INVARIANT GAUSSIAN PROCESSES AND INDEPENDENT SETS ON REGULAR GRAPHS OF LARGE GIRTH

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Abstract. We prove that every 3-regular, n-vertex simple graph with sufficiently large girth contains an independent set of size at least $0.4361n$. (The best known bound is $0.4352n$.) In fact, computer simulation suggests that the bound our method provides is about $0.438n$.

Our method uses invariant Gaussian processes on the d-regular tree that satisfy the eigenvector equation at each vertex for a certain eigenvalue λ. We show that such processes can be approximated by i.i.d. factors provided that $|\lambda| \leq 2\sqrt{d-1}$. We then use these approximations for $\lambda = -2\sqrt{d-1}$ to produce factor of i.i.d. independent sets on regular trees.

1. Introduction

An *independent set* is a set of vertices in a graph, no two of which are adjacent. The *independence ratio* of a graph is the size of its largest independent set divided by the total number of vertices. Let $d \geq 3$ be an integer and suppose that G is a d-regular finite graph with sufficiently large girth, that is, G does not contain cycles shorter than a sufficiently large given length. In other words, G locally looks like a d-regular tree. What can we say about the independence ratio of G?

In a regular (infinite) tree every other vertex can be chosen, so one is tempted to say that the independence ratio should tend to $1/2$ when the girth goes to infinity. This is not the case, however: Bollobás [2] showed that (uniform) random d-regular graphs have essentially large girth (i.e., the number of short cycles is small) and their independence ratios are bounded away from $1/2$ with high probability. Asymptotically (as $d \to \infty$) the independence ratio of the random d-regular graph is $2(\log d)/d$ (the lower bound is due to Frieze and Łuczak [3]). The best known upper bound for random 3-regular graphs is 0.45537 due to McKay [10], who sharpened [2].

Shearer [11] showed that for any triangle-free graph with average degree d the independence ratio is at least

$$\frac{d \log d - d + 1}{(d-1)^2}.$$

For regular graphs of large girth, Shearer himself found an improvement [12]. Lauer and Wolmard further improved that bound for $d \geq 7$ by analyzing a simple greedy algorithm [9]. All of these bounds are the same asymptotically: $(\log d)/d$. For small values of d more sophisticated algorithms have been analyzed using computer-assisted proofs: in his thesis Hoppen presents an approach that outdoes the above-mentioned bounds when $d \leq 10$ [7, Table 5.3.1]. For $d = 3$ Kardoš, Král and Volec improved Hoppen's method and obtained the bound 0.4352 [8]. Compare this to McKay's upper bound 0.45537.

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The above lower bounds are based on local improvements of the standard greedy algorithm. Our main theorem is based on a different approach: we use Gaussian wave functions to find independent sets.

Theorem 1. *Every* 3*-regular graph with sufficiently large girth has independence ratio at least* 0.4361*.*

A related problem is finding induced bipartite subgraphs with a lot of vertices. (Equivalently, we are looking for two disjoint independent sets with large total size.) This problem was studied for random 3-regular graphs in [6, 5].

Theorem 2. *Every* 3*-regular graph with sufficiently large girth has an induced subgraph that is bipartite and that contains at least a*

$$1 - \frac{3}{4\pi} \arccos\left(\frac{5}{6}\right) > 0.86$$

fraction of the vertices.

To illustrate our strategy for proving Theorem 1, suppose that there is a real number assigned to each vertex of G, called the value of the vertex. We always get an independent set by choosing those vertices having larger values than each of their neighbors. If we assign these values to the vertices in some random manner, then we get a random independent set. If the expected size of this random independent set can be computed, then it gives a lower bound on the independence ratio. In many cases, the probability that a given vertex is chosen is the same for all vertices, in which case this probability itself is a lower bound.

The idea is to consider a random assignment that is *almost* an eigenvector (with high probability) with some negative eigenvalue λ. Then we expect many of the vertices with positive values to be chosen. The spectrum of the d-regular tree is $[-2\sqrt{d-1}, 2\sqrt{d-1}]$, so it is reasonable to expect that we can find such a random assignment for $\lambda = -2\sqrt{d-1}$. As we will see, the approach described above can indeed be carried out, and it produces a lower bound

$$\frac{1}{2} - \frac{3}{4\pi} \arccos\left(\frac{1+2\sqrt{2}}{4}\right) \approx 0.4298$$

in the $d = 3$ case. This natural bound is already sharper than all previous bounds that are not computer-assisted.

Using the same random assignment but a more sophisticated way to choose the vertices for our independent set provides a better bound. We fix some threshold $\tau \in \mathbb{R}$, and we only keep those vertices that are below this threshold. We choose τ in such a way that the components of the remaining vertices are small with high probability. We omit the large components and we choose an independent set from each of the small components. (Note that the small components are all trees provided that the girth of the original graph is large enough. Since trees are bipartite, they have an independent set containing at least half of the vertices.) We simulated this random procedure on computer and the probability that a given vertex is in the independent set seems to be above 0.438 in the 3-regular case. The best bound we could obtain with a rigorous proof is 0.4361. The proof is computer-assisted in the sense that we used a computer to find certain numerical integrals.

If one wants to avoid using computers, then one can set $\tau = 0$ and use simple estimates to obtain a bound as good as 0.43. (The best previous bound obtained without the use of computers is 0.4139 and is due to Shearer, see [9, Table 1].) Note that one can also choose an independent set from the vertices above the threshold in the same manner. This other independent set is clearly disjoint from the first one and has the same expected size when $\tau = 0$. This is how Theorem 2 will be obtained.

Random processes on the regular tree. Instead of working on finite graphs with large girth, it will be more convenient for us to consider the regular (infinite) tree and look for independent sets on this tree that are i.i.d. factors.

Let T_d denote the d-regular tree for some positive integer $d \geq 3$, $V(T_d)$ is the vertex set, and $\mathrm{Aut}(T_d)$ is the group of graph automorphisms of T_d. Suppose that we have independent standard normal random variables Z_v assigned to each vertex $v \in V(T_d)$. We call an instance of an assignment a configuration. A *factor of i.i.d. independent set* is a random independent set that is obtained as a measurable function of the configuration and that commutes with the natural action of $\mathrm{Aut}(T_d)$. By a *factor of i.i.d. process* we mean random variables X_v, $v \in V(T_d)$ that are all obtained as measurable functions of the random variables Z_v and that are $\mathrm{Aut}(T_d)$-invariant (that is, they commute with the natural action of $\mathrm{Aut}(T_d)$). Actually, in this paper we will only consider *linear factor of i.i.d. processes* defined as follows.

Definition 1.1. We say that a process X_v, $v \in V(T_d)$ is a *linear factor* of the i.i.d. process Z_v if there exist real numbers $\alpha_0, \alpha_1, \ldots$ such that

$$X_v = \sum_{u \in V(T_d)} \alpha_{d(v,u)} Z_u = \sum_{k=0}^{\infty} \sum_{u : d(v,u)=k} \alpha_k Z_u, \tag{1}$$

where $d(v,u)$ denotes the distance between the vertices v and u in T_d. Note that the infinite sum in (1) converges almost surely if and only if $\alpha_0^2 + \sum_{k=1}^{\infty} d(d-1)^{k-1}\alpha_k^2 < \infty$.

These linear factors are clearly $\mathrm{Aut}(T_d)$-invariant. Furthermore, the random variable X_v defined in (1) is always a centered Gaussian.

Definition 1.2. We call a collection of random variables X_v, $v \in V(T_d)$ a *Gaussian process on T_d* if they are jointly Gaussian and each X_v is centered. (Random variables are said to be jointly Gaussian if any finite linear combination of them is Gaussian.)

Furthermore, we say that a Gaussian process X_v is invariant if it is $\mathrm{Aut}(T_d)$-invariant, that is, for arbitrary graph automorphism $\Phi : V(T_d) \to V(T_d)$ of T_d the joint distribution of the Gaussian process $X_{\Phi(v)}$ is the same as that of the original process.

