

## Models of random knots

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**Abstract** The study of knots and links from a probabilistic viewpoint provides insight into the behavior of “typical” knots, and opens avenues for new constructions of knots and other topological objects with interesting properties. The knotting of random curves arises also in applications to the natural sciences, such as in the context of the structure of polymers. We present here several known and new randomized models of knots and links. We review the main known results on the knot distribution in each model. We discuss the nature of these models and the properties of the knots they produce. Of particular interest to us are finite type invariants of random knots, and the recently studied Petaluma model. We report on rigorous results and numerical experiments concerning the asymptotic distribution of such knot invariants. Our approach raises questions of universality and classification of the various random knot models.

**Keywords** Model · Random · Knot

**Mathematics Subject Classification** 57M25 · 60B05

### 1 Knots

There is an increasing interest in random knots by both topologists and probabilists, as well as researchers from other disciplines. Our aim in this survey article is to provide an accessible overview of the many different approaches to this topic.

We start with a very brief introduction to knot theory, and in Sect. 2 we describe the motivation to introduce randomness into this field. The various models are

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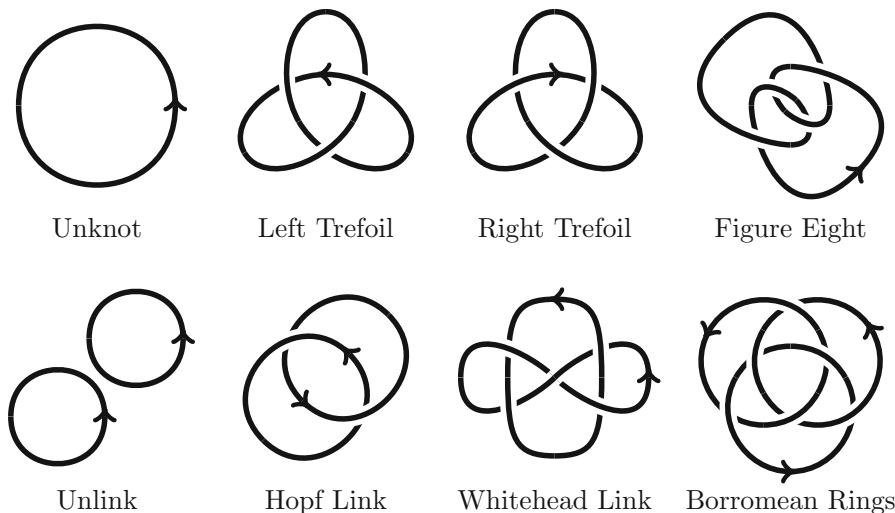
surveyed in Sect. 3, and some specific aspects are further discussed in Sect. 4. Some thoughts and open problems are presented in Sect. 5.

Intuitively, a knot is a simple closed curve in the three dimensional space, considered up to continuous deformations without self-crossing. More formally, a *knot* is a smoothly embedded oriented circle  $S^1 \hookrightarrow \mathbb{R}^3$ , with the equivalence relation of ambient isotopies of  $\mathbb{R}^3$ . A *link* is a disjoint union of several such embedded circles, called *components*, with the same equivalence. An alternative definition uses polygonal paths without the smoothness condition. There are several good general introductions to knot theory such as Adams (1994) or Lickorish (1997).

Knots and links can also be described via planar *diagrams*, which are their generic projections to  $\mathbb{R}^2$ . The projection is injective except for a finite number of traverse double points. Each such *crossing* point is decorated to indicate which preimage is over and which is under, with respect to the direction of the projection. See Fig. 1 for diagrams of some well-known knots and links.

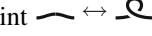
The set of nonequivalent knots is infinite, without much structure and organization. Some order arise from the operation of *connected sum* of knots,  $\mathcal{K}_1 \# \mathcal{K}_2 = \mathcal{K}_1 \cup \mathcal{K}_2$  for example. A theorem by Schubert (Lickorish 1997, Chapter 2) states that every knot can be uniquely decomposed as a connected sum of *prime* knots, which are knot that cannot be decomposed further. However, there are infinitely many nonequivalent prime knots as well.

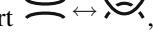
A problem that motivated much of the developments in knot theory since its early days was finding and tabulating all prime knots that can be represented by diagrams with a small number of crossings. As of today, knot tables with up to 16 crossings have been compiled (Jim Hoste et al. 1998). This classification mission called for tools for telling whether or not two given knots are equivalent, even though represented differently.

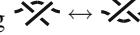


**Fig. 1** Selected knot and link diagrams

By the classical Reidemeister theorem (Lickorish 1997, Chapter 1), two diagrams define equivalent knots if and only if one can be transformed into the other by a sequence of local *moves* of three types:

(I) twisting the curve at some point   $\leftrightarrow$  

(II) sliding one part of the curve under an adjacent part   $\leftrightarrow$  

(III) sliding under an adjacent crossing   $\leftrightarrow$  

As for the complementary purpose of distinguishing one knot from another, a wide variety of *knot invariants* were defined. Here one constructs a well-defined function from the set of all knots to any other set, that attains different values for the two knots in question. Either representation, by diagrams or by curves in  $\mathbb{R}^3$ , may be used to define invariants, as long as one shows that it respects equivalence. In a broader perspective, knot invariants may be viewed as tools to classify knots and understand their properties.

