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An Introduction to Random Geometric Graphs for Physicists

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Abstract

The goal of the project is to understand the critical behaviour of randomly generated Directed Acyclic Graphs (DAG), with particular interest in infinite clusters, connectivity, and network geodesics. In this sense, the hope is to elucidate the nature of information flow in complex, real world systems. This writing will give overview similar results for undirected, Random Geometric Graphs (RGGs) as background. It will cover the Poisson Point Process, Campbell's Theorems, typical connection models, and monotonic, infinite cluster, and full connectivity phase transitions.

1 Introduction

The purpose of our project will be to understand the nature of the Directed Acyclic Graph (DAG). In particular, we hope to understand the critical behaviour of DAGs from the point of view of their random generation. Although nearly no work has been done on this, lots of work has been done on the Random Geometric Graph (RGG), a random graph model in which a set of points are randomly selected from a space (typically a metric space), then connected according to their relative positions. Although one can just as easily add directedness to a normal E-R random graph, where points are connected independent of any background topology, it is much more difficult to add acyclicity. On RGGs, this can be done by manipulating the nature of Lorentz separations (see Section 3), thus motivating their study for this project.

Furthermore, most study on RGGs has been limited to either the highly rigorous (notably, [15]), or purely computational. Given their breadth of applicability [7][16][3][18], it seems valuable to offer an accessible introduction for researchers covering those tools which are frequently reused throughout the field. In particular, this writing will give an informal introduction to the point selection process and Campbell's Theorem's, the point connection process, and the basic phase transitions of RGGs.

2 Poisson Point Process

The first step in forming an RGG is to select the points P from a space $\mathcal{M}$. Consider a Binomial process where each point is in P with probability p. Then the number of points n selected from the region $B \subseteq \mathcal{M}$ will be binomially distributed according to $Bn(n, p, |B|)$. If we take $|\mathcal{M}|, |B| \to \infty$,

and $p = \rho\delta V$ a vanishing probability, then this binomial distribution will limit to a Poisson distribution

$$p_n(B) = \frac{(\rho V_B)^n}{n!} e^{-\rho V_B} \tag{1}$$

where ρ is the point selection density and V_B the volume of the region B. We can then consider using a non-uniform density $\rho(x)$ such that Eqn. (1) is only valid in a local neighbourhood of the point x. The distribution in that neighbourhood then becomes

$$p_{n_x} = \frac{(\rho(x)\delta^d x)^{n_x}}{n_x!} e^{-\rho(x)\delta^d x} \tag{2}$$

where d is the dimension of the space and $\delta^d x$ the volume element. It is well known that the sum of Poisson distributed random variables is itself a Poisson distributed random variable, whose average is the sum of the averages of the original distributions. Thus if $n = \sum n_x$ is the total number of points selected from the region B, then

$$p_n(B) = \frac{\Lambda(B)^n}{n!} e^{-\Lambda(B)} \tag{3}$$

where

$$\Lambda(B) = \int_B \Lambda(d^d x) = \int_B d^d x \rho(x) \tag{4}$$

is the average number of points selected from B, and is typically called the intensity measure. To select points in this way is called a Poisson Point Process (PPP), and has the important property that the probabilities of selecting points in disjoint regions are mutually independent. This independence then gives rise to Campbell's theorem, which states that for some function $f(x)$

$$\mathbb{E}[\Sigma] = \int_B \Lambda(d^d x) f(x) \tag{5}$$

where

$$\Sigma = \sum_{x \in P \cap B} f(x) \tag{6}$$

is the sum over points selected from the region B, and $\mathbb{E}[\cdot]$ is the expectation value. Although intuitive, this notation leads to a useful result. First note that

$$\frac{1}{m!}\theta^m \Sigma^m = \theta^m \sum_{x \in V \cap B} f(x)^m \tag{7}$$

where θ is just some complex number. Using Eqn. (5) then summing over m gives

$$\mathbb{E}[e^{\theta\Sigma}] = 1 + \sum_{m=1} \int \Lambda(d^d x) f(x)^m \theta^m \tag{8}$$

which with a straightforward expansion is equivalent to

$$\mathbb{E}[e^{\theta\Sigma}] = \exp\left(\int \Lambda(d^d x) e^{\theta f(x)} - 1 \right) \tag{9}$$

therefore giving us the characteristic equation for Σ. This will become important later in studying full connectivity, and is in general quite useful for practical applications.