The following invariant processes will be of special interest for us.

Theorem 3. *For any real number λ with $|\lambda| \leq d$ there exists a non-trivial invariant Gaussian process X_v on T_d that satisfies the eigenvector equation with eigenvalue λ, i.e., (with probability 1) for every vertex v it holds that*

$$\sum_{u \in N(v)} X_u = \lambda X_v,$$

where $N(u)$ denotes the set of neighbors of v.

The joint distribution of such a process is unique under the additional condition that the variance of X_v is 1. We will refer to this (essentially unique) process as the Gaussian wave function *with eigenvalue λ.*

These Gaussian wave functions can be approximated by linear factor of i.i.d. processes provided that $|\lambda| \leq 2\sqrt{d-1}$.

Theorem 4. *For any real number λ with $|\lambda| \leq 2\sqrt{d-1}$ there exist linear factor of i.i.d. processes that converge in distribution to the Gaussian wave function corresponding to λ.*

The Gaussian wave function for negative λ has negative correlations for neighbors. The set where the process takes values below a threshold τ is a percolation process, which – with the right choice of parameters – has high density but no infinite clusters. We will use this percolation to construct independent sets. Our first step, of independent interest, is to bound the critical threshold for this percolation.

Theorem 5. *Let X_v, $v \in T_3$ be the Gaussian wave function with eigenvalue $\lambda = -2\sqrt{2}$, and consider the percolation $S_\tau = \{v \in V(T_d) \ : \ X_v \leq \tau\}$. If $\tau \leq 0.086$, then each cluster of S_τ is finite almost surely. (Note that for $\tau = 0.086$ the density of the percolation is above 0.534, yet the clusters are finite almost surely.)*

Asymptotically, for large values of d, Gamarnik and Sudan [4] have recently showed that factor of i.i.d. processes can only produce independent sets with size at most $1/2 + 1/\sqrt{8}$ times the largest in random regular graphs. This means that upper bounds coming from random regular graphs (such as the Bollobás and McKay bounds) cannot be matched by factor of i.i.d. algorithms.

For $d = 3$, it is an open problem whether the best asymptotic independence ratio can be achieved with factor-of-i.i.d. algorithms such as ours.

The rest of the paper is organized as follows: in Section 2 we prove Theorems 3 and 5, and derive other useful properties of Gaussian wave functions, in Section 3 we give a proof for Theorem 4, and in Section 4 we show how one can use these random processes to find large independent sets.

2. Gaussian wave functions

We call the random variables X_v, $v \in V(T_d)$ a Gaussian process if they are jointly Gaussian and each X_v is centered (see Definition 1.2). The joint distribution is completely determined by the covariances $\operatorname{cov}(X_u, X_v)$, $u, v \in V(T_d)$. A Gaussian process with prescribed covariances exists if and only if the corresponding infinite "covariance matrix" is positive semidefinite.

From this point on, all the Gaussian processes considered will be $\operatorname{Aut}(T_d)$-invariant. For an invariant Gaussian process X_v the covariance $\operatorname{cov}(X_u, X_v)$ clearly depends only on the distance $d(u, v)$ of u and v. (The distance between the vertices u, v is the length of the shortest path connecting u and v in T_d.) Let us denote the covariance corresponding to distance k by σ_k. So an invariant Gaussian process is determined (in distribution) by the the sequence $\sigma_0, \sigma_1, \ldots$ of covariances.

Theorem 3 claims that for any $|\lambda| \leq d$ there exists an invariant Gaussian process that satisfies the eigenvector equation $\sum_{u \in N(v)} X_u = \lambda X_v$ for each vertex v. What would be the covariance sequence of such a *Gaussian wave function*? Let $v_1, \ldots, v_d$ denote the neighbors of an arbitrary vertex v_0. Then

$$0 = \operatorname{cov}(X_{v_0}, 0) = \operatorname{cov}(X_{v_0}, X_{v_1} + \cdots + X_{v_d} - \lambda X_{v_0}) = d\sigma_1 - \lambda\sigma_0.$$

Also, if u is at distance k from v_0, then it has distance $k-1$ from one of the neighbors $v_1, \ldots, v_d$, and has distance $k+1$ from the remaining $d-1$ neighbors of v_0. Therefore

$$0 = \operatorname{cov}(X_u, 0) = \operatorname{cov}(X_u, X_{v_1} + \cdots + X_{v_d} - \lambda X_{v_0}) = (d-1)\sigma_{k+1} + \sigma_{k-1} - \lambda\sigma_k.$$

After multiplying our process with a constant we may assume that the variance of X_v is 1, that is, $\sigma_0 = 1$. So the covariances satisfy the following linear recurrence relation:

$$\sigma_0 = 1;\ d\sigma_1 - \lambda\sigma_0 = 0;\ (d-1)\sigma_{k+1} - \lambda\sigma_k + \sigma_{k-1} = 0,\ k \geq 1. \tag{2}$$

There is a unique sequence σ_k satisfying the above recurrence. Therefore to prove the existence of the Gaussian wave function we only need to check that the corresponding infinite matrix is positive semidefinite. This does not seem to be a straightforward task, though, so we take another approach instead, where we recursively consruct the Gaussian wave function. (This approach will also yield some interesting and useful properties of Gaussian wave functions, see Remark 2.2 and 2.3.)

Remark 2.1. The case $|\lambda| \leq 2\sqrt{d-1}$ also follows from the results presented in the next section, where we construct factor of i.i.d. processes, the covariance matrices of which converge to the "covariance matrix" of the (supposed) Gaussian wave function. As the limit of positive semidefinite matrices, this "covariance matrix" is positive semidefinite, too, and thus the Gaussian wave function indeed exists.

Proof of Theorem 3. Let σ_k be the solution of the recurrence relation (2), in particular,

$$\sigma_0 = 1;\ \sigma_1 = \frac{\lambda}{d};\ \sigma_2 = \frac{\lambda^2 - d}{d(d-1)}.$$

We need to find a Gaussian process X_v, $v \in V(T_d)$ such that

$$\operatorname{cov}(X_u, X_v) = \sigma_{d(u,v)} \tag{3}$$

holds for all $u, v \in V(T_d)$.

We will define the random variables X_v recursively on larger and larger connected subgraphs of T_d. Suppose that the random variables X_v are already defined for $v \in S$ such that (3) is satisfied for any $u, v \in S$, where S is a (finite) set of vertices for which the induced subgraph $T_d[S]$ is connected. Let v_0 be a leaf (i.e., a vertex with degree 1) in $T_d[S]$, v_d denotes the unique neighbor of v_0 in $T_d[S]$, and $v_1, \dots, v_{d-1}$ are the remaining neighbors in T_d. We now define the random variables $X_{v_1}, \dots, X_{v_{d-1}}$. Let $(Y_1, \dots, Y_{d-1})$ be a multivariate Gaussian that is independent from X_v, $v \in S$ and that has a prescribed covariance matrix that we will specify later. Set

$$X_{v_i} \overset{\text{def}}{=} \frac{\lambda}{d-1} X_{v_0} - \frac{1}{d-1} X_{v_d} + Y_i\ ,\ i = 1, \dots, d-1.$$

For $1 \leq i \leq d-1$ we have

$$\operatorname{cov}\left(X_{v_i}, X_{v_0}\right) = \frac{\lambda}{d-1} - \frac{1}{d-1}\sigma_1 = \sigma_1,$$

and if $u \in S \setminus \{v_0\}$ is at distance $k \geq 1$ from x_0, then

$$\operatorname{cov}\left(X_{v_i}, X_u\right) = \frac{\lambda}{d-1}\sigma_k - \frac{1}{d-1}\sigma_{k-1} = \sigma_{k+1}.$$

We also need that

$$\operatorname{var}\left(X_{v_i}\right) = \sigma_0 \ \text{ and } \operatorname{cov}\left(X_{v_i}, X_{v_j}\right) = \sigma_2, \text{ whenever } 1 \leq i, j \leq d-1,\ i \neq j. \tag{4}$$

