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– CENTRUM SCIENTIARUM MATHEMATICARUM –

Critical Scaling in Particle Systems and Random Graphs

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Mathematical Statistics



Critical Scaling in Particle Systems and Random Graphs

Critical Scaling in Particle Systems and Random Graphs

by

VASILII GORIACHKIN



LUND
UNIVERSITY

Thesis for the degree of Doctor of Philosophy
Thesis advisor: Professor Tatyana Turova
Faculty opponent: Associate Professor Johan Tykesson

To be presented, with the permission of the Faculty of Science of Lund University, for public criticism on Thursday, the 2nd of November 2023, at 13:00 in the lecture hall MH:Hörmandersalen at the Centre for Mathematical Sciences, Sölvegatan 18A, Lund.

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Abstract <p>The purpose of this thesis is to study the behavior of macro-systems through their micro-parameters. In particular, we are interested in finding critical scaling in various models.</p> <p>Paper I investigates the influence of discrete-time collisions on particle dynamics. By analyzing two models — one involving external forces and friction, and another incorporating collisions with lighter particles — a nuanced understanding of particle trajectories emerges. Conditions for the equivalence of these models are established, encompassing both deterministic and stochastic collision scenarios.</p> <p>Paper II focuses on scaling properties within critical geometric random graphs on a 2-dimensional torus. This is an example of an inhomogeneous random graph that is not of rank 1. Drawing parallels with classic Erdős-Rényi graphs, the study unveils scaling patterns of the size of the largest connected component and its diffusion approximation.</p> <p>In Paper III and Paper IV, we examine axon tree growth models in dimensions 2 and 3. We uncover the relationship between the probability of neuron connections and micro-level growth parameters. Notably, we demonstrate that connection probabilities do not strictly decrease exponentially or polynomially with the distance between neurons. While finding the critical scaling for the connection probability over time (determined by distance) remains challenging, the insights from Papers III and IV will aid in addressing this issue.</p>			
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VASILII GORIACHKIN



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A doctoral thesis at a university in Sweden takes either the form of a single, cohesive research study (monograph) or a summary of research papers (compilation thesis), which the doctoral student has written alone or together with one or several other author(s).

In the latter case the thesis consists of two parts. An introductory text puts the research work into context and summarizes the main points of the papers. Then, the research publications themselves are reproduced, together with a description of the individual contributions of the authors. The research papers may either have been already published or are manuscripts at various stages (in press, submitted, or in draft).

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List of publications

This thesis is based on the following publications, referred to by their Roman numerals:

- I **Linear Dissipative Force as a Result of Discrete Time Collisions**
Vasilii Goriachkin, Tatyana Turova
Markov Processes and Related Fields 26, 2 (2020), 315-337
- II **Scaling of Components in Critical Geometric Random Graphs on 2-dim Torus**
Vasilii Goriachkin, Tatyana Turova
arXiv:2308.07696 (2023)
- III **Decay of connection probabilities with distance in 2D and 3D neuronal networks**
Vasilii Goriachkin, Tatyana Turova
BioSystems 184 (2019), 103991
- IV **Properties of Randomly Grown 2D and 3D Networks**
Vasilii Goriachkin
Manuscript, (2023)

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Lund, September 2023

Vasilii Goriachkin

Popular summary

The purpose of this thesis is to study the behavior of macro-systems through their micro-parameters. In particular, we are interested in finding critical scaling in various models.

In Paper I, we explore two models. In the first one, the particle moves under the action of an external force, and a dissipative force acts on it, which depends linearly on the velocity of the particle. In the second model, the same external force acts on the particle, but instead of a dissipative force, it collides with particles of small masses m_k at some time intervals. We have found conditions on the model parameters such that the particle motion in the first model will be equivalent (in some sense) to the particle motion in the second model. In particular, we determined that the masses of small particles should be of the same order as the time period τ between collisions. That is, we found the correct scale with m_k tending to zero.

In Paper II, we consider a random graph with N^2 vertices on a 2-dimensional torus, such that the connection probabilities between the vertices depend on the distance between them. We consider the critical case, that is, the one where in the average each vertex has exactly one neighbor. It turns out that in this case, the largest connected component is of the order of $N^{4/3}$, and it is possible to construct a diffusion approximation similar to the classical Erdős-Rényi model. We make a conjecture that the same approach will work for models of higher dimensions and that the critical scaling will be the same, namely $n^{2/3}$, where n is the number of vertices in the graph.

In Paper III and Paper IV, we consider the growth model of neuron axon trees in dimensions 2 and 3. We find how such a macro indicator as the probability of connection between neurons depends on the micro indicators that determine the growing tree. In particular, we show that connection probabilities do not necessarily decrease exponentially or polynomially with increasing distance between neurons. At the moment, it remains a challenge to find the critical scaling for the distance d between particles as a function of time t , at which the probability of connection between neurons starts to decrease from 1, but the results of Paper III and Paper IV will definitely help in solving this problem.

Collectively, these explorations illuminate the interwoven fabric of diverse phenomena across physics, random graphs, neuroscience, and probabilistic modeling. As I undertake the endeavor of synthesizing these insights into my impending thesis, I am keenly aware of the intrinsic unity underlying seemingly disparate facets of scientific inquiry.

Introduction

The thesis is based on four papers. In this chapter, we provide some definitions and theorems necessary for understanding the papers.

I Conservation Laws and Stokes' Law

The laws of physics are often empirical and are based on experimental data. In addition, some laws work only for a certain set of parameters, while for other parameters, completely different laws work, which are in no way related to the first ones. Examples of such theories are Newton's Classical Mechanics [16] and Quantum Mechanics [17].

