Nearest-Neighbor Graphs

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Consider a set P of n points that are independently and uniformly distributed in the d-dimensional unit cube. Let $p \in P$. There exists almost-surely $q \in P$ such that $q \neq p$ and |p-q| < |p-r| for all $r \in P$, $r \neq p$, $r \neq q$. The point q is called the **nearest neighbor** of p and we write $p \prec q$. Note that $p \prec q$ does not imply $q \prec p$. Draw an edge connecting p and q if and only if $p \prec q$; the resulting graph of n vertices and $\leq n$ edges is called the **nearest-neighbor graph** G on P.

What is the probability, $\alpha(d)$, given $p \in P$, that $p \prec q$ implies $q \prec p$? Such a pair is **isolated** from the rest of G, in the sense that the only edge touching p or q is the edge that connects p and q. We have [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]

$$\alpha(1) = \frac{2}{3}, \qquad \alpha(2) = \frac{6\pi}{8\pi + 3\sqrt{3}} = 0.6215048968..., \qquad \alpha(3) = \frac{16\pi}{27}$$

and, more generally [9],

$$\alpha(d) = \begin{cases} \left[\frac{3}{2} + \frac{1}{2}\sum_{k=1}^{\ell} \frac{1 \cdot 3 \cdots (2k-1)}{2 \cdot 4 \cdots (2k)} \left(\frac{3}{4}\right)^{k}\right]^{-1} & \text{if } d = 2\ell + 1, \\ \left[\frac{4}{3} + \frac{\sqrt{3}}{2\pi} \left(1 + \sum_{k=1}^{\ell-1} \frac{2 \cdot 4 \cdots (2k)}{3 \cdot 5 \cdots (2k+1)} \left(\frac{3}{4}\right)^{k}\right)\right]^{-1} & \text{if } d = 2\ell. \end{cases}$$

Here is a variation of the preceding. Draw an edge connecting p and q if and only if $q \prec p$; the resulting graph of n vertices and $\leq n$ edges is called the **nearest-neighbor anti-graph** H on P. What is the probability, $\beta(d)$, that $p \in P$ is isolated from the rest of H? That is, what proportion of points in P are not nearest neighbors of any other points? We have [16, 17, 18, 19, 20, 21]

$$\beta(1) = \frac{1}{4}, \qquad \beta(2) \approx 0.28, \qquad \beta(3) \approx 0.30$$

but the latter two estimates are only simulation-based. To further understand $\beta(2)$ will occupy us for the remainder of this essay.

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Define constants C(0, d) = 1 and

$$C(k,d) = \int_{\Omega(k,d)} \exp\left[-\operatorname{Vol}\left(\bigcup_{j=1}^{k} S(x_j)\right)\right] dx_1 dx_2 \dots dx_k$$

for $k \geq 1$, where $S(x_j)$ is the ball in \mathbb{R}^d of radius $|x_j|$, centered at x_j , and

$$\Omega(k,d) = \{ (x_1, x_2, \dots, x_k) \in \mathbb{R}^{dk} : |x_i| \le |x_i - x_j| \text{ for all } 1 \le i \ne j \le k \}.$$

It is known that [19, 22, 23, 24, 25]

$$\beta(2) = \sum_{k=0}^{6} \frac{(-1)^k}{k!} C(k,2), \qquad \beta(3) = \sum_{k=0}^{12} \frac{(-1)^k}{k!} C(k,3)$$

and clearly C(1, d) = 1, C(2, 1) = 1/2. The upper limits of summation are the *kissing* numbers in \mathbb{R}^2 and \mathbb{R}^3 , respectively. A proof that 24 is the kissing number in \mathbb{R}^4 was given only recently [26, 27]. Also, C(6, 2) = 0 since $\Omega(6, 2)$ is of measure zero.

Henze [24, 25] showed that

$$C(2,d) = \frac{2^{d+1}\pi^{d-1}}{\Gamma(d-1)} \int_{0}^{\infty} \int_{0}^{\xi} \int_{\theta_0}^{\pi} \xi^{d-1} \eta^{d-1} \sin(\theta)^{d-2} F_d(\xi,\eta) \, d\theta \, d\eta \, d\xi$$

where

$$\theta_0 = \arccos\left(\frac{\eta}{2\xi}\right),$$

$$F_d(\xi,\eta) = \exp\left[-f_d(\xi,\gamma) - f_d(\eta,\delta)\right],$$

$$\gamma = \frac{\xi(\xi - \eta\cos(\theta))}{\sqrt{\xi^2 + \eta^2 - 2\xi \eta\cos(\theta)}}, \quad \delta = \frac{\eta(\eta - \xi\cos(\theta))}{\sqrt{\xi^2 + \eta^2 - 2\xi \eta\cos(\theta)}},$$

$$f_d(x,y) = \frac{\pi^{d/2}x^d}{2\Gamma(d/2+1)} \left[1 + I\left(\frac{y^2}{x^2}, \frac{1}{2}, \frac{d+1}{2}\right)\right]$$

and I is the regularized beta function

$$I(z,a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \int_{0}^{z} w^{a-1} (1-w)^{b-1} dw.$$