Since

$$\operatorname{var}\left(X_{v_i}\right) = \left(\frac{\lambda}{d-1}\right)^2 + \left(\frac{1}{d-1}\right)^2 - \frac{2\lambda}{(d-1)^2}\sigma_1 + \operatorname{var}(Y_i) \text{ and}$$
$$\operatorname{cov}\left(X_{v_i}, X_{v_j}\right) = \left(\frac{\lambda}{d-1}\right)^2 + \left(\frac{1}{d-1}\right)^2 - \frac{2\lambda}{(d-1)^2}\sigma_1 + \operatorname{cov}(Y_i, Y_j),$$

we can set $\operatorname{var}(Y_i)$ and $\operatorname{cov}(Y_i, Y_j)$ such that (4) is satisfied, namely let

$$\operatorname{var}(Y_i) = a \overset{\text{def}}{=} \frac{(d-2)(d^2-\lambda^2)}{d(d-1)^2} \text{ and } \operatorname{cov}(Y_i, Y_j) = b \overset{\text{def}}{=} \frac{-(d^2-\lambda^2)}{d(d-1)^2}.$$

We still have to show that there exist Gaussians $Y_1, \ldots, Y_{d-1}$ with the above covariances. The corresponding $(d-1) \times (d-1)$ covariance matrix would have a's in the main diagonal and b's everywhere else. The eigenvalues of this matrix are $a + (d-2)b$ and $a - b$ (with $a - b$ having multiplicity $d - 2$). Therefore the matrix is positive semidefinite if $a \geq b$ and $a \geq -(d-2)b$. It is easy to check that these inequalities hold when $|\lambda| \leq d$. (In fact, $a = -(d-2)b$, so the covariance matrix is singular, which means that there is some linear dependence between $Y_1, \ldots, Y_{d-1}$. Actually, this linear dependence is $Y_1 + \cdots + Y_{d-1} = 0$, and that is why the eigenvector equation $X_{v_1} + \cdots + X_{v_d} = \lambda X_{v_0}$ holds.)

So the random variables X_v are now defined on the larger set $S' = S \cup \{v_1, \ldots, v_{d-1}\}$ such that (3) is satisfied for any $u, v \in S'$. Since

$$\begin{pmatrix} 1 & \sigma_1 \\ \sigma_1 & 1 \end{pmatrix}$$

is positive semidefinite for $|\lambda| \leq d$, we can start with a set S containing two adjacent vertices, and then in each step we can add the remaining $d-1$ vertices of a leaf to S. The statement then follows from the Kolmogorov extension theorem. □

Remark 2.2 (*Markov field property*)**.** There is an important consequence of the proof above, which we will make use of when we will be computing the probability of certain configurations for a particular Gaussian wave function in Section 4. Let u and v be adjacent vertices in T_d. They cut T_d (and thus the Gaussian wave function on it) into two parts. Our proof yields that the two parts of the process are independent under the condition $X_u = x_u; X_v = x_v$ for any real numbers x_u, x_v.

Remark 2.3. If $d = 3$ and $\lambda = -2\sqrt{d-1} = -2\sqrt{2}$, then we have $Y_2 = -Y_1$ in the above proof with $\operatorname{var}(Y_1) = a = 1/12$. So we can express X_{v_1} and X_{v_2} with the standard Gaussian $Z = 2\sqrt{3}Y_1$ as follows:

$$X_{v_1} = -\sqrt{2}X_{v_0} - \frac{1}{2}X_{v_3} + \frac{1}{2\sqrt{3}}Z \text{ and}$$
$$X_{v_2} = -\sqrt{2}X_{v_0} - \frac{1}{2}X_{v_3} - \frac{1}{2\sqrt{3}}Z.$$

Note that Z is independent from the random variables $X_v, v \in S$, in particular, it is independent from X_{v_0}, X_{v_3}.

2.1. **Percolation corresponding to Gaussian wave functions.** Let X_v, $v \in V(T_d)$ be some fixed invariant process on T_d. For any $\tau \in \mathbb{R}$ we define

$$S_\tau \overset{\text{def}}{=} \{v \in V(T_d) \ : \ X_v \leq \tau\},$$

that is, we throw away the vertices above some threshold τ. (If the random variables X_v are independent, then we get the Bernoulli site percolation. Otherwise S_τ is a *dependent percolation.*) One very natural question about this random set S_τ is whether its components are finite almost surely or not. Clearly, there exists a *critical threshold* $\tau_c \in [-\infty, \infty]$ such that for $\tau < \tau_c$ the component of any given vertex is finite almost surely, while if $\tau > \tau_c$, then any given vertex is in an infinite component with some positive probability.

First we explain why it would be extremely useful for us to determine this critical threshold (or bound it from below). Let τ be below the critical threshold τ_c and let I_τ be the "largest" independent set contained by S_τ. More precisely, we choose the largest independent set in each of the (finite) components of S_τ and consider their union. If the largest independent set is not unique, then we choose one in some invariant way. This way we get an invariant independent set I_d. (Moreover, if X_v can be approximated by i.i.d. factors, then so is I_d.) Clearly, the larger τ is, the larger the independent set we get. So we want to pick τ close to the critical threshold.

The next lemma provides a sufficient condition for the components to be finite in the case when our process X_v is a Gaussian wave function. Let us fix a path in T_d containing $m+2$ vertices for some positive integer m and fix the values assigned to the first and second vertex: x and y, respectively. The sufficient condition is roughly the following: for any $x, y \leq \tau$, the conditional probability of the event that the random values assigned to the remaining m nodes are also below τ is less than $1/(d-1)^m$. In fact, the only thing that we will use about Gaussian wave functions is the Markov field property pointed out in Remark 2.2.

Lemma 2.4. *Let $X_v, v \in T_d$ be a Gaussian wave function on T_d and let $v_{-1}, v_0, v_1, \ldots, v_m$ be any fixed path in T_d containing $m+2$ vertices for some positive integer m. Suppose that there exists a real number $c < 1/(d-1)^m$ such that*

$$P\left(X_{v_i} \leq \tau\ ,\ 1 \leq i \leq m | X_{v_{-1}} = x_{v_{-1}}; X_{v_0} = x_{v_0}\right) < c$$

holds for any real numbers $x_{v_{-1}}, x_{v_0} \leq \tau$. Then each component of

$$S_\tau = \{v \in V(T_d)\ :\ X_v \leq \tau\} \subset V(T_d)$$

is finite almost surely.

Proof. Let u be an arbitrary vertex and let us consider the component of u in S_τ. Let s be any positive integer. We want to count the number of vertices in the component at distance $sm+1$ from u. The number of such vertices in T_d is $d(d-1)^{sm}$. For any such vertex w the path from u to w can be split into s paths, each having $m+2$ vertices and each overlapping with the previous and the next one on two vertices. The Gaussian wave function on such a path depends on the previous pathes only through the first two (overlapping) vertices of the path (see Remark 2.2). Using this fact and the assumption of the lemma, one can conclude that the probability that w is in the component is less than c^s. Consequently, the expected number of vertices in the component at distance $sm+1$ from u is at most $d(d-1)^{sm}c^s$, which is exponentially small in s. Thus, by Markov's inequality, the probability that the component has at least one vertex at distance $sm+1$ is exponentially small, too. It follows that each component must be finite with probability 1. □

Now we will use the above lemma to give a lower bound for the critical threshold in the case $d = 3$, $\lambda = -2\sqrt{2}$.