A more in depth overview of the PPP can be found in [11].

3 Typical Models and Local Degree Distribution

The second step in forming the RGG is to form the set of edges E, and therefore the graph $G = (P, E)$. Most broadly, edges are formed between points according to the probability H(x,y), called the connection function, where x and y are the positions of the points. Some typical models are hard RGG (hRGG)

$$H(x,y) = \begin{cases} 0 & \text{if } \|x-y\| > \text{r} \\ 1 & \text{if } \|x-y\| \leq \text{r} \end{cases} \tag{10}$$

where points are connected if they fall within some mutual distance r of one another, or the soft RGG (sRGG) Rayleigh decay model

$$H(x,y) = Ae^{-\beta\|x-y\|^\eta} \tag{11}$$

which can proxy for signal decay [12]. Although $\|x-y\|$ is typically just the d-dimensional Eucildean distance and $\mathcal{M} = \mathbb{R}^d$, sometimes authors will use the l_p metrics

$$\|x\|^p = \sum_{i=1}^{d} |x_i|^p \tag{12}$$

where p is just some number, and when $p \to \infty$

$$\|x\| = \max(|x_1|, |x_2|, \cdots) \tag{13}$$

which is useful for the analysis of abstract datasets [3][13][13]. In the case of causal sets and discretized spacetime, authors will use hRGG with Lorentzian separations

$$dx^2 = \sum_{\mu,\nu=0}^{d} g_{\mu\nu} dx^\mu dx^\nu \tag{14}$$

where greek indices indicate we are summing over spacetime coordinates, and typically the connectivity radius will be set to $r = 0$ such that only timelike or null separated points are connected. Demanding points are only connected in the past to future direction induces causality in the graph, and thus a directed acyclicity. Again, we will not dwell on DAGs for now.

One of the features of RGGs which makes them so difficult to analyze is that connectivity information about a pair of points will almost always give some information about the location of all the other points in the RGG. For example, if we have an RGG where a single point has lots of neighbours, then we know that many of those neighbours are likely connected to eachother, and that all other points in P are on average not very close to the point in question. This leads to different clustering behaviour than in standard E-R random graphs.

The closeness of connected points can be captured by the probability density of there existing a point at y which is connected to a known point at x. Such points exist independently of one another, and are therefore Poisson distributed

$$p_k(x, B) = \frac{\Lambda_H(B)^k}{k!} e^{-\Lambda_H(B)} \tag{15}$$

where

$$\Lambda_H(B) = \int_B \Lambda_H(d^d y) = \int_B d^d y \rho(y) H(x, y) \tag{16}$$

and $p_k(x, B)$ is the probability the point at x has k neighbours in the region B. The probability that two points connected to x are also connected to eachother is then given by

$$C(x) = \int_{\mathcal{M}} dy dz H(x, y) \rho(y) H(x, z) \rho(z) H(y, z) \tag{17}$$

where we have just integrated over all possible positions for two points connected to x, multiplied by the probability that the two points are connected

to eachother. $C(x)$ is called the clustering coefficient, and for an hRGG like Eqn.(10) is

$$C = \frac{2^{d+1}\pi_{d-1}^2}{\pi_d^2} \int_{V_0} du \int_0^{\arccos u} d\theta u^{d-1} (\sin\theta)^d \tag{18}$$

where π_d is the volume of a d-dimensional unit ball. A proof for this can be found in Appendix A of [8]. Interestingly, the cluster coefficient is purely geometrical, and does not depend on the connectivity radius.