As V.A. Malyshev wrote in [19], the fact that physics is only an approximation of reality does not mean that mathematics contradicts physics. The standard mathematical approach should aim for the following things:

1. There should be axioms, the less the better. However, for some values of parameters, they should be as close as possible to the basics of theoretical physics.
2. The range of corollaries and coordination with theoretical physics should be as wide as possible.

In the first paper we aim to describe the macro-level law for dissipation force (Stoke's law) through micro-level collisions with small particles, where we use only laws of conservation of energy and momentum. We start with some definitions.

Let V be a set of point particles that interact only with each other, i.e. do not interact with any foreign bodies. Such a system is called a *closed* system.

Consider the first law that we will use, which deals with uniformity of time. It is the law of conservation of energy. For closed system V we write the Lagrangian function in Cartesian

coordinates

$$L = \sum_{a \in V} \frac{m_a \mathbf{v}_a^2}{2} - U(\mathbf{r}_1, \mathbf{r}_2, \dots), \quad (1.1)$$

where m_a is a mass of a particle a , \mathbf{v}_a is its velocity, and \mathbf{r}_a is its radius-vector. Since \mathbf{v}_a is a vector we need to mention that \mathbf{v}_a^2 is a scalar product of \mathbf{v}_a with itself. U is a function that stands for the interaction between particles in system V . We call U a *potential energy* of the system and the first term in (1.1)

$$T = \sum_{a \in V} \frac{m_a \mathbf{v}_a^2}{2} \quad (1.2)$$

we call a *kinetic energy* of the system.

Let us denote the generalized coordinates for the i -th particle by q_i, \dot{q}_i . From Lagrange equations, it follows that

$$\frac{d}{dt} \left(\sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L \right) = 0. \quad (1.3)$$

Hence, we can conclude that the value

$$E = \sum_i \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} - L \quad (1.4)$$

does not depend on time. We call this value the *energy* of the system. In Cartesian coordinates, the energy is written as

$$E = \sum_{a \in V} \frac{m_a \mathbf{v}_a^2}{2} + U(\mathbf{r}_1, \mathbf{r}_2, \dots). \quad (1.5)$$

Thus, the energy of the system can be expressed as a sum of kinetic and potential energies, and it does not depend on time.

Next, we consider the second law which deals with uniformity of space distance-wise. It is the law of conservation of linear momentum. For closed system V from Lagrange equations it follows that

$$\sum_{a \in V} \frac{d}{dt} \frac{\partial L}{\partial \mathbf{v}_a} = \frac{d}{dt} \sum_{a \in V} \frac{\partial L}{\partial \mathbf{v}_a} = 0, \quad (1.6)$$

which implies that the value

$$\mathbf{P} = \sum_{a \in V} \frac{\partial L}{\partial \mathbf{v}_a} \quad (1.7)$$

does not depend on time. We call this value the *momentum* of the system. In Cartesian coordinates it becomes

$$\mathbf{P} = \sum_{a \in V} m_a \mathbf{v}_a. \quad (1.8)$$

Let us derive now simple examples of these two laws. Consider a closed system V which consists of only two particles a and b . We also assume that there is no potential force between them, i.e. $U = 0$, but there are interactions caused by collisions between the particles.

Definition 1.1. A collision of two particles is said to be *elastic* if it is not accompanied by a change in their internal state. Accordingly, when applying the energy conservation law to such a collision, one can ignore the internal energy of particles.

For elastic collision the following propositions hold.

Proposition 1.2 (Laws of conservation of energy and momentum). *Assume that two particles, with masses m_1 and m_2 , collide elastically. Denote the velocities of them before the collision as \mathbf{u}_1 and \mathbf{u}_2 and after the collision as \mathbf{v}_1 and \mathbf{v}_2 . Then*

$$\frac{m_1 \mathbf{u}_1^2}{2} + \frac{m_2 \mathbf{u}_2^2}{2} = \frac{m_1 \mathbf{v}_1^2}{2} + \frac{m_2 \mathbf{v}_2^2}{2}, \quad (1.9)$$

$$m_1 \mathbf{u}_1 + m_2 \mathbf{u}_2 = m_1 \mathbf{v}_1 + m_2 \mathbf{v}_2, \quad (1.10)$$

where (1.9) is the law of conservation of energy and (1.10) is the law of conservation of momentum.

From Proposition 1.2 we derive formulas of velocities of the particles after the collision.

Proposition 1.3. *Given masses m_1 and m_2 of two particles, and the velocities \mathbf{u}_1 and \mathbf{u}_2 before the collision, we derive equations for velocities after the collision:*

$$\mathbf{v}_1 = \frac{m_1 - m_2}{m_1 + m_2} \mathbf{u}_1 + \frac{2m_2}{m_1 + m_2} \mathbf{u}_2, \quad (1.11)$$

$$\mathbf{v}_2 = \frac{m_2 - m_1}{m_1 + m_2} \mathbf{u}_2 + \frac{2m_1}{m_1 + m_2} \mathbf{u}_1. \quad (1.12)$$

Consider also Newton's laws of motion, in particular the second law. The momentum of a point particle is

$$\mathbf{p} = m\mathbf{v}. \quad (1.13)$$

Taking the derivative with respect to time we get

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} = m \frac{d\mathbf{v}}{dt} = m\mathbf{a}. \quad (1.14)$$

Newton's second law of motion states that this derivative \mathbf{F} is a *force* (sum for all forces acted upon the particle) and \mathbf{a} is an *acceleration* of the particle.

The last law we consider is Stoke's law [28] which describes force arising in fluid dynamics [18], such as a frictional (drag) force for a spherical object with very small Reynolds numbers [25] in a viscous fluid.

Proposition 1.4 (Stoke's law). *The force of viscosity (Stoke's drag) on a small sphere moving through a viscous fluid is given by*

$$\mathbf{F}_d = 6\pi\mu R\mathbf{v}, \quad (1.15)$$

where μ is a dynamic viscosity, R is a radius of the spherical object, \mathbf{v} is the flow velocity relative to the object.