(In [24], the definitions of γ and δ were mistakenly reversed; also, the expression within square brackets for $f_d(x, y)$ was unclear.) We obtain

$$C(2,2) = 0.63317... = 2(0.316585...), \quad C(2,3) = 0.70888....$$

Tao & Wu [19] independently showed that

$$C(2,2) = \pi \int_{\pi/2}^{\pi} \int_{0}^{\infty} \frac{\tau}{(g(\tau,\theta) + \tau^2 h(\tau,\theta))^2} d\tau \, d\theta + \int_{\pi/3}^{\pi/2} \int_{2\cos(\theta)}^{1/(2\cos(\theta))} \frac{\tau}{(g(\tau,\theta) + \tau^2 h(\tau,\theta))^2} d\tau \, d\theta$$

where

$$g(\tau,\theta) = \pi - \varphi + \frac{1}{2}\sin(2\varphi), \qquad h(\tau,\theta) = \pi - \psi + \frac{1}{2}\sin(2\psi),$$
$$\varphi = \arcsin\left(\frac{\tau\sin(\theta)}{\sqrt{1 + \tau^2 - 2\tau\cos(\theta)}}\right), \qquad \psi = \arcsin\left(\frac{\sin(\theta)}{\sqrt{1 + \tau^2 - 2\tau\cos(\theta)}}\right).$$

(Several underlying details in [19] are clarified in [28].) Even more elaborate integral formulas apply for C(3,2), C(4,2), C(5,2). Given the discrepancy between our estimate of C(2,2) and their estimate (see the Table), it seems doubtful that their approximation $\beta(2) = 0.284051...$ is entirely correct.

Table 1 Old and New Calculations of Constants

k	Tao & Wu estimate of $C(k,2)/k!$	Current estimate of $C(k,2)/k!$
2	0.3163335	0.316585
3	0.0329390	0.033056
4	0.0006575	still open
5	0.0000010	still open

A discrete version of the latter problem appears in [29, 30, 31, 32]. Let all the vertices of the lattice \mathbb{Z}^d be initially occupied by particles which can annihilate oneby-one their 2*d* nearest neighbors. More precisely, for each unit-length edge $\{u, v\}$ of the lattice, there is a Uniform [0, 1] random variable $T_{\{u,v\}}$ representing the time of an attack along the edge. If vertices u, v are both occupied immediately prior to time $T_{\{u,v\}}$, then at time $T_{\{u,v\}}$ either vertex u or vertex v (each with probability 1/2) becomes vacant (that is, one particle annihilates the other). If u, v are not both occupied at time $T_{\{u,v\}}$, then there is no change. Once a vertex becomes vacant, it remains vacant permanently. The variables $T_{\{u,v\}}$, considered over all unit-length edges $\{u, v\}$, are independent. By time 1, no two surviving particles can be adjacent. When d = 1, the probability that a given vertex remains occupied is 1/e = 0.3678794411.... When d = 2, this probability is known to be in the interval (0.227, 0.306) and is approximately 0.25 via simulation. Greater accuracy is desired.