4 Phase Transitions

As with any percolation model, RGGs exhibit numerous phase transitions. In particular, the behaviour of the RGG can be split into two regimes: the subcritical regime, with $P_\infty = 0$, and the supercritical regime, with $P_\infty > 0$, where P_k is the probability that a given vertex lies in a cluster of size k [20]. Although very few critical points are known for RGGs, they are relatively well bounded. Unfortunately, finding these bounds is quite mathematically involved. The goal of this section will then be to present the important proofs concerning monotonic properties, infinite clustering, and full connectivity in an informal way, as well as provide some original heuristics leading to broader forms of the same results.

4.1 Monotonic Properties

Monotonic properties are properties which a graph maintains upon the addition of edges. Under this edge addition process, monotonic properties are both irreversible and probabilistically cumulative, indicating that perhaps monotonic properties exhibit phase transitions. This was proven rigorously by A. Goel, S Rai, and B. Krishnamachari (GRK) [1] for the case of hRGGs in a d-dimensional unit cube. We will now informally repeat this proof

Let us dentote the set of RGG-valid graphs with monotonic property Γ by Γ. Consider two hard RGG graphs $G = G(N, r) = (P, E)$ and $G' = G(N, r + 2\gamma(N)) = (P', E')$, where N is the number of points, r the connectivity radius (see Eqn. (10)), and $\gamma(N)$ just some function. Because they have the same number of points, we can form a bijection $\phi : P \to P'$. Given two connected points $u, v \in P$ in G, the triangle inequality then ensures that

$$\begin{aligned} \|\phi(u) - \phi(v)\| &= \|\phi(u) - u + u - v + v - \phi(v)\| \\ &\leq \|\phi(u) - u\| + \|u - v\| + \|v - \phi(v)\| \\ &\leq \|\phi(u) - u\| + r + \|v - \phi(v)\| \end{aligned} \tag{19}$$

Now, let M be the greatest possible distance between corresponding points in the two graphs, ie. the maximum possible $\|\phi(x) - x\|$. Then we just have

$$\|\phi(u) - \phi(v)\| \leq 2M + r$$

If we choose the bijection such that $M \leq \gamma(N)$ then

$$\|\phi(u) - \phi(v)\| \leq 2\gamma(N) + r \tag{20}$$

meaning the two edges are also connected in G'. Thus $(u, v) \in E \implies (\phi(u), \phi(v)) \in E'$, and so G' contains a copy of G within it (call this $G \subset G'$). Of course, the vertices in the two graphs are randomly distributed, and so we might not be able to find a bijection where $M \leq \gamma(N)$. If this occurs with probability $\mathbb{P}[M \leq \gamma(N)] \geq 1 - p$, then $\mathbb{P}[G \subseteq G'] \geq 1 - p$, implying $\mathbb{P}[G \not\subset G'] \leq p$

Let us now imagine that $G \in \Gamma$, but $G' \notin \Gamma$. Because Γ is monotonic, we know $G \not\subset G'$. Thus

$$\mathbb{P}[G \in \Gamma]P[G' \notin \Gamma] \leq \mathbb{P}[G \not\subset G'] \leq p \tag{21}$$

If we now define $R(N, \epsilon)$ as the connectivity radius an RGG with N vertices must have such that it has the property Γ with probability ϵ, then set $r = R(N, \epsilon)$, from Eqn. (21) we get

$$\begin{aligned} \epsilon\mathbb{P}[G' \notin \Gamma] &\leq p \\ \mathbb{P}[G' \in \Gamma] &\geq 1 - \frac{p}{\epsilon} \end{aligned} \tag{22}$$

Because increasing the connectivity radius can only add edges, for monotonic properties $a \geq b \implies R(N, a) \geq R(N, b)$. Applying this to Eqn. (22) gives

$$R\bigg(N, P[G' \in \Gamma]\bigg) \geq R\bigg(N, 1 - \frac{p}{\epsilon}\bigg) \tag{23}$$

