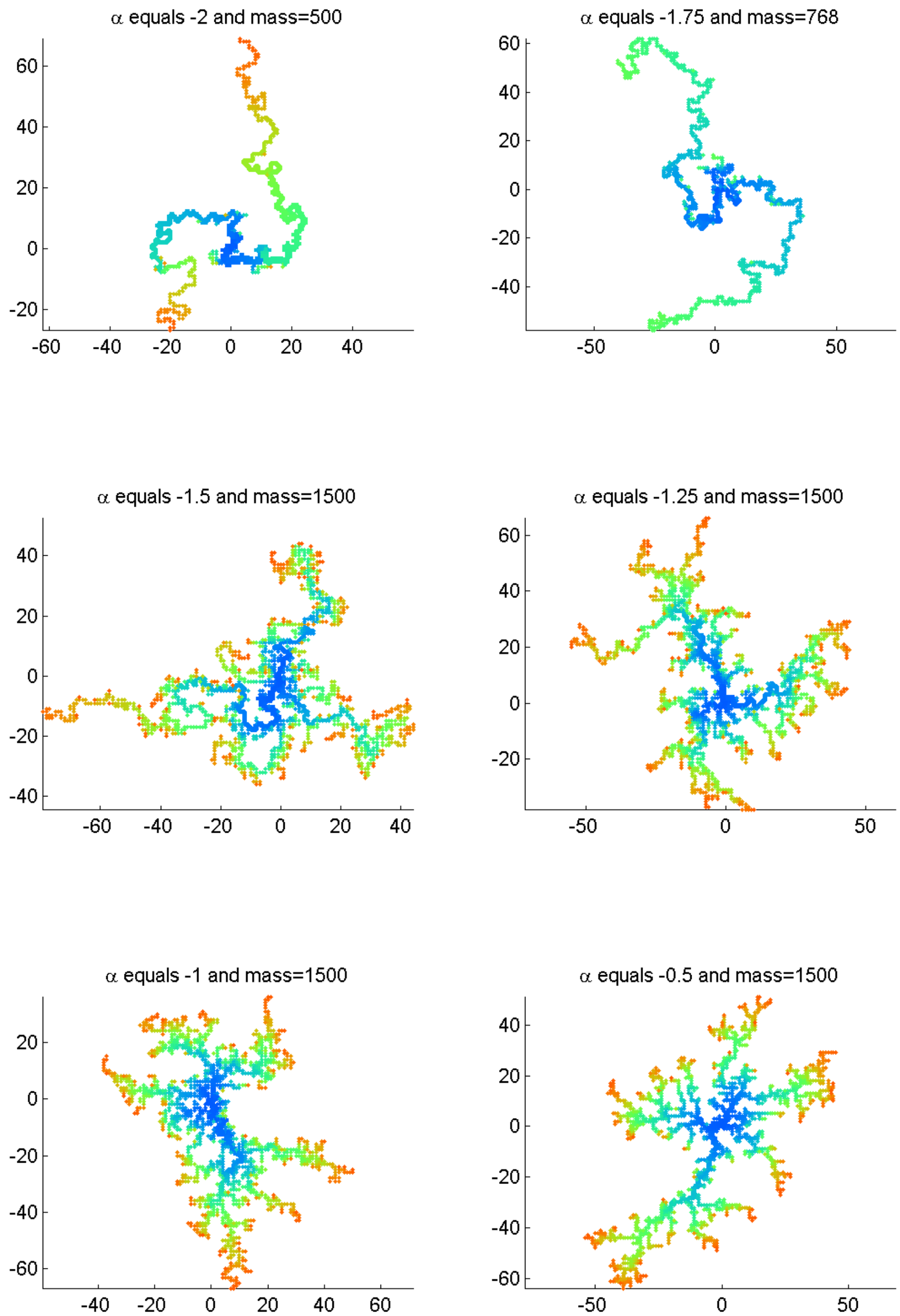
where c_G is the normalization factor. An ideal normalization factor c_G is the minimum of all values $c(v)$ over all vertices v of G. Nevertheless, instead of calculating this number directly we approximate it by taking c_G to be the minimum of all possible $c(v)$ that have been calculated before (including the current one). When $\alpha \geq 0$ we have $c_G = 1$, and when $\alpha < 0$ then c_G becomes a small positive number. So for each v, $p(v) \leq 1$ as $c_G \leq c(v)$.

