In de verdediging

| In defence

Pas gepromoveerden brengen hun werk onder de aandacht. Heeft u tips voor deze rubriek of bent u zelf pas gepromoveerd? Laat het weten aan onze redacteur.

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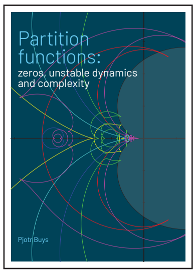

Partition Functions: Zeros, Unstable Dynamics and Complexity
Pjotr Buys

In October 2022, Pjotr Buys from the University of Amsterdam successfully defended his PhD thesis with the title *Partition Functions: Zeros, Unstable Dynamics and Complexity*. Pjotr carried out his research under the supervision of prof. dr. Han Peters (UvA) and dr. Guus Regts (UvA).

From Gases to Magnets on Graphs

Researchers in statistical physics use interaction particle models to understand the behaviour of various systems, for example charged particles in a magnetic field. To describe such systems a positive weight $w(\sigma)$ is assigned to each possible state σ of the system. This means that the probability of observing σ is proportional to its weight, and to find the exact probability you need to normalize. The exact probability is given by $w(\sigma)/Z$, where

$$Z = \sum_{\sigma \in \Sigma} w(\sigma),$$

and Σ is the space of all possible states. This normalizing constant, Z, is called the partition function of the model, and it depends on the parameters of the system at study. The goal is to understand what kind of states are likely to occur. It turns out that these types of questions can be answered by having a good understanding of the partition function and how its properties change as the parameters change. In his thesis Pjotr was interested in two models, the *Ising model* and the *hard-core* model.

Of magnets, sizes, and independence polynomials

The Ising model, introduced by Lenz and Ising around 1920, is used to study magnetism. The underlying structure is a finite simple graph $G=(V,E)$, where the vertices represent particles and the edges represent those pairs of particles that can interact directly (typically those which are close enough to each other). Each particle can be in one of two states, either spin $+$ or $-$. The possible states of the system are therefore described by functions $\sigma : V \to \{+,-\}$.

Pjotr considered the Ising model with two parameters: a magnetic field parameter λ and an interaction parameter b. The weight of a state σ is then equal to

$$w(\sigma) = \lambda^{n_+(\sigma)} b^{\delta(\sigma)},$$

where $n_+(\sigma)$ is the number of vertices that get assigned the spin $+$ under σ, and $\delta(\sigma)$ is the number of edges with differing spins. Here you observe the interplay between the two quantities, when the number of vertices with a positive spin increases the edge-interactions will decrease. The partition function is therefore equal to

$$Z_G^{\mathrm{Is}}(\lambda, b) := \sum_{\sigma : V \to \{+,-\}} \lambda^{n_+(\sigma)} b^{\delta(\sigma)}.$$

If $\lambda \in (0,1)$ the magnetic field points down and states with more particles that have a negative spin are generally more likely. If $\lambda \in (1,\infty)$ the magnetic field points up and states with more particles that have spin + are generally more likely.

The parameter b represents an interaction parameter between neighbouring particles. If $b \in (0,1)$, then neighbouring particles will have with higher probability the same spin. In this case, the model is *ferromagnetic*. If $b \in (1,\infty)$, then neighbouring particles will have with higher probability opposite spins. In this case, the model is called *antiferromagnetic*, which is also the model Pjotr focused on.

In the hard-core model the underlying structure is again a finite simple graph $G=(V,E)$. The vertices represent lattice sites that may or may not be occupied by particles. These particles have a certain size, which prevents two neighbouring sites being occupied. Therefore the possible states are subsets $I \subset V$ such that no pair $u,v \in I$ forms an edge. Such a subset is called an *independent set*. The weight of a state I is equal to $w(I) = \lambda^{|I|}$ for some positive parameter λ, referred to as the *fugacity parameter*. The partition function in this model can thus be written in the following form

$$Z_G^{\text{ind}}(\lambda) = \sum_{I \subset V:\, I \text{ an independent set}} \lambda^{|I|}.$$

This function is also commonly known as the *independence polynomial*.