But the radius on the LHS is exactly the radius of G', which is related to $r = R(N, \epsilon)$ by $r' = r + 2\gamma(N)$. Substituting this into Eqn. (22), then choosing $\epsilon = \sqrt{p}$ we get

$$2\gamma(N) \geq R(N, 1 - \sqrt{p}) - R\bigg(N, \sqrt{p}\bigg) \tag{24}$$

thus with just the condition $\mathbb{P}[M \leq \gamma(N)] \geq 1 - p$, we can get a bound on the size of the range of radii over which the probability of having some monotonic property goes from $\sqrt{p}$ to $1 - \sqrt{p}$.

GRK then use the following result by Shor and Yukich [19]. Let there be an RGG in dimension d with N vertices. Let $r_c = \left(\frac{\ln(N)}{\pi_d N}\right)^{1/d}$ and $a > 0$, where π_d is the volume of a d-dimensional unit ball. Then

$$\mathbb{P}(M = O(r_c)) \geq 1 - N^{-a} \tag{25}$$

Here, the asymptotic notation $f(N) = O(g(N))$ means that there exists N_0, α such that for all $N > N_0$, $f(N) < \alpha g(N)$. Less formally, $g(N)$ bounds $f(N)$ from above asymptotically. From this result we can now identify $\gamma(N) = r_c$ and $p = N^{-a}$, such that

$$R(N, 1 - N^{-a/2}) - R(N, N^{-a/2}) = O(r_c) \tag{26}$$

In the limit of large N, we see that the probability that $G \in \Gamma$ runs from 0 to 1 over a change of radius of $\sim O(0)$, ie. there is a phase transition. This completes the proof by GRK. This works for any finite square system, however can be generalized by taking the volume of the system to infinity, and replacing N with ρ.

Perhaps frustratingly, this proof doesn't build particularly well on intuitions one might have about why monotonic properties result in phase transitions for dense systems, but instead is dependent on bijections between graphs in a relatively involved way. Let us then present a nice heuristic using just the monotonic properties and the probabilities of their emergence.

Let $Q(r)$ be the probability that $G(\rho, r) \in \Gamma$, and $u(r, r')$ be the probability that if we r to r' the graph will acquire the property Γ, assuming it didn't have the property already. Here, r is some order parameter. Now increase r by a small amount δr and Taylor expand

$$\begin{aligned} Q(r + \delta r) &= Q(r) + \big(1 - Q(r)\big)u(r, r + \delta r) \\ Q(r) + \frac{dQ(r)}{dr}\delta r &= Q(r) + \big(1 - Q(r)\big)\Big(u(r, r) + \frac{du(r, r')}{dr'}_{r'=r}\delta r\Big) \end{aligned} \tag{27}$$

by definition $u(r, r) = 0$, so

$$\frac{dQ(r)}{dr} = \big(1 - Q(r)\big)\frac{du(r, r')}{dr'}_{r'=r} \tag{28}$$

solving

$$Q(r) = 1 - \exp\left(-\int dr \frac{du(r, r')}{dr'}_{r'=r}\right) \tag{29}$$

the nature of monotonic properties implies that $u(r, r')$ should be increasing in both r and ρ. Graphically, it is then easy to see (Fig. 1) that $Q(r)$ exhibits a phase transition in the limit of large ρ. Note that this works for any RGG.