We mention some important knot invariants. The *crossing number*  $c(K)$  is the least number of crossing points in a diagram of a knot  $K$ . The *genus*  $g(K)$  is the least genus of an embedded oriented compact surface with boundary  $K$ . Several other invariants, such as the *bridge number*, *unknotting number*, and *stick number* (Adams 1994), are similarly defined by taking the minimum value of some complexity measure over certain descriptions of the knot.

It is conjectured that knots can be fully classified by Vassiliev's *finite type invariants* (Vassiliev 1990; Bar-Natan 1995b; Chmutov et al. 2012). See Sect. 4.1 for a definition. This infinite collection of numerical invariants includes Gauss's *linking number* and the *Casson invariant*, coefficients of the *Alexander–Conway polynomial*, the modified *Jones polynomial*, and the *Kontsevich integral*.

Other invariants are defined via properties of the knot complement, such as its fundamental group  $\pi_1(\mathbb{R}^3 \setminus K)$ , the *knot group* of  $K$ . A knot is called *hyperbolic* if its complement can be given a metric of constant negative curvature. In this case  $\text{Vol}(S^3 \setminus K)$ , the *hyperbolic volume* of  $K$ , is a well-defined and useful knot invariant (Thurston 1978).

## 2 Randomness

There are several motivations to study randomized knot models. They emerge from different perspectives. Below we mention several aspects and applications of knot theory where it is natural to adopt a probabilistic point of view.

### 2.1 Study typical knots

As mentioned, the space of knots is infinite and poorly structured. Usually, the particular examples of knots one considers are either very simple with only a few crossings, or they are explicit constructions of knots of quite specific forms. These

can be members of well-known families such as torus knots, pretzel knots, and rational knots, or ad hoc constructions tailored for the problem under investigation.

Similarly, often one considers knots of some particular type, such as alternating or hyperbolic. Do these classes represent the general case, and if so in what sense?

It is natural and desirable to understand what typical knots are like and what properties they tend to have.

We specify a probability distribution over knots in search of a framework to investigate such questions. Often we consider a sequence of such distributions, supported on increasingly larger sets of knots. These distributions may be defined via random planar diagrams or random curves in  $\mathbb{R}^3$ , but ultimately only the resulting knot type is considered.

Rather than focus on particular constructions and classes, we ask what knot properties hold with high probability. Knot invariants become random variables on the probability space, and we study their distribution and interrelations.

It is not apriori clear which distributions, or *models of random knots*, are worth studying. It is reasonable to require that every knot have positive probability. We also do not want the measure to be highly concentrated on some overly specific class of knots. At present it remains debatable how good any concrete distribution that one suggests is.

## 2.2 Probabilistic existence proofs

A more definite goal of studying random knot models is the application of the probabilistic method in knot theory. The basic idea is to prove the existence of certain objects by showing that in some random model they occur with positive probability. This influential methodology has yielded many unexpected results in combinatorics and other fields (Alon and Spencer 2000). In many cases, the existence of objects with some given properties can be established using probabilistic methods, while finding matching explicit constructions remains elusive.

To illustrate this idea, consider the Jones polynomial  $V_K(t) \in \mathbb{Z}[t, t^{-1}]$ . The discovery of this important knot invariant in 1984 was hailed as a breakthrough in the field (Lickorish 1997, Chapter 3). By definition  $V_{\text{unknot}}(t) = 1$ , and it is unknown whether there exists a non-trivial knot  $K$  for which  $V_K(t) = 1$  (Jones 2000). It is believed though, that if such knots exist, then they are plentiful. If so, it is reasonable to expect that in some random model it should be possible to prove the probability of this trivial Jones polynomial is strictly larger than that of the unknot.

For this approach to work we clearly need a random model that allows us to estimate the probability of the relevant events and the distributions of the invariants at hand.

Random knot models come handy also in computer experiments, where one non-exhaustively searches for a specific exemplar to demonstrate some properties, thus providing explicit examples and counterexamples in a more direct way.

### 2.3 Knots in nature

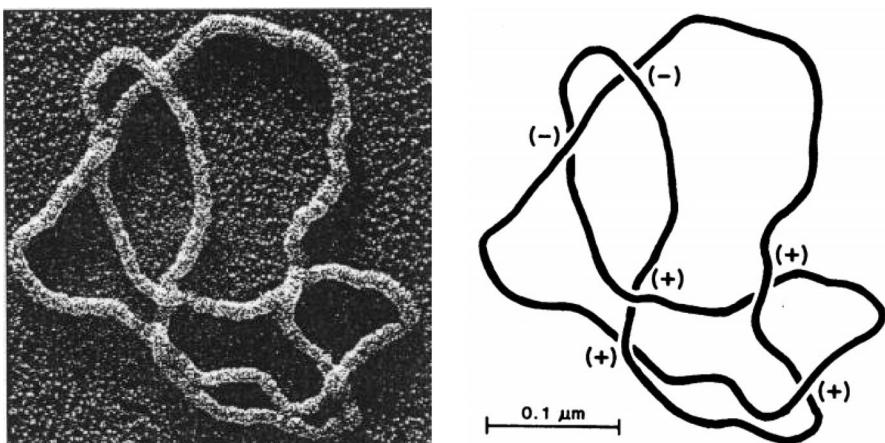
The occurrence of knots and links in the natural sciences has been a fruitful source for several studies of randomized knot models.