In particular, this states that the drag force is linearly dependent on the flow velocity.

2 Markov Chains and Branching Processes

We present some results related to Markov chains from [24]. A *Markov Process* $\{X_t\}$ is a stochastic process with the property that, given the value of X_t , the values of X_s for $s > t$ are not influenced by the values of X_u for $u < t$. A *discrete-time Markov chain* is a Markov process whose state space S is a finite or countable set, and whose (time) index set is $T = (1, 2, \dots)$. In formal terms, the Markov property is that

$$\begin{aligned} \mathbb{P}(X_{n+1} = j | X_n = i, X_{n-1} = i_{n-1}, \dots, X_1 = i_1) \\ = \mathbb{P}(X_{n+1} = j | X_n = i), \end{aligned} \quad (2.1)$$

for all time points n and all states $i_1, \dots, i_{n-1}, i, j \in S$. The latter probability is called the *one-step transition probability* and is denoted by $P_{ij}^{n, n+1}$. When the one-step transition probabilities are independent of the time variable n , i.e. $P_{ij}^{n, n+1} = P_{ij}$, we say that the Markov chain has *stationary transition probabilities*. Set $S = 1, 2, \dots$. It is customary to arrange numbers P_{ij} in a matrix, in the infinite square array

$$P = \begin{pmatrix} P_{11} & P_{12} & P_{13} & \dots \\ P_{21} & P_{22} & P_{23} & \dots \\ \vdots & \vdots & \vdots & \dots \\ P_{i1} & P_{i2} & P_{i3} & \dots \\ \vdots & \vdots & \vdots & \dots \end{pmatrix}, \quad (2.2)$$

which is called a *transition probability matrix*.

Suppose that $S = \{1, \dots, N\}$, finite, and a transition probability matrix P on S has the property that when raised to the power k , the matrix P^k has all of its elements strictly positive. Such a transition probability matrix and the corresponding Markov chain are called *regular*. The important fact concerning a regular Markov chain is the existence of a *limiting probability distribution* $\pi = (\pi_1, \dots, \pi_N)$, where $\pi_j \geq 0$ for $j = 1, \dots, N$ and $\sum_{j=1}^N \pi_j = 1$, and this distribution is independent of the initial state, i.e. there is a convergence

$$\lim_{n \rightarrow \infty} P_{ij}^n = \pi_j, \text{ for } j = 1, \dots, N. \quad (2.3)$$

Theorem 2.1. *Let P be a regular transition probability matrix on the states $1, \dots, N$. Then the limiting distribution $\pi = (\pi_1, \dots, \pi_N)$ is the unique non-negative solution of the equations*

$$\pi_j = \sum_{i=1}^N \pi_i P_{ij}, \quad j = 1, \dots, N \quad (2.4)$$

$$\sum_{j=1}^N \pi_j = 1. \quad (2.5)$$

A transition probability matrix is called *doubly stochastic* if the columns sum to one as well as the rows, i.e.

$$P_{ij} \geq 0 \text{ and } \sum_k P_{ik} = \sum_k P_{kj} = 1 \text{ for all } i, j. \quad (2.6)$$

Consider a doubly stochastic transition probability matrix on the N states $1, 2, \dots, N$. If the matrix is regular, then the limiting distribution is the uniform distribution $\pi = (1/N, \dots, 1/N)$, since it is a solution of the equations (2.4) and (2.5) and by Theorem 2.1 this solution is unique.

Let us now consider a branching process. Suppose an organism at the end of its life produces a random number ξ of offspring with the probability distribution

$$\mathbb{P}(\xi = k) = p_k, \text{ for } k = 0, 1, \dots, \quad (2.7)$$

where $p_k \geq 0$ and $\sum_{k=1}^{\infty} p_k = 1$. We assume that all offspring act independently of each other and at the end of their lifetimes individually have progeny in accordance with the probability distribution (2.7). The process $\{X_n\}$, where X_n is the population size at the n th generation, is a Markov chain of special structure called a *branching process* or *the Galton-Watson process* [32].

Suppose that the process starts with only one organism $X_1 = 1$. An important characteristic of a branching process is the probability that the process ever becomes extinct, i.e.

$$q = \mathbb{P}(X_i = 0 \text{ for some } i \geq 2) = \lim_{n \rightarrow \infty} \mathbb{P}(X_n = 0). \quad (2.8)$$

Consider also the probability generating function of the random variable ξ

$$g(s) = \mathbb{E}s^\xi = \sum_{k=0}^{\infty} s^k p_k, \quad |s| \leq 1. \quad (2.9)$$

Then the following theorems hold true:

Theorem 2.2 (From [5]). *The extinction probability of the $\{X_n\}$ is the smallest non-negative root q of the equation*

$$t = g(t), \quad (2.10)$$

and

- if $\mathbb{E}\xi \leq 1$, then $q = 1$;
- if $\mathbb{E}\xi > 1$, then $q < 1$.

Theorem 2.3 (From [11]). *No matter what is the finite value of $m = \mathbb{E}\xi$, we have*

$$\lim_{n \rightarrow \infty} \mathbb{P}(X_n = k) = 0, \quad k = 1, 2, \dots \quad (2.11)$$

Moreover $X_n \rightarrow \infty$ with probability $1 - q$ and $X_n \rightarrow 0$ with probability q .

3 Random Graphs

Consider some classical results for Erdős-Rényi graphs [10]. Let $V = \{1, 2, \dots, n\}$ be a set of vertices and let $X_{i,j} : 1 \leq i < j \leq n$ be independent Bernoulli random variables with parameter p . Then for each pair of vertices $i \neq j$ we place an edge between them if $X_{i,j} = 1$. The resulting graph we denote as $G(n, p)$. Note that there are no loops and double edges in the graph. We can vary the parameter p (for example, $p = \lambda/n$), and consider the structure of $G(n, p)$ in the limit $n \rightarrow \infty$.