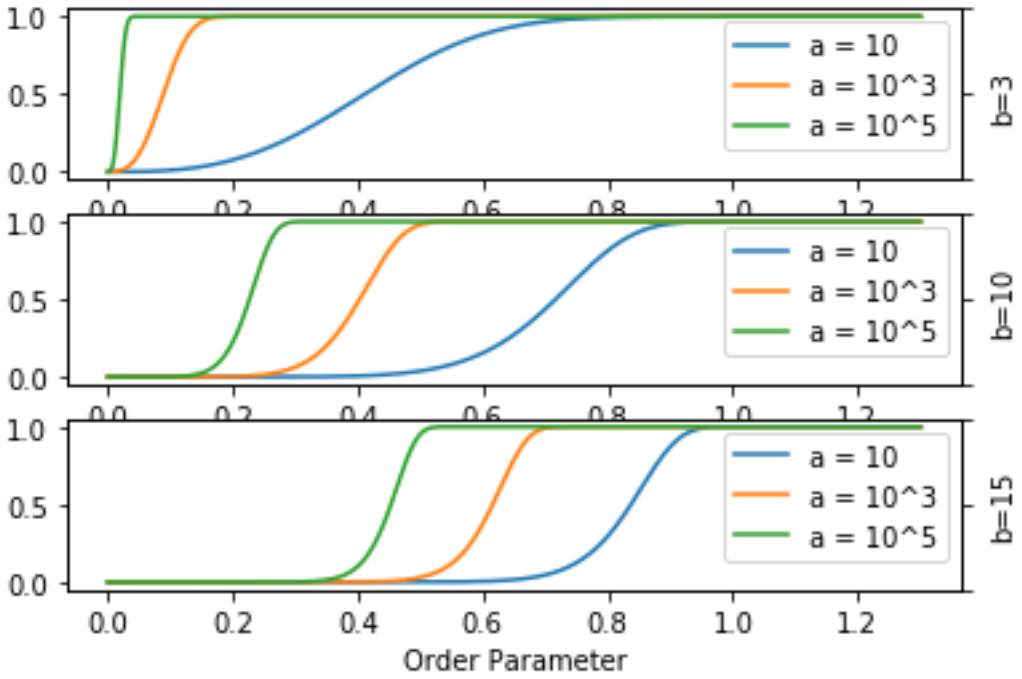

Figure 1: The probability that some graph $G(\rho, r)$ has the monotonic property Γ, where ρ is the point density, and r some monotonic order parameter of the connection function. Here the probability that G gains Γ going from r to r' is $u(r, r') = abr^{b-1}r'$, where a and b are just some parameters. a and b would likely increase with ρ.

4.2 Infinite Cluster

The infinite cluster, or Giant Connected Cluster (GCC), is a cluster in an infinite RGG containing a finite fraction of the graphs points. Obviously the existence of an infinite cluster is a monotonic property, and so we expect for a phase transition to arise in P_∞. Although the exact critical point for most RGGs is unknown, we can at least set bounds for hRGGs using tessellation arguments [20].

Consider performing RGG on $\mathbb{R}^d$ with connectivity radius r and density $\rho = const$. Now tessellate the space into d-dimensional hypercubes of sidelength l. Choosing l such that

$$\begin{aligned} r &= \sqrt{(2l)^2 + (d-1)l^2} \\ \implies l &= \frac{r}{\sqrt{d+3}} \end{aligned} \tag{30}$$

means points in adjacent hypercubes will be guaranteed to be connected. Now perform percolation on the hypercubes by demanding that if a hypercube contains a point selected in the PPP process, the cube is "filled". This occurs with probability

$$\begin{aligned} z(r) &= 1 - e^{-\rho l^d} \\ &= 1 - \exp\Big(- \frac{\rho r^d}{(d+3)^{\frac{d}{2}}} \Big) \end{aligned} \tag{31}$$

Because of the way we selected l, we know that if the filling of the hypercubes forms an infinite cluster, then so does the hRGG process. Thus we know that $z(r_c) > z_c^+$ for critical radius r_c and probability z_c^+. Using Eqn. (31)

$$\bar{k_c} = \rho \pi_d r_c^d > \pi_d (d+3)^{\frac{d}{2}} \ln\Big(\frac{1}{1-z_c^+}\Big) \tag{32}$$

where we note that $\bar{k} = \rho V = \rho \pi_d r^d$ is the average degree of a point in hRGG (see Eqns. (1) and (10)).