Experiments in the complex plane

An important quantity when studying these models is called the pressure

$$p_G(\lambda) = \frac{1}{|V|} \cdot \log(Z_G(\lambda)).$$

This logarithmic rescaling of the partition function is important to be able to study its behaviour as the system grows large, since there are exponentially many configurations that correspond to the same observable. The graphs that are relevant from a physical perspective usually are quite structured. The vertices might form part of a lattice for example. Moreover, these graphs typically contain a very large number of vertices. To analyse such large quantities mathematically we would like to speak about the pressure and the density on infinite graphs (usually a lattice $\mathcal{L}$). To make this formal a sequence of finite graphs $G_1, G_2, \ldots$ converging to $\mathcal{L}$ is considered. A famous result in this area is due to Lee and Yang, who showed that the functions p_{G_n} converge to a continuous function $p_{\mathcal{L}}$.

While $p_{\mathcal{L}}$ is continuous on the whole positive real axis, its derivatives may not be. A model is said to undergo a *phase transition* at a parameter λ_0 if $p_{\mathcal{L}}$ is not analytic at λ_0. Lee and Yang gave a condition that is sufficient to guarantee the absence of a phase transition. But this demands a venture in the complex plane! Lee and Yang proved that if $G_1, G_2, \ldots$ is a sequence of graphs converging to a lattice $\mathcal{L}$, and there is a complex domain U that is zero-free for Z_{G_n} for all n, then the limit $p_{\mathcal{L}}$ is analytic on U.

Pjotr investigated what happens when the family of graphs on which the Ising or the hard-core model is considered is the family of bounded degree graphs (the lattice is thus a special case). For an integer $\Delta \in \mathbb{Z}_{\geq 2}$ we let $\mathcal{G}_\Delta$ denote the class of graphs with maximum degree at most Δ. The domain U being zero-free for $\mathcal{G}$ means that $Z_G(\mu) \neq 0$ for any $\mu \in U$ and $G \in \mathcal{G}$.

Understanding the zeros

For the ferromagnetic Ising model this problem is fully solved. The Lee-Yang circle theorem states that the complex zeros of Z_G^{Is} all lie on the unit circle in the complex plane for any graph. This result was refined by Han Peters and Guus Regts, Pjotr's supervisors, who proved that, depending on the degree bound Δ and the interaction parameter b, the closure of the zeros is either equal to the unit circle or equal to a circular arc strictly contained in the unit circle. Pjotr investigated in detail the locations of the zeros of the partition function for the family of bounded degree graphs for both the antiferromagnetic Ising model and the hard-core model.

To understand the zeros of the partition function a new quantity needs to be defined. We consider a graph G and a specific vertex u, and the restrictions of the partition function to those configurations assigning a + or − to u. For the hard-core model the restriction is to those configurations for which u is in (denoted with a +) an independent set or not (denoted with a −). These restrictions are denoted by $Z_{G,+u}(\lambda)$ and $Z_{G,-u}(\lambda)$. A useful quantity to define is the ratio, or occupation ratio, between these contributions, namely

$$R_{G,u}(\lambda) = Z_{G,+u}(\lambda) / Z_{G,-u}(\lambda).$$

This ratio represents the odds that u gets assigned a + (positive spin or present in the independence set). In general, $R_{G,u}$ is a rational function in λ. We can thus interpret $R_{G,u}$ as a function from the Riemann sphere $\hat{C}$ to itself. It follows that complex zeros λ_0 of Z_G correspond one to one with parameters λ_0 for which $R_{G,u}(\lambda_0) = -1$. Understanding the zeros of Z_G is thus essentially equivalent to understanding the -1-parameters of $R_{G,u}$. It turns out that the presence of zeros of Z_G is related to the local dynamical behaviour of the family of occupation ratios defined as

$$R_\Delta = \left\{ Z_{G,+u}(\lambda) / Z_{G,-u}(\lambda) \colon G \text{ a graph of max degree } \Delta \right\}.$$