Proof of Theorem 5. Let X_v, $v \in T_3$ be the Gaussian wave function with eigenvalue $\lambda = -2\sqrt{2}$. We need to prove that S_τ has finite components almost surely for $\tau = 0.086$. We will use Lemma 2.4 with $m = 2$. Let us fix a path containing four vertices of T_3, we denote the random variables assigned to the first, second, third, and fourth vertex of the path by X, Y, U, and V, respectively. Let x, y be arbitrary real numbers not more than τ. From now on, every event and probabilitiy will be meant under the condition $X = x; Y = y$. According to Remark 2.3 there exist independent standard normal random variables Z_1, Z_2 such that

$$U = -\sqrt{2}y - \frac{1}{2}x + \frac{1}{2\sqrt{3}}Z_1;$$

$$V = -\sqrt{2}U - \frac{1}{2}y + \frac{1}{2\sqrt{3}}Z_2 = \frac{3}{2}y + \frac{1}{\sqrt{2}}x - \frac{1}{\sqrt{6}}Z_1 + \frac{1}{2\sqrt{3}}Z_2.$$

Our goal is to prove that the probability of $U \le \tau; V \le \tau$ is less than $1/4$ for any fixed $x, y \le \tau$. If we increase y by some positive Δ, and decrease x by $2\sqrt{2}\Delta$ at the same time, then U does not change, while V gets smaller, and thus the probability in question increases. Thus setting y equal to τ and changing x accordingly always yield a higher probability. So from now on we will assume that $y = \tau$. Then

$$U \le \tau \Leftrightarrow Z_1 \le \sqrt{3}x + 2\sqrt{6}\tau + 2\sqrt{3}\tau;$$

$$V \le \tau \Leftrightarrow -Z_1 + \frac{1}{\sqrt{2}}Z_2 \le -\sqrt{3}x - \frac{\sqrt{3}}{\sqrt{2}}\tau.$$

We notice that the sum of the right hand sides does not depend on x:

$$a \overset{\text{def}}{=} \tau\left(2\sqrt{6} + 2\sqrt{3} - \frac{\sqrt{3}}{\sqrt{2}}\right).$$

Therefore we have to maximize the following probability in d_1:

$$P\left(Z_1 \le d_1; Z_2/q \le Z_1 + a - d_1\right), \text{ where } q = \sqrt{2}.$$

This can be expressed as a two-dimensional integral:

$$f(d_1) \overset{\text{def}}{=} \int_{-\infty}^{d_1}\int_{-\infty}^{q(z_1+a-d_1)} \frac{1}{2\pi}\exp\left(-\frac{z_1^2+z_2^2}{2}\right) \mathrm{d}z_2\,\mathrm{d}z_1. \tag{5}$$

To find the maximum of the function $f(d_1)$, we take its derivative, which can be expressed using the cumulative distribution function Φ of the standard normal distribution:

$$f'(d_1) = \frac{1}{\sqrt{2\pi}}\exp\left(\frac{-d_1^2}{2}\right)\Phi(qa) - \frac{\sqrt{1+q^2}}{\sqrt{2\pi}q}\exp\left(\frac{-d_2^2}{2}\right)\Phi\left(\sqrt{1+q^2}a - d_2/q\right),$$

$$\text{where } d_2 = \frac{q}{\sqrt{1+q^2}}(a - d_1).$$

The derivative has a unique root, belonging to the maximum of f. Solving $f'(d_1) = 0$ numerically ($d_1 \approx 0.555487$), then computing the integral (5) (≈ 0.249958) shows that $\max f < 1/4$ as claimed. (Both finding the root of the derivative and computing the integral numerically are easy to do, and $\max f < 1/4$ can be made rigorous using simple error bounds.) □

3. Approximation with factor of i.i.d. processes

Our goal in this section is to prove Theorem 4: there exist linear factor of i.i.d. processes approximating (in distribution) the Gaussian wave function with eigenvalue λ provided that $|\lambda| \leq 2\sqrt{d-1}$. This will follow easily from the next lemma.

Lemma 3.1. *Let $|\lambda| \leq 2\sqrt{d-1}$ be fixed. For a sequence of real numbers $\alpha_0, \alpha_1, \ldots$ we define the sequence $\delta_0, \delta_1, \ldots$ as*

$$\delta_0 \overset{def}{=} d\alpha_1 - \lambda\alpha_0; \;\; \delta_k \overset{def}{=} (d-1)\alpha_{k+1} - \lambda\alpha_k + \alpha_{k-1}, \;\; k \geq 1. \tag{6}$$

Then for any $\varepsilon > 0$ there exists a sequence α_k such that

$$\alpha_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\alpha_k^2 = 1 \text{ and } \delta_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\delta_k^2 < \varepsilon.$$

We can clearly assume that only finitely many α_k are nonzero.

Remark 3.2. We can think of such sequences α_k as invariant approximate eigenvectors on T_d. Let us fix a root of T_d and write α_k on vertices at distance k from the root. Then the vector $f \in \ell_2(V(T_d))$ obtained is spherically symmetric around the root (i.e., f is invariant under automorphisms fixing the root). Furthermore, $\|f\|^2 = \alpha_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\alpha_k^2$.

As for the sequence δ_k, it corresponds to the vector $A_{T_d}f - \lambda f \in \ell_2(V(T_d))$, where A_{T_d} denotes the adjacency operator of T_d. Therefore $\|A_{T_d}f - \lambda f\|^2 = \delta_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\delta_k^2$. So the real content of the above lemma is that for any $\varepsilon > 0$ there exists a spherically symmetric vector $f \in \ell_2(V(T_d))$ such that $\|f\| = 1$ and $\|A_{T_d}f - \lambda f\| < \varepsilon$.

In the best scenario $\delta_k = 0$ would hold for each k, that is, α_k would satisfy the following linear recurrence:

$$d\alpha_1 - \lambda\alpha_0 = 0; (d-1)\alpha_{k+1} - \lambda\alpha_k + \alpha_{k-1} = 0, \;\; k \geq 1. \tag{7}$$

However, for a non-trivial solution α_k of the above recurrence we always have $\alpha_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\alpha_k^2 = \infty$. This follows from the fact that the point spectrum of A_{T_d} is empty.

First we show how Theorem 4 follows from the above lemma.

Proof of Theorem 4. Let Z_v, $v \in V(T_d)$ be independent standard normal random variables. Let $\varepsilon > 0$ and let α_k as in Lemma 3.1. Let X_v be the linear factor of Z_v with coefficients α_k as in (1). Then

$$\operatorname{var}(X_v) = \alpha_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\alpha_k^2 = 1.$$

Let v_0 be an arbitrary vertex with neighbors $v_1, \ldots, v_d$. It is easy to see that

$$X_{v_1} + \ldots + X_{v_d} - \lambda X_{v_0} = (d\alpha_1 - \lambda\alpha_0)Z_{v_0} + \sum_{k=1}^{\infty} \sum_{u:d(v_0,u)=k} \left((d-1)\alpha_{k+1} - \lambda\alpha_k + \alpha_{k-1}\right) Z_u.$$

So $X_{v_1} + \ldots + X_{v_d} - \lambda X_{v_0}$ is also a linear factor with coefficients δ_k as defined in (6). Therefore the variance of $X_{v_1} + \ldots + X_{v_d} - \lambda X_{v_0}$ is $\delta_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\delta_k^2 < \varepsilon$.

What can we say about the covariance sequence σ_k of the Gaussian process X_v? We have $\sigma_0 = 1$ and

$$|d\sigma_1 - \lambda\sigma_0|, |(d-1)\sigma_{k+1} - \lambda\sigma_k + \sigma_{k-1}| \leq \sqrt{\operatorname{var}(X_u)\operatorname{var}\left(X_{v_1} + \cdots + X_{v_d} - \lambda X_{v_0}\right)} < \sqrt{\varepsilon}.$$

In other words, the equations in (2) hold with some small error $\sqrt{\varepsilon}$. If K is a positive integer and $\delta > 0$ is a real number, then for sufficiently small ε we can conclude that for $k \leq K$ the covariance σ_k is closer than δ to the actual solution of (2). It follows that if ε tends to 0, then the covariance sequence of X_v pointwise converges to the unique solution of (2). It follows that X_v converges to the Gaussian wave function in distribution as $\varepsilon \to 0$. □

Proof of Lemma 3.1. It is enough to prove the statement for $|\lambda| < 2\sqrt{d-1}$, the case $\lambda = \pm 2\sqrt{d-1}$ then clearly follows. Excluding $\pm 2\sqrt{d-1}$ will spare us some technical difficulties.