Most prominently, biologists are interested in the three-dimensional shape of proteins, DNA and RNA molecules (Fig. 2). Their geometric and topological features affect their functionality in a variety of biological processes, such as protein folding and DNA replication and transcription. Physicists and chemists look into the formation of entanglements in polymeric materials. The topological structure of such substances is reflected macroscopically in its features, such as elasticity, viscosity, diffusion rate, and purity of crystallization. There is plenty of literature on the modeling of knots in thread-like molecules. Find some expositions and surveys in Wasserman and Cozzarelli (1986), Vologodskii (1992), Sumners (1992), Sumners (1995), Grosberg et al. (1997), Bates and Maxwell (2005), Orlandini and Whittington (2007), McLeish (2008), Fenlon (2008), Buck (2009), Sumners et al. (2009), Micheletti et al. (2011) and Lim and Jackson (2015).

Numerous numerical simulations and experiments have been preformed to investigate the topological properties of such filamentary molecules. These involved the invention of several mathematical models that produce random paths in  $\mathbb{R}^3$  to simulate the conformation of molecules in natural environments. In particular, such a model defines a distribution over knot types, often parametrized by the length of the path.

Naturally, these models are designated to emulate natural features and processes, with different degrees of simplification. Most often they incorporate physical constraints such as non-zero thickness, self interaction, restricted bending, and spatial confinement. Additionally, this line of research calls for random models that can be easily sampled in numerical studies.

The study of knotted structures in three-dimensional fields dates back to early fluid dynamics and Kelvin's vortex atom hypothesis (von Helmholtz 1867; Kelvin



**Fig. 2** Knotted DNA. Figure is courtesy of Wasserman et al. (1985)

1867). Knots and links are formed in a three-dimensional flow  $\mathbf{u} : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  by the vortex lines that follow  $\nabla \times \mathbf{u}$ , or similarly by the nodal set  $\psi = 0$  of a wavefunction  $\psi : \mathbb{R}^3 \rightarrow \mathbb{C}$ .

In current research, such knotting phenomena are theoretically analyzed, numerically simulated, and experimentally created or identified in various physical systems. To mention some examples: knotted vortices in classical fluid flow (Kleckner and Irvine 2013) and in superfluids (Hall et al. 2016; Kleckner et al. 2016), optical vortices in laser beams (Dennis et al. 2010), magnetic fields in plasma (Berger 1999), superposition of states in quantum mechanics (Berry 2001), and also nonlinear waves in biological and chemical excitable media (Winfree and Strogatz 1984).

It seems that the generation of such knotted fields is often dominated by random factors, and it would be interesting to investigate what knots and links are likely to occur in such circumstances. Indeed, a recent work (Taylor and Dennis 2016) simulates random quantum wavefunctions in different potentials, and study the complexity of the vortex knots that show up.

Finally, knots form at random in many objects of everyday practice, from extension cords, ropes, and garden hoses (Raymer and Smith 2007) to umbilical cords (Goriely 2005; Hershkovitz et al. 2001) and eels (Zintzen et al. 2011).

## 2.4 Computational aspects

The study of random knot models is also motivated by the important role of randomness in the design and analysis of algorithms and in computational complexity theory (Mitzenmacher and Upfal 2005).

It is a central computational challenge in knot theory to determine how hard it is to detect unknots, and more generally to decide the equivalence of two given knots (Haken 1961; Hass et al. 1999; Kuperberg 2014; Lackenby 2016). Specifically it is interesting to bound the number of Reidemeister moves that yield the equivalence of two representations (Hass and Nowik 2010; Lackenby 2015; Coward and Lackenby 2014). It is generally believed that some of these problems are hard, and consequently cryptosystems were proposed that are based on such problems (Farhi et al. 2012). To this end it is necessary to know the complexity of typical instances of problems. Random knot models are clearly needed in such pursuits.

The computation of various invariants also leads to interesting complexity problems. Hardness results are known for the knot genus (Agol et al. 2006; Lackenby 2016) and for the Jones polynomial (Jaeger et al. 1990; Aharonov et al. 2009; Kuperberg 2009). Other invariants such as the Alexander–Conway polynomial and finite type invariants are computable in polynomial time (Alexander 1928; Bar-Natan 1995a; Chmutov et al. 2012). Many such algorithms are implemented in software packages, such as *SnapPy* (Culler et al. 2016), *KnotTheory* (Bar-Natan et al. 2016b) and *KnotScape* (Hoste and Thistlethwaite 2016). These are used in practice for the compilation of knot databases and are important tools in research and applications (Bar-Natan et al. 2016a; Cha and Livingston 2016; Jim Hoste et al.

1998). Random knot models could serve as the basis for average-case analysis of such algorithms.

## 2.5 Random 3-manifolds

The probabilistic method has had a great success in many areas. The study of random knots can be viewed as part of a broader research effort to apply this approach to the study of geometric and topological objects.

In recent years, there have been interesting developments in the study of random simplicial complexes (Linial and Meshulam 2006; Adler et al. 2010; Kahle 2016), random groups (Gromov 2003; Ollivier 2005), random manifolds (Brooks et al. 2004; Dunfield and Thurston 2006; Pippenger and Schleich 2006; Farber and Kappeler 2008), and more.