Using machinery from complex dynamical systems Pjotr investigated when this family of complex functions hits -1, which would yield regions where the partition function attains a zero. Central in Pjotr's research is the theorem of Montel from Complex Analysis. Applying Montel's theorem it can be proven that if U is a zero-free area for the partition functions then the family R_Δ is a normal family of holomorphic functions. In his research Pjotr proved this is an equivalence, hence finding zero-free regions for the partition function is equivalent to proving that the family R_Δ is a normal family. Intuitively this means that the presence of zeros is equivalent to chaotic behavior of this family of partition functions.

Rooted trees show the way

A very important result for both models states that for any (G,u) there exists a rooted tree (T,u) with the same maximum degree as G for which $R_{G,u} = R_{T,u,\tau}$. Here the τ represents a boundary condition on a subset of the leaves of T. Hence it suffices to understand the behaviour of the occupation ratios for rooted trees.

Any rooted tree can be generated by recursively applying a simple scheme, starting with single vertices. It therefore follows that the ratio $R_{G,u}(\lambda)$ of any rooted graph (G,u) of degree at most $d+1$ can be written as a composition of maps $F_{1,\lambda}, \ldots, F_{d,\lambda}$, where

$$F_{k,\lambda}(z_1, z_2, \ldots, z_k) = \lambda \prod_{i=1}^{k} \frac{z_i + b}{b z_i + 1},$$

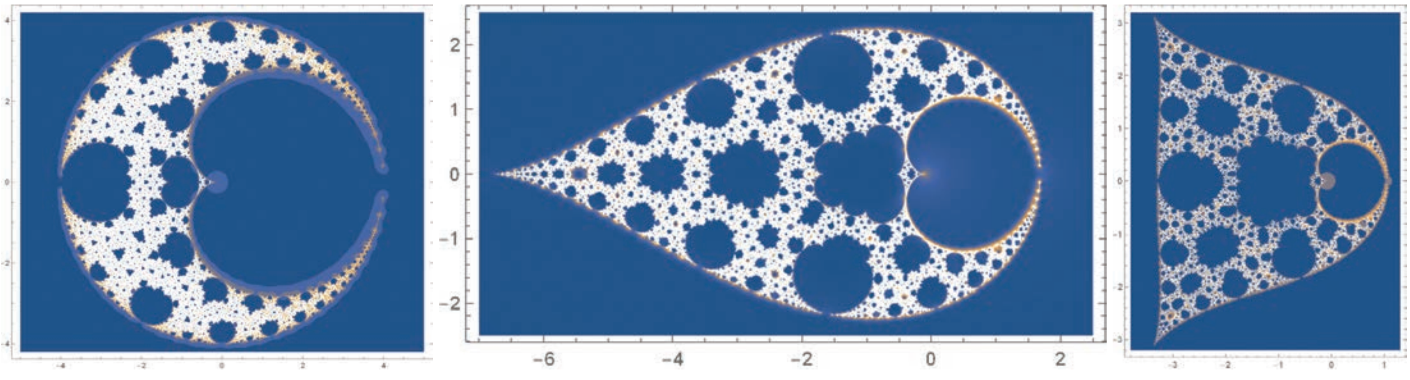

Figure 1 The activity-locus of Cayley trees in the hard-core model for down-degrees $2, 4$ and 3. For each pixel the spherical derivative of the occupation ratio is computed for the Cayley tree of depth 120. Pixels for which this derivative is sufficiently large are depicted in white, suggesting that the corresponding parameter λ lies approximately on the activity locus.

applied to initial values. These initial values are the ratios R_v of single vertices. The iteration of functions with complex parameters is a setting that is common in the field of complex dynamics. Pjotr started by investigating a nicer and more structured class of trees, that of Cayley trees. A perfect d-ary tree is a rooted tree such that every node that is not a leaf has exactly d children, and all the leaves have the same distance to the root.