Let β_k be a solution of the following recurrence

$$d\beta_1 - \lambda\sqrt{d-1}\beta_0 = 0; \beta_{k+1} - \frac{\lambda}{\sqrt{d-1}}\beta_k + \beta_{k-1} = 0,\ k \geq 1. \tag{8}$$

(This is the recurrence that we would get from (7) had we made the substitution $\beta_k = (d-1)^{k/2}\alpha_k$.) Since $|\lambda| < 2\sqrt{d-1}$, the quadratic equation $x^2 - \frac{\lambda}{\sqrt{d-1}}x + 1 = 0$ has two complex roots, both of norm 1, which implies that (8) has bounded solutions. Set

$$\alpha_k \overset{\text{def}}{=} \varrho^k (d-1)^{-k/2}\beta_k \tag{9}$$

for some positive real number $1/2 \leq \varrho < 1$. Since β_k is bounded, $\alpha_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\alpha_k^2$ is finite for any $\varrho < 1$. It is also easy to see that $\alpha_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\alpha_k^2$ tends to infinity as $\varrho \to 1-$. Furthermore,

$$\delta_k = (d-1)\alpha_{k+1} - \lambda\alpha_k + \alpha_{k-1} = (d-1)^{-(k-1)/2}\varrho^k\left(\varrho\beta_{k+1} - \frac{\lambda}{\sqrt{d-1}}\beta_k + \varrho^{-1}\beta_{k-1}\right) =$$

$$(d-1)^{-(k-1)/2}\varrho^k(\underbrace{\beta_{k+1} - \frac{\lambda}{\sqrt{d-1}}\beta_k + \beta_{k-1}}_{0} + (\varrho-1)\beta_{k+1} + (\varrho^{-1}-1)\beta_{k-1}).$$

Thus

$$\sum_{k\geq 1} d(d-1)^{k-1}\delta_k^2 \leq d\sum_{k\geq 1}\varrho^{2k}\left((\varrho-1)\beta_{k+1} + (\varrho^{-1}-1)\beta_{k-1}\right)^2.$$

Using that $\varrho^{-1} - 1 = (1-\varrho)/\varrho \leq 2(1-\varrho)$ and the fact that β_k is bounded we obtain that

$$\sum_{k\geq 1} d(d-1)^{k-1}\delta_k^2 \leq C(1-\varrho)^2\sum_{k\geq 1}\varrho^{2k} = C(1-\varrho)^2\frac{\varrho^2}{1-\varrho^2} = C\frac{\varrho^2}{1+\varrho}(1-\varrho) \leq C(1-\varrho),$$

where C might depend on d and λ, but not on ϱ. Therefore the above sum tends to 0 as $\varrho \to 1-$. A similar calculation shows that $\delta_0 \to 0$, too. Therefore $\delta_0^2 + \sum_{k\geq 1} d(d-1)^{k-1}\delta_k^2 \to 0$. Choosing ϱ sufficiently close to 1 and rescaling α_k completes the proof. □

4. Independent sets

In this section we explain how one can find large independent sets in d-regular, large-girth graphs using the Gaussian wave functions on T_d and their linear factor of i.i.d. approximations.

Let X_v be a linear factor of i.i.d. process on the d-regular tree T_d that has only finitely many nonzero coefficients:

$$X_v = \sum_{k=0}^{N} \sum_{u:d(v,u)=k} \alpha_k Z_u, \text{ where } \alpha_0, \alpha_1, \dots, \alpha_N \in \mathbb{R}. \tag{10}$$

We will present different ways to produce independent sets on T_d using the random variables X_v. In each case the decision whether a given vertex v is chosen for the independent set will depend (in a measurable and invariant way) only on the values of the random variables X_u, $|d(v,u)| < N'$, where N' is some fixed constant. Therefore the obtained random independent set will be a factor of the i.i.d. process Z_v. Moreover, whether a given vertex v is chosen will depend only on the values in the $N + N'$-neighborhood of v. It follows that the same random procedure can be carried out on any d-regular finite graph provided that its girth is sufficiently large, and the probability that a given vertex is chosen will be the same.

So we can work on T_d (instead of graphs with sufficiently large girth). We will choose the coefficients $a_0, \dots, a_N$ in such a way that the process (10) approximates the Gaussian wave function with eigenvalue $\lambda = -2\sqrt{d-1}$ (see Theorem 4). In the limit we can actually replace the underlying process X_v with the Gaussian wave function. So from this point on, let X_v, $v \in V(T_d)$ denote the Gaussian wave function with eigenvalue $-2\sqrt{d-1}$. We will define random independent sets on T_d that are measurable and invariant functions of this process X_v. Then the probability p that v is in the independent set is the same for every vertex v. We will call this probability p the *size* of the random independent set. (If we replace the underlying Gaussian wave function X_v with an approximating process in the form (10), but otherwise use the same measurable and invariant way to produce a random independent set from the underlying process, then we get a factor of i.i.d. independent set with size arbitrarily close to p. Once we work with processes like (10), we can carry out the procedure on finite regular graphs as well provided that the girth is sufficiently large. Thus for any $\varepsilon > 0$ and for any n-vertex, d-regular graph G with girth sufficiently large (depending on ε) we have a random independent set in G with expected size at least $(p - \varepsilon)n$. It means that the lim inf (as the girth goes to infinity) of the independence ratio is at least p.)

Our method works best when the degree d is equal to 3.

4.1. **The 3-regular case.** Let $d = 3$, then $\lambda = -2\sqrt{d-1} = -2\sqrt{2}$ and the covariance sequence of X_v is

$$\sigma_0 = 1; \sigma_1 = \frac{-2\sqrt{2}}{3}; \sigma_2 = \frac{5}{6}; \dots.$$

First approach. We choose those vertices v for which $X_v > X_u$ for each neighbor $u \in N(v)$.

We need to compute the probability

$$P\left(X_{v_0} > X_{v_1}; X_{v_0} > X_{v_2}; X_{v_0} > X_{v_3}\right),$$

where v_0 is an arbitrary vertex with neighbors v_1, v_2, v_3. We will use the fact that if (Y_1, Y_2, Y_3) is a non-degenerate multivariate Gaussian, then the probability that each Y_i is positive can be expressed in terms of the pairwise correlations as follows:

$$P\left(Y_1 > 0; Y_2 > 0; Y_3 > 0\right) = \frac{1}{2} - \frac{1}{4\pi} \sum_{1 \le i < j \le 3} \arccos\left(\operatorname{corr}(Y_i, Y_j)\right). \tag{11}$$

Indeed, the probability on the left can be expressed as the standard Gaussian measure of the intersection of three half-spaces through the origin. This, in turn, equals the relative area of a spherical triangle with angles $\pi - \arccos\left(\mathrm{corr}(Y_i, Y_j)\right)$, which is given by the standard formula (11).

Let $Y_i = X_{v_0} - X_{v_i}$, $i = 1, 2, 3$, then we have

$$\mathrm{corr}(Y_1, Y_2) = \frac{\mathrm{cov}(Y_1, Y_2)}{\sqrt{\mathrm{var}(Y_1)\,\mathrm{var}(Y_2)}} = \frac{1 + \sigma_2 - 2\sigma_1}{2 - 2\sigma_1} = \frac{11 + 8\sqrt{2}}{12 + 8\sqrt{2}} = \frac{1 + 2\sqrt{2}}{4}.$$

The two other correlations are the same, therefore

$$P\left(v_0 \text{ is chosen}\right) = \frac{1}{2} - \frac{3}{4\pi} \arccos\left(\frac{1 + 2\sqrt{2}}{4}\right) = 0.4298245...$$

So by simply choosing each vertex that is larger than its neighbors, we get an independent set of size larger than 0.4298. Note that we could choose the vertices that are smaller than their neighbors and would get an independent set of the same size. Moreover, these two independent sets are clearly disjoint.