In particular, several models for random 3-manifolds have been presented and studied in the past decade (Dunfield and Thurston 2006; Lutz 2008; Maher 2010; Kowalski 2010; Dunfield and Wong 2011; Maher et al. 2011; Maher 2012; Lubotzky et al. 2016; Rivin 2014). Since every closed orientable 3-manifold can be generated by performing Dehn surgeries on links in  $S^3$  (Lickorish 1997, Chapter 12), models for random links give rise to random 3-manifold whose properties are interesting to study (Even-Zohar et al. 2017b).

In another direction, random knot models may extend to knotted 2-spheres or other surfaces in a 4-sphere, and further to randomly embedded manifolds in higher dimensions (Soteros et al. 2012; Atapour et al. 2015).

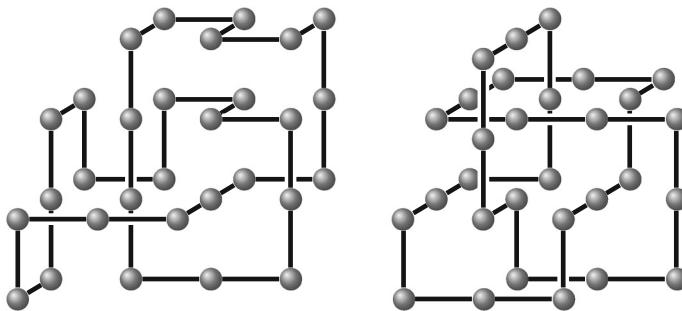
## 3 Models

Before listing some specific models, a few words on the general framework. A *random knot model* is a distribution over the set of all knots, which we represent by a random variable  $K$ . We usually consider a sequence  $K_n$  of such distributions, where  $n \in \mathbb{N}$  naturally appears in the construction. This parameter  $n$  can often be viewed as a complexity measure of the typical resulting knots. All unspecified asymptotic statements that we make here are w.r.t.  $n \rightarrow \infty$ .

Variations abound: We also encounter some multi-parameter constructions and some models that yield random links of any number of components, or focus on some subclass such as prime or alternating knots.

### 3.1 Self-avoiding grid walk

As usual, a walk on the three-dimensional lattice  $\mathbb{Z}^3$  is a sequence  $\{X_0, \dots, X_n\}$  such that  $X_0 = (0, 0, 0)$  and  $(X_{i+1} - X_i) \in \{(\pm 1, 0, 0), (0, \pm 1, 0), (0, 0, \pm 1)\}$ . Consider  $n$ -step walks that are *closed*, with  $X_n = X_0$ , and *self-avoiding*, so that  $X_i \neq X_j$  for any other pair of points. Connecting the points of such a walk yields an  $n$ -segment polygonal path, that represents a knot. See Fig. 3 for two examples.



**Fig. 3** The trefoil and figure-eight knots as 30-step walks on  $\mathbb{Z}^3$

Random self-avoiding walks (SAW) on  $\mathbb{Z}^3$  were suggested as a model for polymeric molecules, and their knotting properties have been studied over the past decades in varying degrees of rigor. In the *grid walk model* a random knot  $K_n$  is obtained by sampling from the uniform distribution of all closed self-avoiding  $n$ -step walks. Every knot appears in this model for  $n$  large enough.

It was conjectured by Delbrück (1961) that  $K_n$  is knotted with high probability. This was observed in numerical simulations (Crippen 1974; Frank-Kamenetskii et al. 1975), and proved by Sumners and Whittington (1988) and by Pippenger (1989). Using Kesten's pattern theorem (1963), they showed that the unknot appears with exponentially small probability in  $n$ . Moreover, every prime knot appears in the decomposition of  $K_n$  with multiplicity  $\Theta(n)$ , except for an exponentially small probability (Soteros et al. 1992).

Let  $K'_n$  be a uniformly random connected component of  $K_n$ , conditioned on  $K_n$  being knotted. Note that  $K'_n$  is a natural model for *random prime knots*, and it is suggestive that  $K'_n$  converges in distribution, and yields a random model for all prime knots.

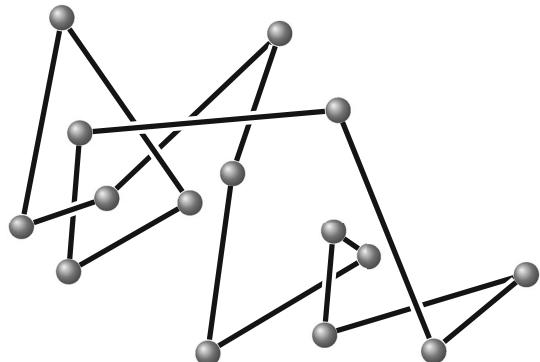
It is of interest to study self-avoiding walks and the resulting knots on other lattices (Janse van Rensburg and Whittington 1990). Also extensions to random 2-component links, and the effect of confinement within a box or a tube, are considered and analyzed (Orlandini et al. 1994; Soteros et al. 1999; Atapour et al. 2010). Madras and Slade's book (2013) offers a rigorous analysis of Monte Carlo sampling methods for self avoiding walks.

### 3.2 Polygonal walks

In the study of polymers, random polygonal paths in  $\mathbb{R}^3$  also play a prominent role. Again we create a closed self-avoiding path by joining  $n$  straight segments, but these are now distributed according to some continuous law. Two common choices for the distribution of the segments are the *equilateral* with uniform distribution on the 2-sphere, and the *Gaussian* with standard 3-normal distribution (see Fig. 4).