A delicate argument of complex nature

In the case of the antiferromagnetic Ising model, the closure of the zeros of graphs of perfect d-ary trees is equal to the *non-stable parameters* of the parametrized family $z \mapsto ((z+b)/(bz+1))^d$. This turns out to be equal to the closure of the zeros of all graphs with degree at most $d+1$. In a nutshell, this means that for the antiferromagnetic Ising model it suffices to study Caley trees to understand the zero-free regions of partition functions of arbitrary rooted trees with bounded degree.

But this is not the case for the hard-core model. In the hard core model Pjotr proved that the behaviour of the family R_Δ is radically different for Cayley trees than for arbitrary rooted trees. This is shown in Figure 1, where the blue regions show the values of λ for which the family of Cayley trees are normal. In all pictures consider the large blue cardioid. Pjotr proved that for all values of λ in the cardioid R_Δ is normal for Caley trees. On the other hand, for the family of rooted trees with bounded degrees there exist parameters inside the cardioid at which the family of ratios is not normal. This means that the cardioid is a zero-free region for Caley trees but not for general bounded degree trees.

To compute them or not

Besides the location of zeros of the partition function Pjotr also investigated a very deep connection between these zeros and the computational complexity of approximating the partition function. The difficulty of computing $Z_G(\lambda)$ is motivated by the importance of the partition function in physics, and it started to receive attention from a computer science perspective in the late 1980s. Suppose that a parameter λ lies in a complex domain U containing 0 that is zero-free for $\mathcal{G}_\Delta$. Then there is a fully polynomial time approximation scheme (we will not explain this now) for approximating $Z_G(\lambda)$ for $G \in \mathcal{G}_\Delta$. Pjotr proved that this result is an equivalence, namely that the closure of the complex zeros of the partition function is contained in the closure of parameters λ for which approximating $Z_G(\lambda)$ for $G \in \mathcal{G}_\Delta$ is #P-hard!

The more personal aspect

As a final note we would like to give the word to the doctor.

Pjotr, how did you get interested in mathematics?

"From a very young age I was already interested in solving puzzles, mostly puzzles involving numbers. This interest persisted during my childhood and thus, at the end of high-school, it was clear to me that I wanted to pursue a degree in mathematics (although I did semi-seriously consider classical languages). My interest in research mathematics came during my master thesis, which I did under Guus Regts, who would later become my PhD supervisor. Research mathematics still involves doing puzzles, but these are puzzles for which nobody knows the solution yet. This adds an extra layer of excitement (and sometimes frustration). My favourite part of being a mathematician is working together with colleagues to solve these problems. The longer it takes to solve a problem, the more satisfying it is when you eventually do crack it!"

Were you also involved in some activities you would like to share with the readers?

"My PhD was largely during the pandemic, which made traveling more difficult, but at the start and at the end I did have the opportunity to go to conferences and research visits. I went to Berkeley twice and I spent three weeks in Chicago. At these conferences you get the chance to listen to and speak to people from all over the world that work on the same (or very similar) problems as you do. It is a lot of fun to talk to and make friends with people that are interested in the same obscure things as you are. I once spoke about a conjecture that I had disproved. Afterwards I talked to the person who had made the conjecture. He told me he was happy that there was a resolution to his conjecture, but that he was sad that it was false."

Concluding

To summarize, in his research Pjotr investigated the locations of zeros of the partition function of the Ising model and the hard-core model. He used techniques from complex dynamical systems to prove that the existence of zeros is equivalent to a chaotic behaviour of the family of occupancy ratios due to its non-normality. In regions where this chaotic behaviour rises the partition function is also, loosely speaking, very difficult to approximate. After his PhD Pjotr started a post-doc at the UvA. We wish him the best and we hope that he keeps enjoying his complex wanderings!