Consider the results for largest connected component of $G(n, p)$ for

$$p = \frac{\lambda}{n}, \quad \lambda > 0. \quad (3.1)$$

Theorem 3.1 (From [10] and [30]). *Let C_1 be the size of the largest connected component in $G(n, p)$, with p defined in (3.1). Then for $\lambda = 1$ the phase transition occurs, and*

i. *If $\lambda < 1$ then*

$$\frac{C_1}{\log n} \xrightarrow{P} \frac{1}{\lambda - 1 - \log \lambda}, \quad n \rightarrow \infty. \quad (3.2)$$

2. If $\lambda > 1$ then

$$\frac{\mathcal{C}_1}{n} \xrightarrow{P} \beta(\lambda), \quad n \rightarrow \infty, \quad (3.3)$$

where $\beta(\lambda) \in (0, 1)$ is the unique solution of

$$\beta + e^{-\lambda\beta} = 1. \quad (3.4)$$

From Theorem 3.1 we see, that in subcritical case $\lambda < 1$ the largest connected component is of order $\log n$. For supercritical case $\lambda > 1$ the largest connected component is of order n .

In the critical case there is a result of Aldous [4].

Theorem 3.2. *Consider the graph $G(n, p)$ with*

$$p = \frac{1}{n} + \frac{t}{n^{4/3}}. \quad (3.5)$$

Let $\mathcal{C}_1, \mathcal{C}_2, \dots$ denote the ordered sizes of the connected components in $G(n, p)$ with \mathcal{C}_1 being the largest one. Let $\gamma_1, \gamma_2, \dots$ denote the ordered lengths of the excursions of the process

$$B(s) = \widetilde{W}(s) - \min_{0 < t < s} \widetilde{W}(t),$$

where

$$\widetilde{W}(s) = W(s) - \frac{1}{2}s^2 + ts \quad (3.6)$$

with W being the standard Brownian motion. Then

$$\frac{1}{n^{2/3}} (\mathcal{C}_1, \mathcal{C}_2, \dots) \xrightarrow{d} (\gamma_1, \gamma_2, \dots), \quad \text{as } n \rightarrow \infty,$$

with respect to l^2 topology on the set of infinite non-decreasing sequences $x = (x_1, x_2, \dots)$ of non-negative values with metric $d(x, y) = \left(\sum_i (x_i - y_i)^2 \right)^{1/2}$.

From Theorem 3.2 we see, that in critical case the largest connected component is of order $n^{2/3}$. Very similar results were obtained in [20].

Erdős-Rényi graph $G(n, p)$ is an example of a homogeneous graph. Let us define the inhomogeneous graph [8]. If instead of the probability of connection p (which does not depend on vertices $i, j \in V$) we consider probabilities $p(i, j)$, then the graph becomes inhomogeneous.

Consider a separable metric space (\mathcal{S}, ρ) . Let μ be a Borel probability measure on \mathcal{S} . Let also $(\mathbf{x}_n) = \{x_1, \dots, x_n\}$ be a sequence (deterministic or random) of points in \mathcal{S} such that for any μ -continuity set $A \subset \mathcal{S}$

$$\frac{\#\{i : x_i \in A\}}{n} \xrightarrow{P} \mu(A). \quad (3.7)$$

Definition 3.3. A *generalized vertex space* \mathcal{V} is a triple $(\mathcal{S}, \mu, (\mathbf{x}_n))$, where (\mathbf{x}_n) satisfies (3.7).

Definition 3.4. A kernel κ is *graphical* on a (generalized) vertex space $\mathcal{V} = (\mathcal{S}, \mu, (\mathbf{x}_n))$ if the following conditions hold:

1. κ is continuous *a.e.* on $\mathcal{S} \times \mathcal{S}$;
2. $\kappa \in L^1(\mathcal{S} \times \mathcal{S}, \mu \times \mu)$;

3.
$$\frac{1}{n} \mathbb{E} \{e(G(\mathcal{V}, n, \kappa))\} = \frac{1}{2} \int_{\mathcal{S}} \int_{\mathcal{S}} \kappa(x, y) d\mu(x) d\mu(y), \quad (3.8)$$

where $G(\mathcal{V}, n, \kappa)$ denotes a random graph where any two vertices x_i and x_j are connected independently of others with probability

$$p(x_i, x_j) = \min \left\{ \frac{\kappa(x_i, x_j)}{n}, 1 \right\}, \quad (3.9)$$

and $e(G)$ denotes the number of the edges in G .

Definition 3.5. Let $\mathcal{V} = (\mathcal{S}, \mu, (\mathbf{x}_n))$ be a (generalized) vertex space and let κ be a kernel on \mathcal{V} . A sequence (κ_n) of kernels on (\mathcal{S}, μ) is *graphical on \mathcal{V} with limit κ* if, for *a.e.* $(y, z) \in \mathcal{S}^2$

$$y_n \rightarrow y \text{ and } z_n \rightarrow z \text{ imply that } \kappa_n(y_n, z_n) \rightarrow \kappa(y, z), \quad (3.10)$$

κ satisfies condition 1 and 2 of Definition 3.4, and

$$\frac{1}{n} \mathbb{E} \{e(G(\mathcal{V}, n, \kappa_n))\} \rightarrow \frac{1}{2} \int_{\mathcal{S}} \int_{\mathcal{S}} \kappa(x, y) d\mu(x) d\mu(y). \quad (3.11)$$

Consider also an integral operator

$$(T_\kappa f)(x) = \int_{\mathcal{S}} \kappa(x, y) f(y) dy \quad (3.12)$$

for any measurable function f such that this integral is defined for *a.e.* x . Define the norm of this operator

$$\|T_\kappa\| := \sup \{ \|T_\kappa(f)\|_{L^2(\mathcal{S})} : f \geq 0, \|f\|_{L^2(\mathcal{S})} \leq 1 \} \leq \infty. \quad (3.13)$$

The following result for the phase transition obtained in [8].