Second approach. We fix some threshold $\tau \in \mathbb{R}$ and we delete those vertices v for which $X_v > \tau$, then we consider the connected components of the remaining graph. If a component is small (its size is at most some fixed N'), then we choose an independent set of size at least half the size of the component. We can do this in a measurable and invariant way. For example, we partition the component into two independent sets (this partition is unique, since each component is connected and bipartite), if one is larger than the other, we choose the larger, if they have equal size, we choose the one containing the vertex with the largest value in the component. If a component is large, then we simply do not choose any vertex from that component. (The idea is to set the parameter τ in such a way that the probability of large components is very small.)

We used a computer to simulate the procedure described above. Setting $\tau = 0.12$ and $N' = 200$ the simulation showed that the probability that a given vertex is chosen is above 0.438. In what follows we will provide rigorous (but – in the case of the best result – computer-assisted) estimates of this probability.

From this point on, we will assume that τ is below the critical threshold, that is, each component is finite almost surely. It follows that with probability arbitrarily close to 1 the component of any given vertex has size at most N' provided that N' is sufficiently large. Let p_s denote the probability that the component of a given vertex has size s. (If a vertex is deleted, then we say that its component has size 0. Thus p_0 is simply the probability that $X_v > \tau$.) If a component has size $2k - 1$ for some $k \geq 1$, then we choose at least k vertices from the component. If a component contains an even number of vertices, then we choose at least half of the vertices. Thus the probability that a vertex is chosen (in the limit as $N' \to \infty$) is at least

$$\sum_{k=1}^{\infty} \frac{k}{2k-1} p_{2k-1} + \frac{1}{2}\left(1 - p_0 - \sum_{k=1}^{\infty} p_{2k-1}\right) = \frac{1}{2}(1 - p_0) + \sum_{k=1}^{\infty} \frac{1}{2(2k-1)} p_{2k-1}. \tag{12}$$

The main difficulty in this approach is to determine (or estimate) the probabilities p_{2k-1} (each can be expressed as an integral of a multivariate Gaussian, where the domain of the integration is an unbounded polyhedron). These integrals can be computed with high precision using a computer (up to p_5).

$\boxed{\tau = 0}$ First we discuss what bound can be obtained with no computer assistance whatsoever. If we set $\tau = 0$, then clearly $p_0 = 1/2$. We can even compute the exact value of p_1. We notice that $X_{v_1} > 0$, $X_{v_2} > 0$ and $X_{v_3} > 0$ imply that $X_{v_0} < 0$, because we have a Gaussian wave function with negative eigenvalue. Thus using (11) we obtain

$$p_1 = P\left(X_{v_0} \leq 0; X_{v_1} > 0; X_{v_2} > 0; X_{v_3} > 0\right) = P\left(X_{v_1} > 0; X_{v_2} > 0; X_{v_3} > 0\right) = \frac{1}{2} - \frac{3}{4\pi}\arccos\left(\mathrm{corr}(X_{v_1}, X_{v_2})\right) = \frac{1}{2} - \frac{3}{4\pi}\arccos\left(\frac{5}{6}\right).$$

Using this and the trivial estimates $p_{2k-1} > 0$ for $k \geq 2$, (12) yields the following lower bound:

$$\frac{1}{2} - \frac{3}{8\pi}\arccos\left(\frac{5}{6}\right) = 0.4300889...$$

As far as the authors know, this is the best bound that is not computer-aided.

Doing the same for vertices above the threshold (i.e., vertices with positive values) clearly results in an another independent set that has the same size and that is disjoint from the other independent set. The induced subgraph on the union of these two disjoint independent sets is a bipartite graph. This proves Theorem 2.

$\boxed{\tau = 0.086}$ Here we discuss how we obtained the bound 0.4361 stated in Theorem 1. We set $\tau = 0.086$ (the largest τ for which we know the components to be finite almost surely, see Theorem 5). Then $p_0 = 1 - \Phi(0.086) = 0.46573321...$, where Φ is the cumulative distribution function of the standard Gaussian. Given a fixed path containing s vertices of T_3, p'_s denotes the probability that the path is a component.

For any $k \geq 2$ the number of paths with $2k-1$ vertices through any given vertex is $(2k-1)\cdot 3 \cdot 4^{k-2}$. Furthermore, a component with 3 vertices must be a path, therefore we have the following relations between p_{2k-1} and p'_{2k-1}:

$$p_1 = p'_1;\ p_3 = 9p'_3;\ p_{2k-1} \geq (2k-1)\cdot 3 \cdot 4^{k-2} p'_{2k-1},\ k \geq 2. \tag{13}$$

As explained in the appendix, the probabilities p'_s can be expressed as integrals. Although the occurring integrals cannot be computed analytically, the approximate values of p'_1, p'_3, and p'_5 can be determined by numerical integration:

$$p'_1 \approx 0.3272861614;\ p'_3 \approx 0.0025551311;\ p'_5 \approx 0.0002640467.$$

Therefore

$$p_1 = p'_1 \approx 0.3272861614;\ p_3 = 9p'_3 \approx 0.0229961799;\ p_5 \geq 60p'_5 \approx 0.0158428.$$

Then the resulting lower bound for (12)

$$\frac{1}{2}(1-p_0) + \frac{1}{2}p_1 + \frac{1}{6}p_3 + \frac{1}{10}p_5 \geq 0.5(1-p_0) + 0.5p'_1 + 1.5p'_3 + 6p'_5 \approx 0.43619355. \tag{14}$$

We proved that the overall error is less than 0.000082, therefore the obtained bound is certainly above 0.4361. (See the appendix for details on the numerical integration and the error bound.)

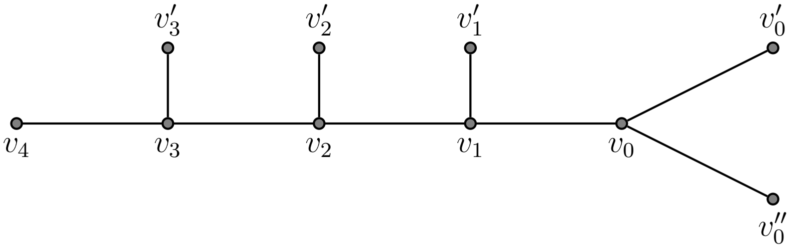
Remark 4.1. The same numerical integrations can be carried out when $\tau = 0$, and thus one can get non-trivial estimates for p_3 and p_5 in that case, too. This way the bound in Theorem 2 can actually be improved to 0.868.

4.2. **The $d \geq 4$ case.** The methods presented above for finding independent sets in T_3 work for regular trees with higher degree, too. However, computing the occurring integrals even numerically (with the required precision) seems very hard. According to our computer simulation the second approach with $\tau = 0.04$ would yield a lower bound 0.3905 for $d = 4$, but we cannot prove this bound rigorously. Note that the current best bound is 0.3901 [7, Table 5.3.1]. When the degree is higher than 4, our approach is not as efficient as previous approaches in the literature.

5. Appendix

Let us consider the Gaussian wave function with eigenvalue $\lambda = -2\sqrt{2}$ on the 3-regular tree T_3. We delete the vertices with value more than τ for some fixed positive real number τ and consider the components of the remaining vertices. For an integer s let p_s denote the probability that the component of a given vertex has size s. These probabilities were used in Section 4 to bound the independence ratio of 3-regular, large-girth graphs, see (12). Therefore, to get actual bounds, we need to determine (or estimate) p_s. In what follows we will explain how p_s can be expressed as an integral in a way that the integration can be performed numerically with high precision (at least for small integers s).