That the walk is self-avoiding is usually satisfied with probability one, but more care is needed to make sure that the walk is closed. Details of this vary with the

**Fig. 4** A closed polygon that realizes the trefoil in  $\mathbb{R}^3$



specific model and sampling method. We remain brief and only mention that it is possible to guarantee this in the Gaussian model by adding a constant drift.

It was conjectured by Frisch and Wasserman (1961) that polygonal walks are also unknotted with vanishing probability. Numerical simulations suggested exponential decay in  $n$  for various different polygonal models (des Cloizeaux and Mehta 1979; Bret 1980; Michels and Wiegel 1982, 1986; Koniaris and Muthukumar 1991). Diao et al. (1994) proved  $\exp(-n^\varepsilon)$  for some  $\varepsilon > 0$  for Gaussian-steps polygons. This was extended to equilateral polygons (Diao 1995) and other models (Janse et al. 2007).

General polygonal walks have an advantage over grid walks, in being space-isotropic. This is more realistic for polymers, and more robust to variations. Here to simulate effects of excluded volume constraints, one often replaces segments with rods and points with beads of positive radius. It is also interesting to consider polygons packed in a confined space such as a cube or a tube. Other variations of the model allow simulating bending rigidity, tension, pressure, thermodynamic entropy, and interaction between particles. See Micheletti et al. (2011) for a thorough review.

For numerical experiments, such models are often approximately sampled via Markov chains in the configuration space, with a variety of local and global moves based on re-ordering, rotation, reflection, and more (Alvarado et al. 2011). There is currently much activity in search of faster rigorous sampling algorithms, with new techniques from symplectic geometry (Cantarella and Shonkwiler 2016; Cantarella et al. 2016) and convexity (Chapman 2016a).

The resulting knots were classified for large samples in the various experiments. It turns out that, in several polygonal and grid models, the frequency at which a knot  $K$  occurs is well approximated by  $P[K_n = K] = C_K(n/N)^{\alpha_K} e^{-(n/N)}$ . The constant  $N$  depends only on the model, while for every knot  $K$  the exponents  $\alpha_K$  seem to be universal among different models (Deguchi and Tsurusaki 1994, 1997; Orlandini et al. 1998; Millett and Rawdon 2005; Janse et al. 2011). Further experiments indicated that the  $m$ th most frequent knot appears with probability of order  $m^{-1.75}$  (Cantarella et al. 2016).

### 3.3 Smoothed Brownian motion

A substantially less studied subject is knotting from non-piecewise-linear three-dimensional random walks. A random polygon in the Gaussian model can be viewed as a linear interpolation between a finite number of points from a continuous Brownian bridge taken at constant time intervals. However, Brownian motion cannot model a knot as it is self-intersecting with probability one. Moreover, Kendall (1979) showed that it would contain infinitely many knots of all types, in the sense of being contained in such knotted tubes. Is there a smooth model that avoids these problems but captures the behavior of Brownian motion other than in small scale?

The *worm-like loop* (Grosberg 2000) from polymer physics is a conituum model that takes curvature into account. A smooth closed curve in  $\mathbb{R}^3$  is given weight proportional to  $\exp(-\ell \int \|\dot{\mathbf{r}}\|^2 ds)$ , where  $\mathbf{r}(s)$  is its arc-length parametrization and  $\ell$  is a typical length of persistence to bending. A more general model of statistical mechanics, designated for ribbons, takes care of the bending direction and persistence to twisting as well (Kessler and Rabin 2003). It is known how to approximately sample from this model for open paths but not for closed ones.

In the search of a more numerically accessible model for worm-like loops, Rappaport et al. (2006) and Rappaport and Rabin (2007) suggested the following mathematical model. One way to construct a Brownian bridge in  $\mathbb{R}^3$  is by the following Fourier series, with  $w_k = 1$ .

$$\mathbf{r}(t) = \sum_{k=1}^{\infty} \frac{w_k}{k} (\mathbf{Z}_k \cos kt + \mathbf{Z}'_k \sin kt) \quad \mathbf{Z}_k, \mathbf{Z}'_k \sim 3\text{-normal iid.}$$

To obtain a smooth approximation, one can truncate the sum by  $w_k = 1_{k \leq n}$  or by  $w_k = e^{-k/n}$ . Computer simulations of the second choice show an exponential decay of the unknotting probability (Rappaport et al. 2006). It is interesting to observe that the cut-off factor  $w_k = e^{-(k/n)^2}$  is equivalent to smoothing the Brownian motion by convolution with a narrow Gaussian, which seems to be an appealing choice.

Recent works (Westenberger 2016; Rivin 2016) study the case of polynomially decaying coefficients  $w_k = k^{-\alpha}$ , where  $\alpha \in \mathbb{R}$ . For  $\alpha > 0.5$  they derive bounds on the expected crossing number of a random knot, and on the variance of the linking number of a random link.

The parametrization of knots by a finite sum of cosines yields *Fourier knots* (Buck 1994; Trautwein 1995; Kauffman 1998). As shown by Lamm (2012), every knot can be obtained by taking  $x(t) = \cos(k_x t + \phi_x)$ ,  $y(t) = \cos(k_y t + \phi_y)$ , and a finite sum of such cosines for  $z(t)$ . This was recently improved by Soret and Ville (2016), who showed that a sum of two cosines is sufficient. Taking a single cosine,  $z(t) = \cos(k_z t + \phi_z)$  defines the well-studied *Lissajous knots* (Bogle et al. 1994; Jones and Przytycki 1998; Lamm 1997; Hoste and Zirbel 2006). In Boocher et al. (2009) and Rivin (2016) experiments on random Fourier and Lissajous knots are reported.