Theorem 3.6. *Let (κ_n) be a graphical sequence of kernels on a (generalized) vertex space \mathcal{V} with limit κ . Then*

1. *If $\|T_\kappa\| \leq 1$, then the size of the largest connected component $\mathcal{C}_1(G(\mathcal{V}, n, \kappa_n)) = o_p(n)$.*
2. *If $\|T_\kappa\| > 1$, then $\mathcal{C}_1(G(\mathcal{V}, n, \kappa_n)) = O(n)$ with high probability.*

If the graphical kernel κ has the form $\kappa(x, y) = \psi(x)\psi(y)$ for some function $\psi > 0$ on \mathcal{S} , then we call this *rank 1* case [8]. The critical regime for rank 1 case has been studied in [6], [7], [29].

Consider now Geometric Random Graphs, which have been actively studied in [23]. We are particularly interested in Geometric Random Graphs on torus [22]. Let $N \in \mathbb{N}$ and consider in dimension $d \geq 2$ the discretized torus $\mathbb{T}_N^d = (\mathbb{Z}/N\mathbb{Z})^d$. Denote the set of vertices on this torus by

$$V_N = \{1, \dots, N\}^d.$$

Hence, the number of vertices in V_N is $|V_N| = N^d$. For any two vertices $u = (u_1, \dots, u_d)$, $v = (v_1, \dots, v_d) \in V_N$ define the torus distance $\rho(u, v)$ between them by

$$\rho(u, v) = \sum_{k=1}^d \rho_N(u_k - v_k),$$

where for any $1 \leq i \leq N$

$$\rho_N(i) = \begin{cases} i, & 0 \leq i \leq N/2, \\ N - i, & N/2 < i < N. \end{cases}$$

Consider a random simple graph on the set of vertices V_N defined as follows. Let $X, X_u, u \in V_N$ be *i.i.d.* non-negative random variables, $0 \leq \alpha < d$ be fixed arbitrarily, and let $G_{N,d}^{\alpha, X}$ denote a random graph on V_N where any two different vertices $u, v \in V_N$ are connected independently of the rest with probability

$$p(u, v) = \min \left\{ \frac{X_u X_v}{N^{d-\alpha} \rho^\alpha(u, v)}, 1 \right\}. \quad (3.14)$$

We shall also write $p(u, u) = 0$ for any $u \in V_N$, meaning that there are no loops in the graph.

This model was introduced in [22] as a generalization of the original model from [15], which is a particular case of (3.14) when $d = 2$, $\alpha = 1$, and $X = \sqrt{c}$ for some constant $c > 0$. Phase transitions in this particular case were studied in [2].

The following result for phase transitions of general graph $G_{N,d}^{\alpha,X}$ was obtained in [22].

Theorem 3.7. *Let C_1 be the size of the largest connected component of the graph $G_{N,d}^{\alpha,X}$ with $\alpha < d$. Assume that*

$$\mathbb{E}X^2 = \int_0^\infty x^2 d\mu_X(x) < \infty. \quad (3.15)$$

Define

$$\lambda = 2^d \int_{\Lambda_d} \frac{dx_1 \dots dx_d}{(x_1 + \dots + x_d)^\alpha}, \quad (3.16)$$

where $\Lambda_d = (0, 1/2]^d$.

1. As $N \rightarrow \infty$ we have

$$\frac{C_1}{N^d} \xrightarrow{P} \beta_\lambda := \int_0^\infty \beta(x) d\mu_X(x), \quad (3.17)$$

where $\beta(x)$ is a maximal solution to

$$f(x) = 1 - \exp \left\{ -\lambda x \int_0^\infty y f(y) d\mu_X(y) \right\}. \quad (3.18)$$

Furthermore, $\beta_\lambda > 0$ if and only if

$$\lambda \mathbb{E}X^2 > 1. \quad (3.19)$$

2. If

$$\lambda \mathbb{E}X^2 < 1 \quad (3.20)$$

and also $\mathbb{E}e^{aX} < \infty$ for some $a > 0$, then

$$\frac{C_1}{d \log N} \xrightarrow{P} \frac{1}{\log \gamma_\lambda}, \quad (3.21)$$

where

$$\gamma_\lambda := \frac{1}{\lambda \mathbb{E} \{ X^2 \exp(\lambda(y-1)X \mathbb{E}X) \}} > 1, \quad (3.22)$$

with $y > 1$ which satisfies

$$y = \frac{1}{\lambda \mathbb{E}X} \frac{\mathbb{E}\{X \exp(\lambda(y-1)X \mathbb{E}X)\}}{\mathbb{E}\{X^2 \exp(\lambda(y-1)X \mathbb{E}X)\}}. \quad (3.23)$$

4 Neural Networks

Let us start with a model of an abstract neuron [26], the structure of which is shown in Figure 1. The model neuron usually has several inputs and 1 output (which, however, can be transmitted to several neurons). Each input channel i can transmit a real value x_i . Each input channel has an associated weight w_i which multiplies with the input x_i . Then the transmitted information is integrated into the neuron (typically just by adding the incoming signals) providing some real value, at which the primitive function f (selected arbitrarily) is evaluated.