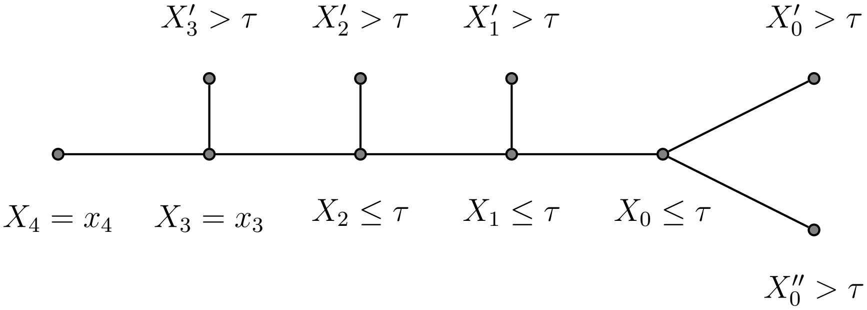
5.1. **Expressing p_s as integrals.** Let $k \geq 0$ be an integer and let us fix a path in T_3 with $k+2$ vertices: $v_0, v_1, \ldots, v_{k+1}$. For $1 \leq i \leq k$ the neighbor of v_i different from v_{i-1} and v_{i+1} is denoted by v_i', while the two neighbors of v_0 different from v_1 are v_0' and v_0''. The random variables (in the Gaussian wave function) assigned to v_i, v_i' and v_i'' will be denoted by X_i, X_i' and X_i'', respectively.



We define the function $f_k : \mathbb{R}^2 \to [0,1]$ as the following conditional probability:

$$f_k(x_{k+1}, x_k) = P\left(X_i \leq \tau, 0 \leq i \leq k-1; X_i' > \tau, 0 \leq i \leq k; X_0'' > \tau | X_{k+1} = x_{k+1}; X_k = x_k\right).$$

The figure below shows the case $k = 3$.



There is a recursive integral formula for these functions. According to Remark 2.3 there exists a standard Gaussian Z_k independent from X_{k+1}, X_k such that

$$X_{k-1} = -\sqrt{2}X_k - \frac{1}{2}X_{k+1} - \frac{1}{2\sqrt{3}}Z_k \text{ and}$$
$$X'_k = -\sqrt{2}X_k - \frac{1}{2}X_{k+1} + \frac{1}{2\sqrt{3}}Z_k.$$

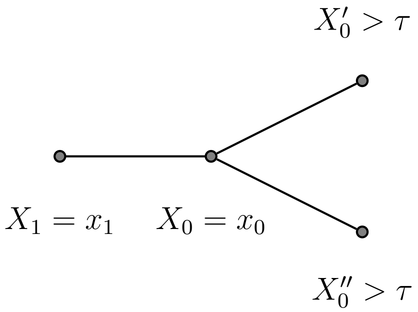
This yields the following formula for the conditional probability $f_k(x_{k+1}, x_k)$ for $k \geq 1$:

$$(15) \quad f_k(x_{k+1}, x_k) = \int_{|2\sqrt{6}x_k+\sqrt{3}x_{k+1}+2\sqrt{3}\tau|}^{\infty} \phi(z_k) f_{k-1}\left(x_k, -\sqrt{2}x_k - \frac{1}{2}x_{k+1} - \frac{1}{2\sqrt{3}}z_k\right) \mathrm{d}z_k,$$

where $\phi(t) = e^{-t^2/2}/\sqrt{2\pi}$ is the density function of the standard normal distribution. As for the case $k = 0$ (see the figure below), we have

$$f_0(x_1, x_0) = \int_{2\sqrt{6}x_0+\sqrt{3}x_1+2\sqrt{3}\tau}^{-(2\sqrt{6}x_0+\sqrt{3}x_1+2\sqrt{3}\tau)} \phi(z_0)\,\mathrm{d}z_0.$$

(We use the convention that $\int_a^b$ is 0 whenever $a > b$.)



So

$$(16) \quad f_0(x_1, x_0) = g_0(2\sqrt{6}x_0 + \sqrt{3}x_1 + 2\sqrt{3}\tau), \text{ where } g_0(t) = \begin{cases} 1 - 2\Phi(t) & \text{if } t < 0 \\ 0 & \text{otherwise.} \end{cases}$$

(Here Φ denotes the cumulative distribution function of the standard normal distribution.)

For a positive integer s let us fix a path in T_3 containing s vertices. Then p'_s will denote the probability that this path is a component, that is, the values on the vertices of the path are all below τ and the values on all the adjacent vertices are above τ. (See (13) for the relation between p_s and p'_s.) In view of Remark 2.2, the probabilities p'_s can be expressed with the functions f_k as follows: if $s \geq 2$, then for any integer $0 \leq m \leq s-2$

$$(17) \quad p'_s = \int_{-\infty}^{\tau}\int_{-\infty}^{\tau} \phi_2(u,v) f_m(u,v) f_{s-2-m}(v,u)\,\mathrm{d}v\,\mathrm{d}u,$$

where ϕ_2 is the density function of the 2-dimensional centered normal distribution with covariance matrix $\begin{pmatrix} 1 & \sigma_1 \\ \sigma_1 & 1 \end{pmatrix}$, where $\sigma_1 = -2\sqrt{2}/3$. As for $s = 1$,

$$p_1 = p'_1 = \int_{\tau}^{\infty}\int_{-\infty}^{\tau} \phi_2(u,v) f_0(u,v)\,\mathrm{d}v\,\mathrm{d}u.$$

Our goal is to find the value of p'_1, p'_3 and p'_5. Using (17) with $s=3, m=0$ and $s=5, m=1$:

$$p'_3 = \int_{-\infty}^{\tau} \int_{-\infty}^{\tau} \phi_2(u,v) f_0(u,v) f_1(v,u) \, \mathrm{d}v \, \mathrm{d}u,$$
$$p'_5 = \int_{-\infty}^{\tau} \int_{-\infty}^{\tau} \phi_2(u,v) f_1(u,v) f_2(v,u) \, \mathrm{d}v \, \mathrm{d}u.$$

5.2. **Numerical integration and bounding the error.** Next we explain how the above integrals (expressing p'_1, p'_3, and p'_5) can be computed numerically. We first have to compute the functions f_0, f_1, f_2. We will store their (approximate) values at the points of a fine grid, and we treat them as if they were 0 outside some bounded region. Once we know f_k, the value of f_{k+1} at each point can be obtained as a one-dimensional integral, see (15). We divide the interval of integration into little pieces and on each piece $[x, x+\delta]$ we approximate the integral using the *trapezoid rule*:

$$\int_x^{x+\delta} f(t) \, \mathrm{d}t \approx \delta \frac{f(x) + f(x+\delta)}{2}.$$

When computing $f_{k+1}(\mathbf{x})$ at some point $\mathbf{x} \in \mathbb{R}^2$ on our grid, we need the values of f_k at points that are not on our grid. These values are interpolated from the values at the closest grid points in a bilinear way in the two coordinates. Once we have computed f_0, f_1, and f_2, the final (two-dimensional) integrals are calculated using the two-dimensional version of the trapezoid rule. The overall run-time is cubic in the resolution of the grid. We have to choose our grid carefully to get a reasonable run-time and reach the needed precision.

Next, we explain how to estimate the numerical error, which comes from the following five sources:

- truncation of the region of integration,
- error in the trapezoid rule,
- using interpolated values of some functions,
- floating point errors, and
- errors carried over from previous integration.