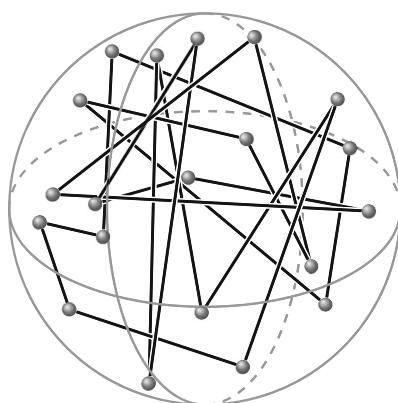
### 3.4 Random jump

In the above random walk models the typical step length is small compared with the diameter of the whole embedded path. Millett (2000) suggests polygonal models where each point  $X_1, \dots, X_n \in \mathbb{R}^3$  is independently sampled from some distribution, such as the uniform distribution on the cube  $[0, 1]^3$ , or a spherically symmetric distribution with a uniform radius in  $[0, 1]$ . To this end any rich enough distribution that almost surely avoids self-intersections will do, such as the 3-normal distribution, or uniform on the unit sphere (O'Rourke 2011).

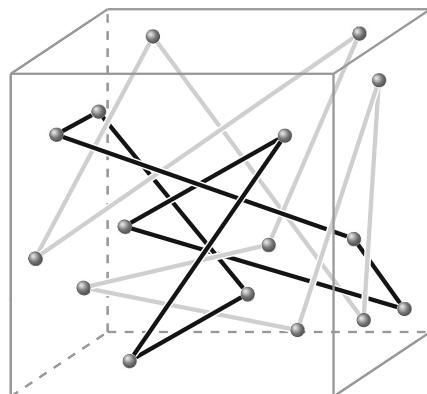
By sampling  $X_1, \dots, X_n$  and  $Y_1, \dots, Y_m$  independently with the same 3-dimensional distribution, the above extends to two-component links (Arsuaga et al. 2007a), and similarly for any number of components (Fig. 5).

We still do not know how likely it is to encounter the unknot in the random jump model. Numerical experiments indicate that this probability vanishes faster than  $\exp(-O(n))$  (Millett 2000; Arsuaga et al. 2007b). This provides evidence for a strong form of the above-mentioned Delbrück–Frisch–Wasserman conjecture in this model. Similar conclusions seem to apply to any fixed knot. Experiments with the cube model suggest that the expected knot *determinant* is  $\omega(\exp n^2)$ . It is proposed in Arsuaga et al. (2007b) that most knots in this model are prime. It was suggested (Thurston 2011) that the expected crossing number in the spherical case is  $\Theta(n^2)$ .

Consider the *linking number*  $L_{mn}$  of a random two-component link with  $n$  and  $m$  segments. It is known (Arsuaga et al. 2007a; Flapan and Kozai 2016) that its variance is  $\Theta(nm)$ , and it is conjectured that  $L_{mn}/\sqrt{nm}$  converges in distribution to a Gaussian (Panagiotou et al. 2010; Karadayi 2010). Based on our analysis of the Petaluma model (Even-Zohar et al. 2016) we tend to doubt this conjecture. Rather, we suspect that the tails of the limit distribution decay exponentially.



A knot in the unit ball



A two-component link in the cube

**Fig. 5** The random jump model

A more symmetric variant of the random jump model has been suggested (Wise 2016), which takes place in  $S^3$  visualized as the unit sphere in  $\mathbb{R}^4$ . A sequence of uniformly random points can be connected along the geodesics, which are the great circles.

These *random jump* or *uniform random polygon* (URP) models, were originally proposed to illustrate the effect of spatial constraints on knotted molecules (Millett 2000). In some bacteriophages, for example, a circular DNA molecule is densely packed inside a spherical capsid. Experiments show that more complex knots are likely to be produced, compared to unconstrained DNA of similar length in free solution (Arsuaga et al. 2002). The observed distribution is also biased towards chiral knots and especially torus knots (Arsuaga et al. 2005).

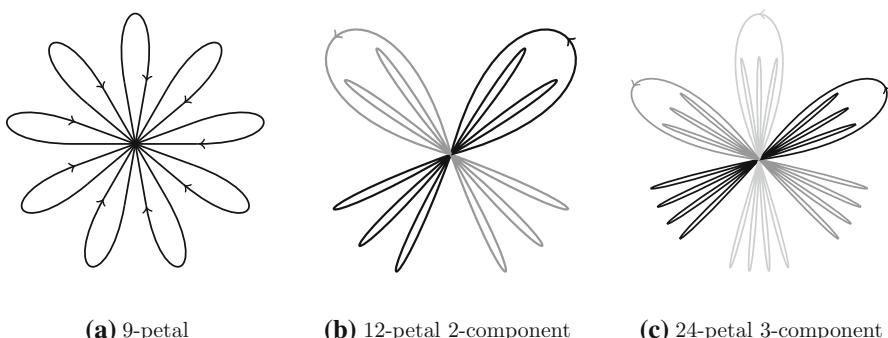
The explanation of these findings requires more realistic simulations that take into account various biophysical features, see e.g. Micheletti et al. (2008) and Marenduzzo et al. (2009). However, the simplicity of the random jump model makes it amenable for rigorous mathematical analysis, while it is arguably a prototype of a polygonal model in spatial confinement (Arsuaga et al. 2007b).