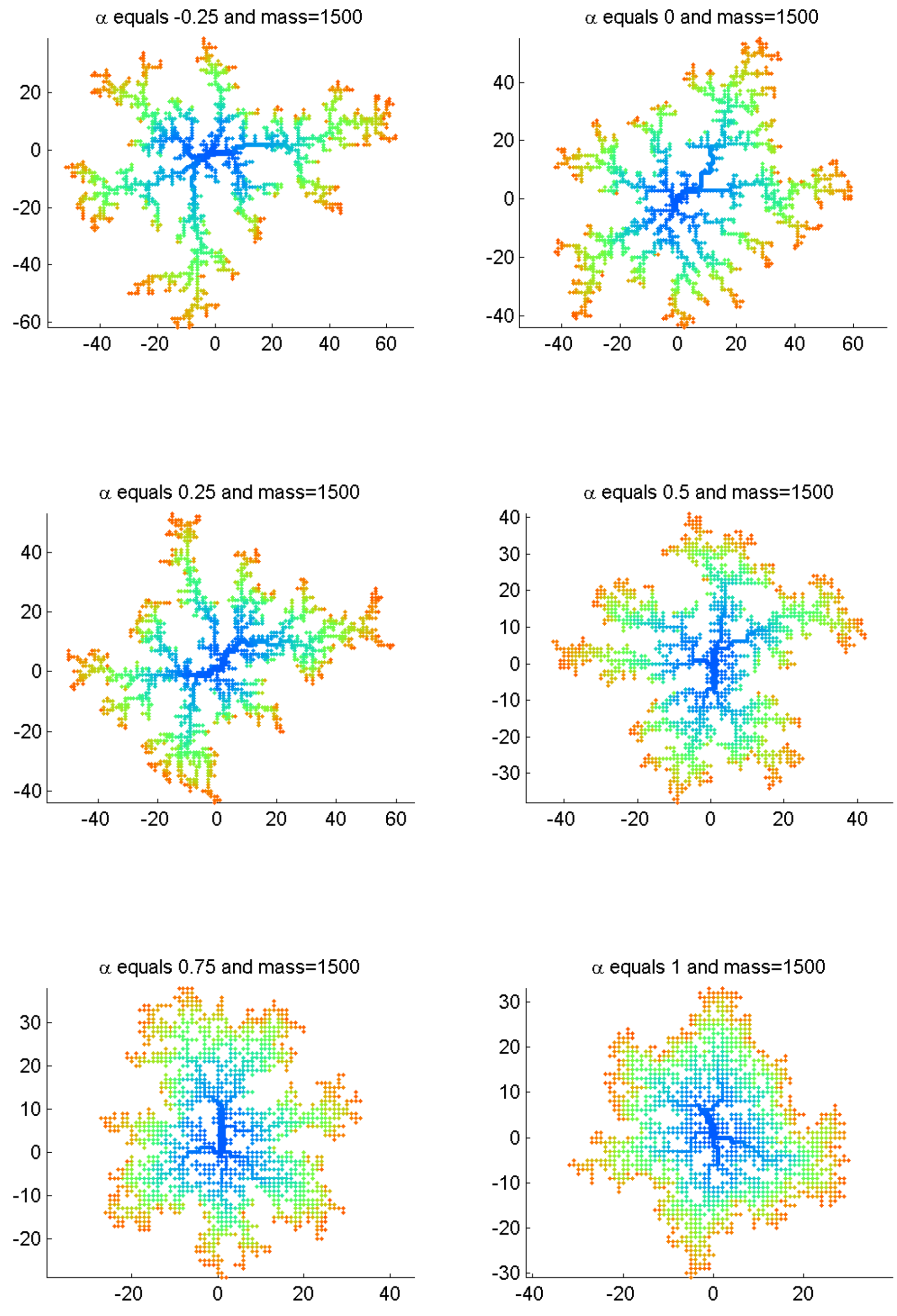
We use the following process to aggregate a cluster:

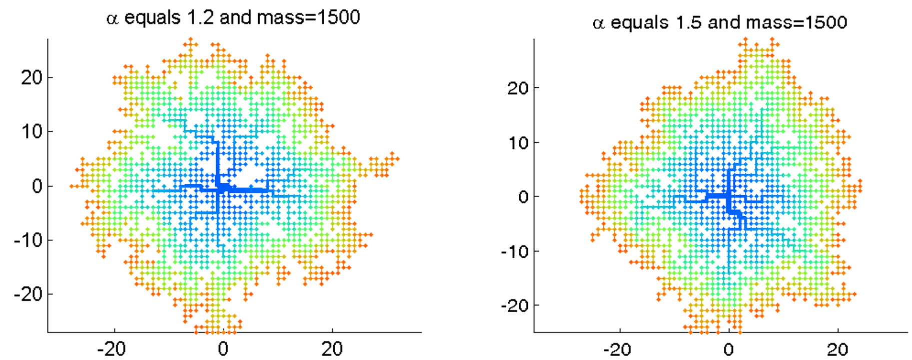
(1) We release a particle from infinity which in practice is a point on a circle whose radius is slightly larger than the maximum radius of the cluster.
(2) The particle undergoes a random walk through unoccupied spaces until it moves adjacent to the cluster.
(3) The additional cost $c(v)$ of attaching to one of the adjacent cluster points is calculated for each adjacent point v and this is translated into a probability $p(v)$.
(4) If the particle sticks, it is added to the cluster and the process starts anew at step 1. If the particle does not stick it continues its random walk from step 2.

Using this algorithm we form the following clusters on a square lattice with different parameters α.




α equals -2 and mass=500
60
40
20
0
-20
-60
-40
-20
0
20
40
α equals -1.75 and mass=768
60
40
20
0
-20
-40
-50
0
50
α equals -1.5 and mass=1500
40
20
0
-20
-40
-60
-40
-20
0
20
40
α equals -1.25 and mass=1500
60
40
20
0
-20
-50
0
50
α equals -1 and mass=1500
20
0
-20
-40
-60
-40
-20
0
20
40
60
α equals -0.5 and mass=1500
40
20
0
-20
-40
-60
-50
0
50


α equals -0.25 and mass=1500
20
0
-20
-40
-60
-40 -20 0 20 40 60
α equals 0 and mass=1500
40
20
0
-20
-40
-40 -20 0 20 40 60
α equals 0.25 and mass=1500
40
20
0
-20
-40
-40 -20 0 20 40 60
α equals 0.5 and mass=1500
40
30
20
10
0
-10
-20
-30
-40 -20 0 20 40
α equals 0.75 and mass=1500
30
20
10
0
-10
-20
-20 0 20 40
α equals 1 and mass=1500
30
20
10
0
-10
-20
-30
-40 -20 0 20



3.1. **Dimensional Analysis.** The modified DLA clusters were analyzed using the standard box counting dimension for different values of the parameter α. We calculated five sets of 5000 particles with α valued in $[-2, 2]$. The following figure is the plot of the average box counting dimensions of these clusters with respect to the variable α.

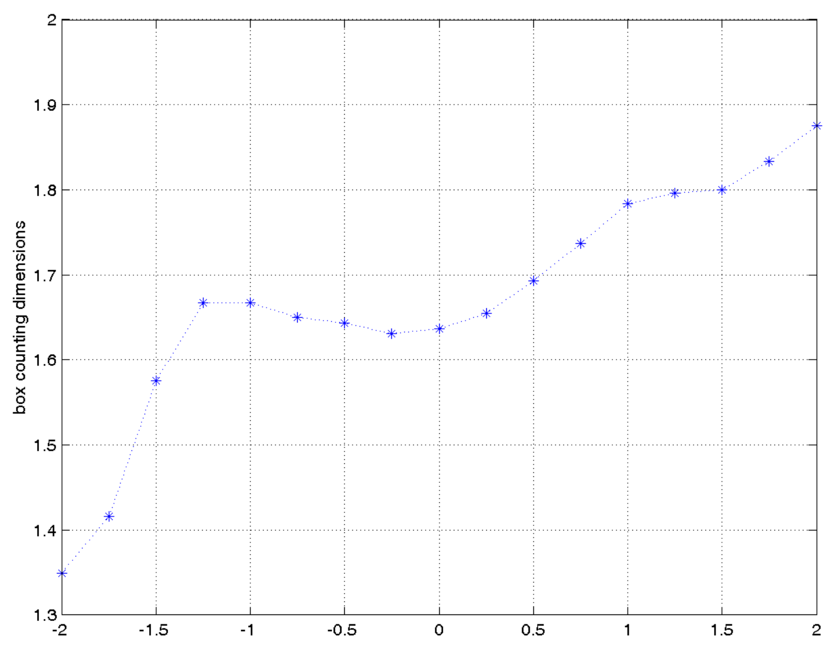
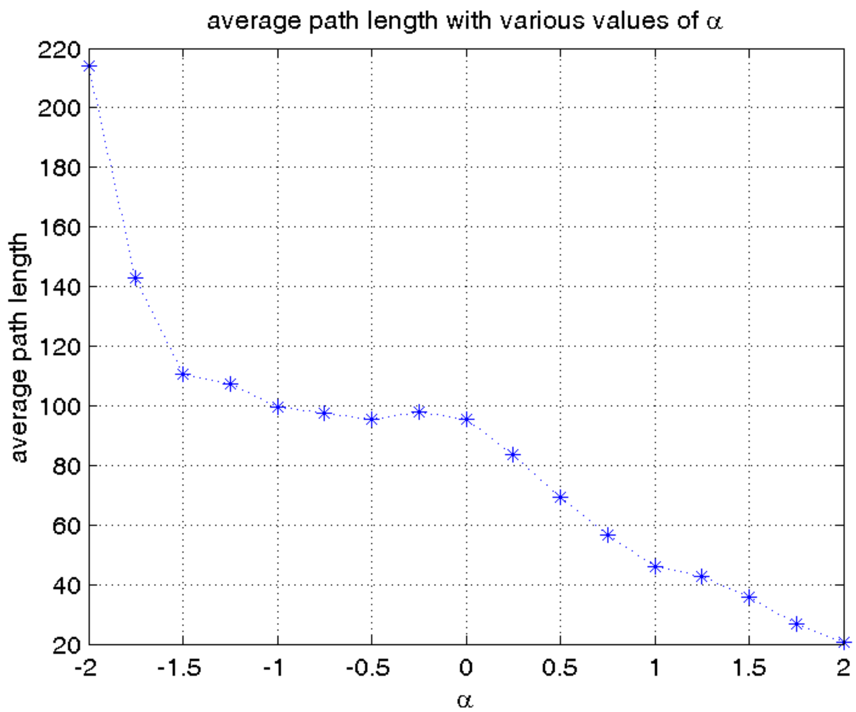