Similarly, if we choose $l = r$, then connected points will be guaranteed to be in either the same hypercube, or an adjacent or diagonal one. If we fill the hypercubes in the same way as before, then the non-existence of an infinite cluster in the hRGG ensures its non-existence in the tessellated hypercubes. Note that the inclusion of diagonal hypercubes means we are dealing with a different infinite cluster, with a different critical z. If we call this z_c^*, then this all means $z(r_c) < z_c^*$ and again with Eqn. (31) we get

$$\bar{k_c} = \rho \pi_d r_c^d < \pi_d (d+3)^{\frac{d}{2}} \ln\Big(\frac{1}{1-z_c^*}\Big) \tag{33}$$

therefore

$$\pi_d (d+3)^{\frac{d}{2}} \ln\Big(\frac{1}{1-z_c^+}\Big) < \bar{k_c} < \pi_d (d+3)^{\frac{d}{2}} \ln\Big(\frac{1}{1-z_c^*}\Big) \tag{34}$$

Experiment has shown that in d-dimensions $\bar{k}_c$ varies according to

$$\bar{k}_c = 1 + A d^{-\gamma} \tag{35}$$

where $A = 11.78$ and $\gamma = 1.74$ [8].

While these arguments are nice, they unfortunately rely on the critical probabilities of two other percolation frameworks, for which neither probability has been exactly solved in any dimension higher than 1. In his original paper, Gilbert used a branching technique to bound $\bar{k}_c$ which is looser but works in all dimensions independently of other models. This technique is rather common in graph theory, and can be found in [10].

4.3 Full Connectivity

A graph is fully connected when it is possible to draw a path between any pair of points. Again, this property is monotonic and so exhibits a phase transition. It was shown by Penrose that in the limit of high density, full connectivity is blocked by the appearance of isolated points [14]. This is because larger, noninfinite clusters require large empty boundaries, while single points just need space for themselves, and the infinite cluster can be a bit more like "swiss cheese" [20].

Full connectivity being correlated with the non-existence of isolated points means all we need to do is find the probability of their non-existence h. Because isolation is a highly local property, the probability $p_0(x)$ a point at x is isolated is independent of other properties in the high density limit [14], thus

$$\begin{aligned} h &= \prod_{x \in P} (1 - p_0(x)) \\ &= \exp\left(\sum_{x \in P} \ln(1 - p_0(x)) \right) \end{aligned} \tag{36}$$

Using Eqns. (9) then (15)

$$\begin{aligned} \mathbb{E}(h) := h &= \exp\left(- \int_{\mathcal{M}} \Lambda(d^d x) p_0(x) \right) \\ &= \exp\left(- \int_{\mathcal{M}} \Lambda(d^d x) e^{-\Lambda_H(\mathcal{M})} \right) \end{aligned} \tag{37}$$

which for hRGGs with $\rho = const.$ is

$$h = e^{-e^{-\rho \pi_d r^d}} \tag{38}$$

and in the limit of high ρ

$$h \approx \frac{1}{1 - e^{-\rho \pi_d r^d}} \tag{39}$$

This clearly has a phase transition, trivially, at $r = 0$, however from Fig. 2 it can be seen how there still exists a sharp transition away from zero for ρ high but still $< \infty$. Practically, one might say that $\frac{d^2 h}{dr^2}_{r=r_c} = 0$ is the centre of that transition, with r_c a good proxy for the critical radius.

These results are the standard in RGGs, but significant progress has been made in full connectivity studies using different approaches. See [6] [9] [15].