The function f_0 can be expressed in terms of the cumulative distribution function of the standard normal distribution Φ, see (16). According to (15) the value f_{k+1} at some point $\mathbf{x} \in \mathbb{R}^2$ is defined as a (one-dimensional) integral of the following form:

$$f_{k+1}(\mathbf{x}) = \int_{|\mathbf{c}^T\mathbf{x}+d|}^{\infty} \phi(z) f_k(A\mathbf{x} + \mathbf{b}z) \, \mathrm{d}z, \tag{18}$$

where A is a 2×2 matrix, $\mathbf{b}$, $\mathbf{c}$ are two-dimensional vectors, and d is a real number. It is clear from (16) that $0 \le f_0(\mathbf{x}) \le 1$. It easily follows by induction that

$$0 \le f_k(\mathbf{x}) \le 2^{-k} \text{ for all } \mathbf{x} \in \mathbb{R}^2.$$

Thus when we change the interval of integration in (18) to $\left[|\mathbf{c}^T\mathbf{x} + d|, R\right]$ for some $R > 0$, we make an error less than the tail probability of a standard Gaussian, which can be bounded as follows:

$$\int_R^{\infty} \phi(z) \, \mathrm{d}z \le \frac{e^{-R^2/2}}{R\sqrt{2\pi}}.$$

Let us now turn to the error of the trapezoid rule. If f is doubly differentiable on the interval $[x, x+\delta]$, then

$$\int_x^{x+\delta} f(t)\,\mathrm{d}t = \delta \frac{f(x)+f(x+\delta)}{2} - \frac{\delta^3}{12} f''(\xi)$$

for some $\xi \in [x, x+\delta]$, see [1, p. 216]. So whenever we have a good uniform bound for $|f''|$ on the interval $[x, x+\delta]$, the trapezoid rule gives a good approximation of the integral:

$$\left| \int_x^{x+\delta} f(t)\,\mathrm{d}t - \delta \frac{f(x)+f(x+\delta)}{2} \right| \leq \frac{\delta^3}{12} \sup_{\xi \in [x,x+\delta]} |f''(\xi)|\,.$$

Unfortunately, in our case f is not always twice differentiable: the absolute value in the integration bound in (18) causes the first derivative to jump. This, however, occurs "rarely" and for those intervals we may use the following weaker bound relying only on the first derivative:

$$\left| \int_x^{x+\delta} f(t)\,\mathrm{d}t - \delta \frac{f(x)+f(x+\delta)}{2} \right| \leq \frac{\delta^2}{3} \sup_{\xi \in [x,x+\delta]} |f'(\xi)|\,.$$

Before we can use these estimates, we need to bound the derivatives of $\phi(z) f_k(A\mathbf{x}+\mathbf{b}z)$ for any fixed $\mathbf{x}$. We start with the derivatives of f_0, f_1, and f_2. These are functions of two variables that are defined recursively by integrals. We have found the following uniform bounds for the ℓ_2 norm of the gradient vector ∂f_k and the $\ell_2 \to \ell_2$ operator norm of the Hessian matrix Hf_k (whenever it exists):

$$\begin{aligned} &\sup_{\mathbf{x}} \|\partial f_0(\mathbf{x})\| \leq 4.2, && \sup_{\mathbf{x}} \|\partial f_1(\mathbf{x})\| \leq 5.9, && \sup_{\mathbf{x}} \|\partial f_2(\mathbf{x})\| \leq 6.4, \\ &\sup_{\mathbf{x}} \|H f_0(\mathbf{x})\| \leq 13.1, && \sup_{\mathbf{x}} \|H f_1(\mathbf{x})\| \leq 96.1, && \sup_{\mathbf{x}} \|H f_2(\mathbf{x})\| \leq 252.8. \end{aligned}$$

On the other hand, for any fixed $\mathbf{x}$ we have the following for the first and second derivative of $\phi(z) f_k(A\mathbf{x}+\mathbf{b}z)$ (with respect to z):

$$\begin{aligned} \left| (\phi(z) f_k(A\mathbf{x}+\mathbf{b}z))' \right| &\leq |\phi(z)| \cdot \|(\partial f_k)(A\mathbf{x}+\mathbf{b}z)\| \cdot \|\mathbf{b}\| + |\phi'(z)| \cdot |f_k(A\mathbf{x}+\mathbf{b}z)|\,, \\ \left| (\phi(z) f_k(A\mathbf{x}+\mathbf{b}z))'' \right| &\leq |\phi(z)| \cdot \|(H f_k)(A\mathbf{x}+\mathbf{b}z)\| \cdot \|\mathbf{b}\|^2 + \\ &\qquad 2\,|\phi'(z)| \cdot \|(\partial f_k)(A\mathbf{x}+\mathbf{b}z)\| \cdot \|\mathbf{b}\| + |\phi''(z)| \cdot |f_k(A\mathbf{x}+\mathbf{b}z)|\,. \end{aligned}$$

Now we are in a position to estimate the integration error when calculating $f_{k+1}(\mathbf{x})$ in (18). We have to add up errors of the trapezoid rule on every small interval. After replacing all $|f_k|$, $\|\partial f_k\|$, and $\|H f_k\|$ with the uniform bounds we have found, it remains to add up $|\phi(\xi_i)|$ where ξ_i is a point from the i-th interval (and similarly for ϕ' and ϕ''). Even though the points ξ_i are not explicitly given, we can estimate these sums using the following simple observation: for a fixed interval length δ and a continuous function f with total variation $V(f) < \infty$ we have

$$\delta \sum_i |f(\xi_i)| \leq \int |f| + \delta V(f).$$

The interpolation errors can be treated similarly. When we calculate f_{k+1} at a grid point $\mathbf{x}$, we need values of f_k at points $A\mathbf{x}+\mathbf{b}z$ where z runs through the points of a one-dimensional grid. Since the values of f_k are given only at the points of our grid, we need to interpolate from the values at those points. Errors coming from such interpolations can be easily bounded using the first and second derivatives, and thus can be treated the same way as errors of the trapezoid rule.

If we carry out the above calculations using a computer, we get an approximate value for f_k at each grid point $\mathbf{x}$. Let us denote this calculated version of f_k by $\hat{f}_k$. We will also use the notation $\tilde{f}_k$, which is the calculated version of f_k assuming that the computer "knows" f_{k-1} precisely at each grid point and that the computer can make precise calculations with real numbers. The difference between $\tilde{f}_k$ and f_k comes from the integration error, the interpolation error and the error coming from the fact that we are integrating on a finite interval. As for the difference between $\tilde{f}_k(\mathbf{x})$ and $\hat{f}_k(\mathbf{x})$, we have to take into account that we only know f_{k-1} with some error ($\hat{f}_{k-1}$) and such errors will be carried over to $\hat{f}_k(\mathbf{x})$. Moreover, we will also have computing errors (i.e., floating point errors). These types of errors are fairly easy to handle. Adding all these up, the obtained error bounds will depend only on the number of grid points N (after fixing $R = 7$ and $\tau = 0.086$):

$$\sup_{\mathbf{x}} \left| \hat{f}_0(\mathbf{x}) - f_0(\mathbf{x}) \right| \leq \frac{20}{N^2} + 1.4 \cdot 10^{-12};$$
$$\sup_{\mathbf{x}} \left| \hat{f}_1(\mathbf{x}) - f_1(\mathbf{x}) \right| \leq \frac{361}{N^2} + 2.0 \cdot 10^{-12};$$
$$\sup_{\mathbf{x}} \left| \hat{f}_2(\mathbf{x}) - f_2(\mathbf{x}) \right| \leq \frac{1606}{N^2} + 2.3 \cdot 10^{-12}.$$

Once we have calculated the approximate values of f_0, f_1, and f_2 at the points of our grid, we are ready to compute the final two-dimensional integrals defining p'_1, p'_3, p'_5. Note that if we use the same grid for the two-dimensional numerical quadrature as we used for storing the values of the functions f_k, then no interpolation errors will occur. Other error terms can be treated along the same lines as in the one-dimensional case.

Our original goal was to find the value of $0.5(1-p_0)+0.5p'_1+1.5p'_3+6p'_5$, recall (14). Setting $N = 20000$ the numerical computations outlined above give 0.43619355 and combining all the errors occurring we get the following upper bound for the overall error:

$$\frac{17094}{N^2} + 3.9 \cdot 10^{-5} + \frac{5 \cdot 10^5}{N^4} < 8.2 \cdot 10^{-5}.$$

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