FIGURE 1. box counting dimensions of clusters with respect to α

Here is another way to compare these clusters. For a particle v on the cluster, we may also calculate the length of the path Γ_v from the particle v to the root. The average length of paths of all particles in the cluster may indicate properties such as roundness of the cluster. Using our data, we have the following plot.



From these figures, we see that different values α do give us quantitatively different clusters. Both the box counting dimension and the average path length of the resulting cluster tends to be nearly monotone with respect to the parameter α. $\alpha = 0$ is the standard DLA. When α becomes negative, particles tend to aggregate near tips. When α is negative enough, the final cluster becomes nearly one dimensional, and the average length of paths in the cluster tends towards the maximum (mass+1)/2 or 50% of the mass. On the other hand, when α is positive, particles tend to aggregate near the root. When α is positive enough, the final cluster approaches a two dimensional disk, and the average length of paths in the cluster decreases.

References

[1] M. T. Barlow, R. Pemantle, and E.A. Perkins: Diffusion-limited aggregation on a tree. Probab. Theory Relat. Fields 107 1-60 (1997)

[2] A. Brancolini, G. Buttazzo, F. Santambrogio, Path functions over Wasserstein spaces. J. Eur. Math. Soc. Vol. 8, No.3 (2006),415–434.

[3] M. Bernot; V. Caselles; J. Morel, Traffic plans. Publ. Mat. 49 (2005), no. 2, 417–451.

[4] T. De Pauw and R. Hardt. Size minimization and approximating problems, Calc. Var. Partial Differential Equations 17 (2003), 405-442.

[5] E.N. Gilbert, Minimum cost communication networks, Bell System Tech. J. 46, (1967), pp. 2209-2227.

[6] F. Maddalena, S. Solimini and J.M. Morel. A variational model of irrigation patterns, Interfaces and Free Boundaries, Volume 5, Issue 4, (2003), pp. 391-416.

[7] P. Meakin, Progress in DLA Research. Physica D 86, 104-112 (1995).
[8] T.A. Witten, L.M. Sander. Diffusion-Limited Aggregation, A Kinetic Critical Phenomenon. Phys. Rev. Lett. 47, 1400-1403 (1981).
[9] T.A. Witten, L.M. Sander. "Diffusion-limited aggregation", Phys. Rev. B, 27, 5686-5697 (1983).
[10] Q. Xia, Optimal paths related to transport problems. Communications in Contemporary Mathematics. Vol. 5, No. 2 (2003) 251-279.
[11] Q. Xia. Interior regularity of optimal transport paths. Calculus of Variations and Partial Differential Equations. 20 (2004), no. 3, 283–299.
[12] Q. Xia. Boundary regularity of optimal transport paths. Preprint.
[13] Q. Xia. The formation of tree leaf. ESAIM Control Optim. Calc. Var. 13 (2007), no. 2, 359–377.
[14] Q. Xia. The geodesic problem in nearmetric spaces. Submitted.

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