### 3.5 The Petaluma model

We now abandon random polygons, and move to more combinatorially oriented models. We start with the Petaluma model, studied by the author and collaborators (Even-Zohar 2017; Even-Zohar et al. 2016, 2017a).

Adams et al. (2015a, b) have shown that every knot or link can be positioned so that its planar projection is injective except for a single point. Several projected strands may smoothly traverse this point of the *über-crossing projection*, each originating at a different height. Moreover, every knot has a *petal projection*, where the loops that emanate from the multi-crossing point have disjoint interiors. Consequently, petal projections are represented by a rose-shaped curve with an odd number of petals, as in Fig. 6a.

In order to reconstruct the original knot we need only the relative ordering of the heights of the strands above the multi-crossing point. This information can be encoded by a permutation  $\sigma \in S_{2n+1}$ . We generate a random knot  $K_{2n+1}$  in the



**Fig. 6** Petal diagrams for knots and links

*Petaluma* model by picking  $\sigma$  uniformly at random (Even-Zohar et al. 2016). By the construction of Adams et al., every knot  $K$  is obtained with positive probability for  $n$  large enough.

The Petaluma model extends to  $k$ -component links, by considering petal diagrams with  $k$  components as in Fig. 6. In Even-Zohar (2017) we study its extension to framed knots, which can be thought as knotted oriented ribbons.

In Even-Zohar et al. (2016), Even-Zohar (2017) we explicitly find the limiting distribution of the linking number of a two-component link, as well as the limiting distribution of the writhe of a random framed knot. We similarly present formulas for the moments of the Casson invariant  $c_2$  and another finite type invariant appearing in the Jones polynomial. We elaborate on finite type invariants of random knots in the Petaluma model in Sect. 4 below.

As we show in a recent paper (Even-Zohar et al. 2017a), every particular knot appears in this model with vanishing probability. We conjecture that this probability decays at least exponentially with  $n$ , but currently the best bounds we have are  $\Omega(n^{-n}) \leq P[K_{2n+1}=K] \leq O(n^{-0.1})$ .

It is of interest to understand the relation between the crossing number  $c(K)$  of a knot and the least number of petals  $p(K)$  needed to represent it. We show in Even-Zohar et al. (2017a) that  $p(K) \leq O(c(K))$ , and this bound is tight by results of Adams et al. (2015a). They have also shown that  $c(K) \leq O(p^2(K))$ , which is also tight.

Numerical simulations for  $n \leq 100$  suggest that most knots in the Petaluma model are prime, and even hyperbolic. See Sect. 4.4 for more details, and further results by Adams (2017), Adams and Kehne (2016) and Kehne (2016). They went on to extend the Petaluma model to the *Überluma* which contains all diagrams of one multi-crossing, allowing for nested loops.

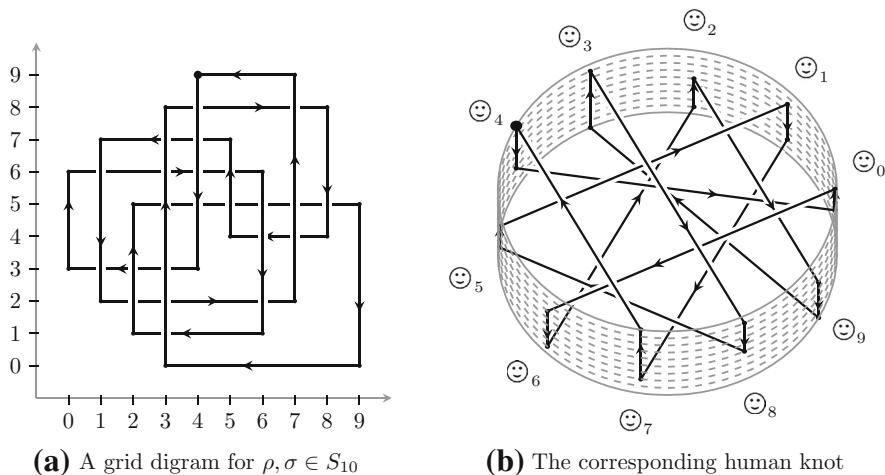
### 3.6 Random grid diagrams

Grid diagrams are a useful kind of regular knot diagrams. They describe all knots and links in a simple way (Brunn 1987; Cromwell 1998). A *grid diagram* consists of  $n$  horizontal segments and  $n$  vertical segments, where vertical segments always pass over horizontal ones. Each of the integers in  $\{1, \dots, n\}$  appears as the  $x$ -coordinates of exactly one vertical segment. Likewise for the  $y$ -coordinates of the horizontal segments.

A grid diagram is encoded by a pair of permutations  $\rho, \sigma \in S_n$  for these horizontal and vertical coordinates respectively. We alternately take steps of the form  $(\rho_i, \sigma_i) \rightarrow (\rho_i, \sigma_{i+1}) \rightarrow (\rho_{i+1}, \sigma_{i+1})$  and so on. See Even-Zohar et al. (2016) for more details, and Fig. 7a for an example.

A random knot in the *random grid* model is obtained by taking  $\rho$  and  $\sigma$  independently uniformly at random. Extensions to  $k$ -component links are easy and we omit further details. A similar model that produces links of varying number of components was considered in a scheme for quantum money (Farhi et al. 2012).