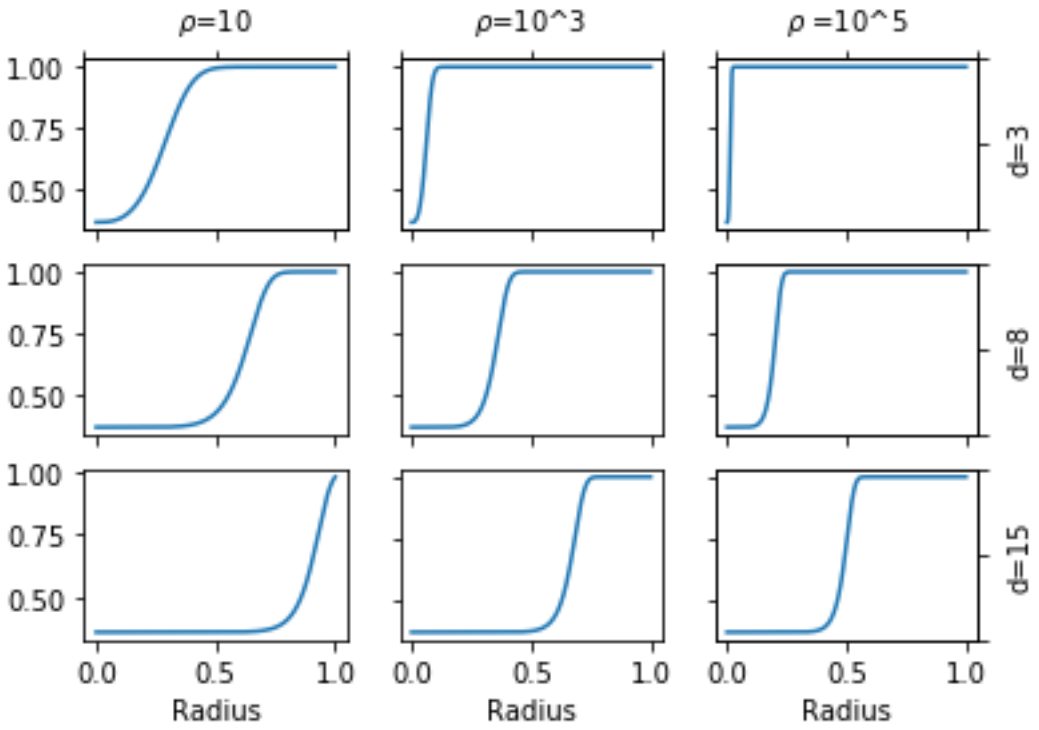

Figure 2: The probability $h(r)$ (see Eqn. (39)) of finding no isolated points in a Euclidean hRGG plotted against connectivity radius for various point densities ρ and dimensions d. As the density increases, the transition becomes sharper and closer to r=0. In higher dimensions the transition becomes sharp faster than it goes to 0, however still does always eventually reach 0. For high ρ this probability is a good approximation for the full connectivity probability.

5 Conclusion

The purpose of this writing was to offer an in depth introduction to RGGs for physicists, ultimately as background to their related DAG. The particular focus was on their structure and phase transitions: In Section 2 the Poisson Point Process was introduced, whose memorylessness ultimately led to Campbell's Theorems. In Section 3 we formed the actual graph by connecting points according to a series of different possible models, finding that the spatial nature of these models resulted in dependencies which would later make the analytical deduction of large scale behaviour very difficult. Although such difficulties were not solved, it was shown that at the very least the dependencies could be quantified through the clustering coefficient. The final section focused on phase transitions, and was broken down into three parts: monotonic properties, where it was shown rigorously for hRGGs, and heuristically for all RGGs, that monotonic properties exhibit phase transitions; the infinite cluster, where tessellation arguments were used to bound the critical radius of its appearance in hRGGs; and full connectivity, where theorems by Penrose and Campbell were used to find an exact, trivial critical radius, as well as an inexact proxy critical radius in the large point density limit.

This writing was of a theoretical focus, and so did not dwell on any experimental results, practical applications, or simulation techniques, although there are many [7][8][2][17]. The writing also did not cover the spectral matrix or topological analysis of RGG phase transitions[4][5], and skipped over some of the less interesting although still practically useful results concerning their asymptotic behaviour by Penrose [15].

6 References

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