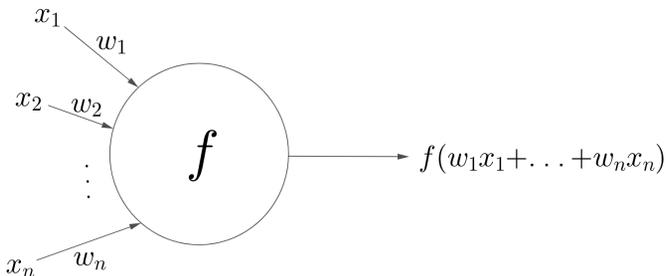


Figure 1: An abstract neuron

One can combine neurons in networks, which are proved to be useful, for instance, in approximation theory. One simple example is the Taylor series for a function F which is being approximated around the point x_0

$$F(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + \cdots + a_n(x - x_0)^n + \cdots, \quad (4.1)$$

where the constants a_0, a_1, \dots depend on the function F and its derivatives at x_0 . We can construct a network, as in Figure 2, which models the first $n + 1$ terms in Taylor series $F_n(x)$ for the function $F(x)$. By changing the number of neurons, connection options, functions, and weights, one can achieve a high precision in approximation.

Another example of a neural network is the Hopfield network [13]. Let V be a graph of $n \in \mathbb{N}$ vertices such that all vertices are connected without loops and double edges. Each

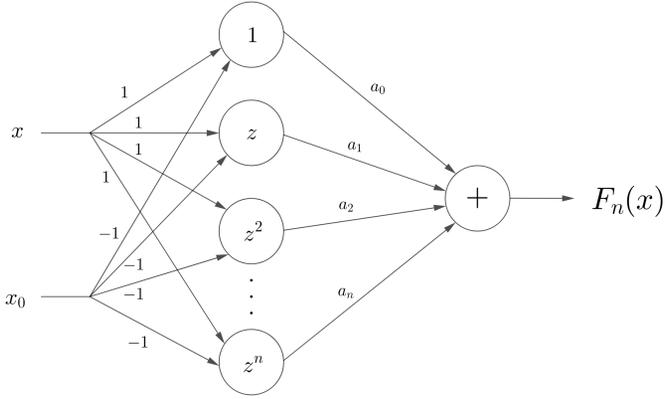


Figure 2: Taylor Network

edge has a weight, i.e. for any two different vertices i and j we assign a number w_{ij} ($w_{ii} = 0$ for any $1 \leq i \leq n$). Then for any set of weights we define a matrix $W = (w_{ij})_{i,j=1}^n$. Since there are no loops in the graph, and there is only one edge between two different vertices, the matrix W is symmetric and has 0's on the diagonal. For each vertex i we also assign a number $x_i \in \{-1, 1\}$ which we call the state of vertex i , and θ_i which we call the threshold of vertex i . For such a network we define an energy function

$$E(x_1, \dots, x_n) = -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_{ij} x_i x_j - \sum_{i=1}^n \theta_i x_i. \quad (4.2)$$

Let us define the updating rule for any particular vertex i :

$$x_i \leftarrow \begin{cases} +1, & \text{if } \sum_{j=1}^n w_{ij} x_j \geq \theta_i. \\ -1, & \text{otherwise.} \end{cases} \quad (4.3)$$

Updates can be performed in two different ways: Asynchronous (only one vertex is updated at a time, it can be picked at random or in a pre-defined order) or Synchronous (all vertices are updated at the same time). The following proposition holds true regarding convergence.

Proposition 4.1 (From [26]). *A Hopfield network with n vertices and asynchronous dynamics, which starts from any given network state, eventually reaches a stable state at a local minimum of the energy function.*

A Hopfield network can be used as an associative memory. If we want to memorize or store m patterns, given as vectors $\mathbf{x}^\mu = (x_1^\mu, \dots, x_n^\mu) \in \{-1, 1\}^n$ where $1 \leq \mu \leq m$, then we

can create a matrix W with the following form (Hebbian learning [12]):

$$w_{ij} = \sum_{\mu=1}^m x_i^{\mu} x_j^{\mu} - m\delta_{ij}, \quad (4.4)$$

where δ_{ij} equals 1, if $i = j$, and 0 otherwise. If $m < n$ and vectors \mathbf{x}^{μ} are close to orthogonal, in most cases, they will be stable with respect to the described dynamics. According to Proposition 4.1 there is a convergence to a stable vector. That is how one can model an associative memory. It is worth noting the equivalence of the Hopfield model and the Perceptron model ([21], [27]), as well as the Ising model [14]. An interesting question for research is to consider the Hopfield model not on a full graph, but on a graph with some structure (for example, \mathbb{Z}^2 -lattice or a star) and find out what patterns this model can remember. It is also interesting to consider this model on geometric graphs, e.g. from Paper II.

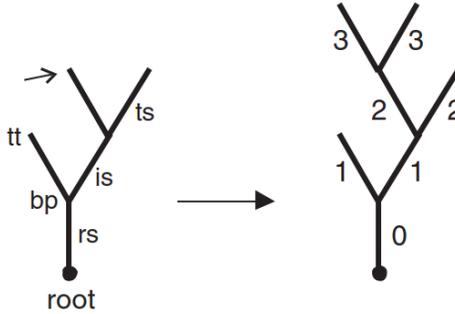


Figure 3: From [31]: A branching event at a terminal segment (open arrow) of a dendritic tree. Terminal (ts), intermediate (is), and root (rs) segments are distinguished, as well as the root, bifurcation points (bp), and terminal tips (tt). In the resultant tree after branching, the segments are labeled according to a centrifugal ordering scheme. By branching, the number of terminal segments has been increased from 3 to 4.