References

- P. J. Clark and F. C. Evans, On some aspects of spatial pattern in biological populations, *Science* 121 (1955) 397–398.
- [2] P. J. Clark, Grouping in spatial distributions, *Science* 123 (1956) 373–374.
- [3] M. F. Dacey, Proportion of reflexive nth order neighbors in spatial distribution, *Geographical Analysis* 1 (1969) 385–388.
- [4] G. F. Schwarz and A. Tversky, On the reciprocity of proximity relations, J. Math. Psych. 22 (1980) 157–175; MR0609119 (82f:92050).
- [5] T. F. Cox, Reflexive nearest neighbours, *Biometrics* 37 (1981) 367–369; MR0673043 (83k:62122).
- [6] D. P. Shine and J. Herbert, Birds on a wire, J. Recreational Math. 11 (1978-79) 227–228; 15 (1982-83) 232.
- [7] S. Morris, Competition winners, *Omni* v. 2 (1980) n. 9, p. 108.
- [8] C. Kluepfel, Birds on a wire, cows in the field, and stars in the heavens, J. Recreational Math. 13 (1980-81) 241–245.
- [9] D. K. Pickard, Isolated nearest neighbors, J. Appl. Probab. 19 (1982) 444–449; MR0649985 (83g:60063).
- [10] M. F. Schilling, Mutual and shared neighbor probabilities: finite- and infinitedimensional results, Adv. Appl. Probab. 18 (1986) 388–405; MR0840100 (87k:60041).
- [11] N. Henze, On the probability that a random point is the j^{th} nearest neighbour to its own k^{th} nearest neighbour, J. Appl. Probab. 23 (1986) 221–226; MR0826925 (87k:60133).
- S. F. F. On [12] D. Eppstein, М. Paterson and Yao, nearest-Geom. 17263 - 282;neighbor graphs, Discrete Comput. (1997)http://www.ics.uci.edu/~eppstein/pubs/EppPatYao-DCG-97.pdf; MR1432064 (98d:05121).
- [13] D. P. Shine and M. P. Cohen, Spread the news, J. Recreational Math. 36 (2007) 277–278.

- [14] C. A. S. Tercariol, F. de Moura Kiipper and A. Souto Martinez, An analytical calculation of neighbourhood order probabilities for high dimensional Poissonian processes and mean field models, J. Phys. A 40 (2007) 1981–1989; condmat/0609210; MR2316309 (2008a:82035).
- [15] P. J. Campbell and B. Atwood, The farmer problem, UMAP Journal 33 (2012) 313–331.
- [16] F. D. K. Roberts, Nearest neighbours in a Poisson ensemble, *Biometrika* 56 (1969) 401–406.
- [17] R. Abilock and M. Goldberg, N riflemen, Amer. Math. Monthly 75 (1968) 1009; 89 (1982) 274–275.
- [18] S. Morris, Rifle puzzle, Omni v. 8 (1986) n. 4, p. 113; v. 9 (1987) n. 7, p. 141.
- [19] R. Tao and F. Y. Wu, The vicious neighbour problem, J. Phys. A 20 (1987) L299–L306; MR0888078 (88d:82021).
- [20] E. G. Enns, P. F. Ehlers and T. Misi, A cluster problem as defined by nearest neighbours, *Canad. J. Statist.* 27 (1999) 843–851; MR1767151 (2001b:60017).
- [21] S. Portnoy, A squirtgun battle, J. Recreational Math. 37 (2008) 39–45.
- [22] C. M. Newman, Y. Rinott and A. Tversky, Nearest neighbors and Voronoi regions in certain point processes, Adv. Appl. Probab. 15 (1983) 726–751; MR0721703 (85m:60023).
- [23] C. M. Newman and Y. Rinott, Nearest neighbors and Voronoi volumes in highdimensional point processes with various distance functions, Adv. Appl. Probab. 17 (1985) 794–809; MR0809431 (87d:60048).
- [24] N. Henze, Über die Anzahl von Zufallspunkten mit typ-gleichem nächsten Nachbarn und einen multivariaten Zwei-Stichproben-Test, *Metrika* 31 (1984) 259–273; MR0773815 (86i:62075).
- [25] N. Henze, On the fraction of random points with specified nearest-neighbour interrelations and degree of attraction, Adv. Appl. Probab. 19 (1987) 873–895; MR0914597 (89c:60063).
- [26] O. R. Musin, The kissing number in four dimensions, Annals of Math. 168 (2008) 1–32; math.MG/0309430; MR2415397.

- [27] F. Pfender and G. M. Ziegler, Kissing numbers, sphere packings, and some unexpected proofs, *Notices Amer. Math. Soc.* 51 (2004) 873–883; MR2145821 (2006a:52015).
- [28] S. R. Finch, Union of *n* disks: remote centers, common origin, arXiv:1511.04968.
- [29] M. O'Hely and A. Sudbury, The annihilating process, J. Appl. Probab. 38 (2001) 223–231; MR1816125 (2001m:60226).
- [30] A. Sudbury, Inclusion-exclusion methods for treating annihilating and deposition processes, J. Appl. Probab. 39 (2002) 466–478; MR1928883 (2003k:60266).
- [31] A. Sudbury, The annihilating process on random trees and the square lattice, J. Appl. Probab. 41 (2004) 816–831; MR2074826 (2005g:82090).
- [32] M. D. Penrose and A. Sudbury, Exact and approximate results for deposition and annihilation processes on graphs, *Annals Appl. Probab.* 15 (2005) 853–889; MR2114992 (2005k:60307).