Let us now look at a model of not artificial neurons, but biological ones. Consider a model which was proposed in [31]. This is a branching process model for growing dendritic trees. We ignore the metric properties such as segment lengths and diameters. Dendritic trees are reduced to their skeletons only characterized by the number and the connectivity of the segments (topological structure). In a rooted binary tree (Figure 3), intermediate segments ending in bifurcation points, and terminal segments ending in terminal tips are distinguished. Segments are labelled by a centrifugal order scheme which counts the number of bifurcation points on the path from the root up to the segment. Branching is assumed to occur at terminal segments only. Let $p_s(t)$ be the branching probability per unit of time of the individual terminal segment, $n(t)$ be the expectation of the number of terminal

segments. It was proposed in [31] that

$$\frac{dn(t)}{dt} = n(t)p_s(t), \quad (4.5)$$

or

$$p_s(t) = \frac{d \log n(t)}{dt}. \quad (4.6)$$

In Paper III and Paper IV, we consider a similar model where all the terminal segments grow independently, and the time until splitting is exponentially distributed with rate λ .

5 Main results of the research papers

5.1 Paper I: Linear Dissipative Force as a Result of Discrete Time Collisions

In this paper, we consider two models: one describes the particle movement under the influence of external force and friction (which refers us to Proposition 1.4), and another one describes the movement of a particle, which is acted upon by the same external force but additionally collides with other particles of much lighter masses (which refers us to laws of conservation of energy and momentum in Proposition 1.2). All models are considered in dimension 1, so to describe the movement of the particle we need to know its position and velocity $(x(t), v(t)) \in \mathbb{R}^2$.

Let $(x_0, v_0) \in \mathbb{R}^2$ be the initial coordinate and speed of the (“main”) particle at time $t = 0$. We assume that the mass of this particle is 1 and that the coordinate $x_0 > 0$. Let $F(x, t)$ denote the external force at time $t \geq 0$ and place x . Using Newton’s second law of motion (1.14) we derive the first model as

$$\begin{cases} \frac{dx}{dt} = v, \\ \frac{dv}{dt} = F(x, t) - av, \end{cases} \quad (5.1)$$

with friction force $-av$, which linearly depends on the velocity as in (1.15). Here the dissipation constant we denote as a .

For the second model, we denote the position and the velocity of the main particle as $(\tilde{x}(t), \tilde{v}(t))$ with the same initial conditions $(\tilde{x}(0), \tilde{v}(0)) = (x_0, v_0)$ as in the first model. Suppose that the particle collides with different light particles at certain moments $0 < t_1 < t_2 < \dots < t_n < \dots$. Until the first collision and between any consecutive collisions the

state and the velocity of the particle are governed by the following law:

$$\begin{cases} \frac{d\tilde{x}}{dt} = \tilde{v}, \\ \frac{d\tilde{v}}{dt} = F(\tilde{x}, t), \end{cases} \quad (5.2)$$

$$t < t_1, \quad t_n < t < t_{n+1}, \quad n \geq 1.$$

We assume that $\tilde{x}(t)$ is a continuous function of t , while the velocity $\tilde{v}(t)$ is a right-continuous function with “jumps” at every t_n caused by the elastic collisions described as follows. Let $m_n < 1$ denote the mass of the light particle which collides with the main particle of mass 1 at the moment t_n , and let w_n be the velocity of this light particle at t_n . Define

$$\alpha_n := \frac{1 - m_n}{1 + m_n}, \quad (5.3)$$

and then from Proposition 1.3 we get

$$\tilde{v}(t_n) = \alpha_n \tilde{v}(t_n-) + (1 - \alpha_n) w_n. \quad (5.4)$$

For various examples of external force $F(x, t)$ we find parameters that yield asymptotic equivalence of the velocities of the particle in different models. We also provide conditions when the trajectories of the particles in different models are close to each other in the Chebyshev norm over a certain finite period of time. In almost all cases if masses of the other particles are equal and small $m_n = m \ll 1$, and if the time between $(n - 1)$ -th and n -th collision $\tau_n = t_n - t_{n-1}$ are either equal to some constant τ , or are *i.i.d* positive random variables with mean τ and variance of order $O(\tau)$ then two models are equivalent if

$$\tau = \frac{2m}{a} + O(m^2), \quad (5.5)$$

from which we see that τ should be of order m multiplying by a constant $2/a$. This is a critical scaling for τ .

5.2 Paper II: Scaling of Components in Critical Geometric Random Graphs on 2-dim Torus

In this paper, we study a random graph on the discrete 2-dimensional torus with probabilities of connection

$$p(u, v) = \min \left\{ \frac{c}{N\rho(u, v)}, 1 \right\}, \quad (5.6)$$

which is special case of (3.14) with $d = 2, \alpha = 1$ and $X = \sqrt{c}$. The phase transition for the special case was studied in [8] and [2], and in the general case in [22]. We study the special case in criticality. The main result of this paper is the following theorem.

Theorem 5.1. *Let G_N^c be a random graph on the set of vertices of \mathbb{T}_N^2 with probabilities of connections*

$$p(u, v) = \min \left\{ \frac{c}{N\rho(u, v)}, 1 \right\},$$

where

$$c = c^{cr} = \frac{1}{4 \log 2}$$

is the critical value.

Let $\mathcal{C}_1, \mathcal{C}_2, \dots$ denote the ordered sizes of the connected components in G_N^c with \mathcal{C}_1 being the largest one. Let $\gamma_1, \gamma_2, \dots$ denote the ordered lengths of the excursions of the process

$$B(s) = \widetilde{W}(s) - \min_{0 < t < s} \widetilde{W}(t),$$

where

$$\widetilde{W}(s) = W(s) - \frac{1}{2}s^2 \tag{5.7}$$

with W being the standard Brownian motion. Then

$$\frac{1}{|V_N|^{2/3}} (\mathcal{C}_1, \mathcal{C}_2, \dots) \xrightarrow{d} (\gamma_1, \gamma_2, \dots), \text{ as } N \rightarrow \infty,$$

with respect to l^2 topology on the set of infinite non-decreasing sequences $x = (x_1, x_2, \dots)$ of non-negative values with metric $d(x, y) = \left(\sum_i (x_i - y_i)^2 \right)^{1/2}$.

Comparing the results of Theorem 5.1 and Theorem 3.7 with Theorem 3.2 and Theorem 3.1 we see, that the results for the connected components in the Geometric Graphs on 2-dimensional torus are similar to the classical Erdős-Rényi graphs. Note that this model is outside the class of models of rank 1.

5.3 Paper III: Decay of connection probabilities with distance in 2D and 3D neuronal networks

In this paper, we study a model that imitates how neurons in the brain grow and form connections through synapses. This model was introduced in [3] as a simplified version of the original model in [31]. We note also a similar model in [9], where the axons are modeled as trajectories of stochastic (but not branching as in our case) processes.

We consider a subset V of a closed bounded area in \mathbb{R}^2 or \mathbb{R}^3 . This set represents the centers of neurons. The dynamics for a randomly growing branching tree (axonal tree) of each neuron are independent of other neurons. At time $t = 0$ a segment starts to grow from each neuron, with uniformly distributed random direction and constant speed. Then each segment splits after exponentially distributed time with rate λ into two segments, which continue to grow in the same manner as the first segment and independently of each other. This creates for any $v \in V$ a tree $\mathbf{T}_v(t)$. We say that a neuron v is connected to a neuron u at time t if the distance between $\mathbf{T}_v(t)$ and u is less than some parameter $r > 0$. If the distance between v and u is equal to d , then, since the direction of each segment in the tree is uniformly distributed, the probability of connection depends on parameters t, d, λ, r .

For the case \mathbb{R}^2 an integral equation for the probability of connection was derived in [3]. In this paper, we derived such an equation also for the case \mathbb{R}^3 and computed numerically this probability for different parameters in both cases \mathbb{R}^2 and \mathbb{R}^3 . Our results show that contrary to a common belief, these probabilities do not necessarily decay polynomially or exponentially in distance, but there are regimes of parameter values when the probability of proximity is not sensitive to the distance. In particular, in \mathbb{R}^3 the Euclidean distance between the neuronal cell body centers of neurons seems to play a very subtle role, as the probabilities of connections are practically constant within a certain finite range of distance.

The model has a sufficient number of parameters to assess networks of neurons of different types. Our results give a firm basis for further modelling of the neuronal connectivity taking into account some realistic bouton distributions for establishing synaptic connections.

5.4 Paper iv: Properties of Randomly Grown 2D and 3D Networks

In this paper, we continue studying the model from Paper III. Some properties (such as degree distribution, average shortest path length, and clustering coefficient) have been studied in [1]. While in the original model from Paper III the branches in the tree $\mathbf{T}_v(t)$ always grow and split into two new branches, in this paper we also consider random stops of growth.

In Section 3.1 we derived the integral formula for the probability of connection for the model with stopping times in \mathbb{R}^2 and \mathbb{R}^3 , and found the expectations and the moment generating functions of the total length of all branches of the tree and of the number of branches which have stopped.

In Section 3.2 we derived some numeric results for the probability of connections. It turned out that for some parameters of the model such probability is very weakly dependent not only on distance d between neurons (as we showed on Paper III), but also on time t .

In Section 3.3 we derived an integral formula for the distribution of the distance between the branching point and the root of the tree.

In Section 3.4 we derived the distribution function for the chord length in the condition that a branch intersects a ball with some radius.

In Section 3.5 we derived an integral formula for the expectation of the number of branching points of the tree inside the ball of radius r which is located at distance d from the root of the tree.

6 Future Development

In Paper I we considered Stokes' Law where the dissipation (drag) force depends linearly on the velocity of the particle. One can ask, what if the drag force has the form $-av^2$ (this is true for higher speeds and higher Reynolds number), or has some other dependence on the velocity. We assume that for this kind of force, it will no longer be possible to build a model with elastic collisions, as we did. Perhaps, here it is necessary to take into account the accumulation of particles or their adhesion.

In Paper II we proved the convergence of scaled components to excursion of diffusion process for the particular case of 2-dimensional torus, when $d = 2, \alpha = 1$. As it was reported in [22] the number of triangles in the graph is of order constant if $\alpha < \frac{2}{3}d$. Therefore we assume, that the same proof should work for all $\alpha < \frac{2}{3}d$ and for all $d \geq 2$. But if α becomes close to d , there are different scalings for the number of triangles, then extra terms may arise in (5.7).

In Papers III and IV, in particular, we considered the probabilities of connection between the axon tree of one neuron and dendrites, which are a ball of radius r , of another neuron. In Paper IV, we also considered the properties of the model, in particular, the density of tree vertices. These results should help us in the problem of investigating the probability of connection, if the dendrites, in turn, also represent growing trees. This is especially interesting in the 3-dimensional case because in this case the trees do not intersect with a high probability and we can talk about a potential connection depending on how far apart the trees are. Also of interest is the question of the distribution of the farthest point of the tree from the root, and how this distribution scales depending on time t .

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Scientific publications

Author contributions

Co-authors are abbreviated as follows:

Tatyana Turova (TT).

Paper I: Linear Dissipative Force as a Result of Discrete Time Collisions

The idea for this project was developed by myself. The analysis and proofs were made by myself with regular discussions and guidance from TT. We collaborated on the writing.

Paper II: Scaling of Components in Critical Geometric Random Graphs on 2-dim Torus

TT had the main idea for the project. The analysis and proofs were made by myself with regular discussions and guidance from TT. We collaborated on the writing.

Paper III: Decay of connection probabilities with distance in 2D and 3D neuronal networks

The initial idea for this project was conceived by TT. I deduced the equations and did the simulations. We collaborated on the writing.

Paper IV: Properties of Randomly Grown 2D and 3D Networks

All the work for this project was performed by myself with the general idea suggested by TT.



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