We numerically compare the distribution of  $c_2$  for the Petaluma and grid models, and find that they share many features, see Sect. 5. As observed in Adams et al.



**Fig. 7** Here  $\rho = (4, 0, 6, 2, 9, 3, 8, 5, 1, 7)$  and  $\sigma = (9, 3, 6, 1, 5, 0, 8, 4, 7, 2)$

(2015a), the Petaluma model is contained in the grid model, and obtained by conditioning on  $\rho(k) = nk \bmod (2n + 1)$ .

Some preliminary work on precise moments' computation for finite type invariants in the random grid model has been done by Gal Lavi, Tahl Nowik, and the author (Lavi and Nowik 2016). We report that  $E[c_2] = n^2/288 + O(n)$  and  $V[c_2] = 7n^4/194400 + O(n^3)$ , which are of the same orders as in the Petaluma model, cf. Sect. 4.

Two grid diagrams of the same knot can be related by a finite sequence of *Cromwell moves*, which are local operations of three types, similar to the Reidemeister moves (Cromwell 1995). Witte et al. (2016) estimate the average writhe of a knot over its  $n \times n$  grids, using a Markov chain of these moves. See also Farhi et al. (2012).

We find a nice interpretation of the grid model in a common group-dynamic game named *the human knot* (Adams 1994). A group of  $n$  two-handed participants stand in a circle. Each player chooses the next one at random and then they hold hands, until the last player holds the free hand of the first one. Their goal is to simplify the knot to a circle without letting their hands go, which is of course not always possible.

To analyze this game, we introduce the assumption of transitivity. Namely, connected pairs of hands are ordered from bottom to top. See Fig. 7b, where the players correspond to axial segments on a cylinder, and connections are horizontal chords at different heights. If this ordering is uniformly random, then this construction is equivalent to a random grid diagram. Horizontal and vertical segments correspond to chords and players respectively. The permutation  $\rho$  records the order at which players are connected, and  $\sigma$  represents the relative order of the hands' heights.

A related model, based on the human knot game, was suggested by Cohen (2007), who conducted computer experiments to study the distribution of the resulting knots.

### 3.7 Random planar diagrams

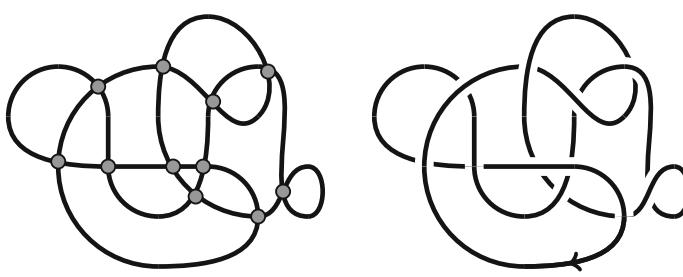
Planar diagrams are routinely used to represent knots and to investigate them. Naturally, this suggests the study of random knots by sampling diagrams with a given number of crossings. Such models were studied by several authors (Schaeffer and Zinn-Justin 2004; Diao et al. 2005, 2010; Dunfield et al. 2014; Cantarella et al. 2016), with various sampling methods.

To this end, we start with a generic smooth immersion of  $S^1$  into  $\mathbb{R}^2$  with  $n$  traverse double points, considered up to diffeomorphism of the plane, as in Fig. 8. This yields a 4-regular plane graph, where loops and multiple edges are allowed. Then each vertex is assigned either of the two possible crossing signs.

The number of  $n$ -vertex 4-valent graphs in  $\mathbb{R}^2$  is asymptotically exponential in  $n$ . However, an algorithm by Schaeffer and Zinn-Justin (2004); Brinkmann (2007) uniformly samples such graphs with a base point, by generating a random rooted binary tree and matching leaves to non-leaves in some clever way. Some of the resulting graphs correspond to curves with several components, which is a problem if one is interested only in knots rather than links. One can either reject (Dunfield et al. 2014; Cantarella et al. 2016) these curves, or modify (Diao et al. 2005, 2010) them, but this, however, ruins uniformity.

Some delicate issues of symmetry arise. Namely, do we care about orientation and mirror images? Should we distinguish between different planar diagrams which are equivalent in the sphere  $S^2$ ? Do we want a base point on some edge? Finally, are different  $n$ -vertex graphs to be weighted equally or according to the number of non-equivalent diagrams they give rise to, which might be smaller than  $2^n$  due to symmetries? However, all subtleties of this sort become negligible as  $n$  grows (Richmond and Wormald 1995; Chapman 2016c).

A recent advance in the study of this model is the establishment of a pattern theorem for diagrams by Chapman (2016b, c). This extends pattern theorems for



**Fig. 8** A random assignment of crossings to an 11-vertex 4-regular plane graph

planar maps (Bender et al. 1992), and parallels the above-mentioned results for grid and polygonal knots. Chapman showed that small sub-diagrams appear  $\Theta(n)$  times in an  $n$ -crossing knot or link diagram, except for an exponentially small probability. In particular, as  $n$  grows the diagram contains a 3-crossing trefoil summand and is hence nontrivial with high probability. Similar results hold if one restricts to *prime* diagram, ones whose underlying graph is 4-edges-connected.

Numerical experiments tell us more. Dunfield et al. (2014) and Obeidin (2016) study random links, knots, and prime connected summands of knots in this model. Their results suggest that several invariants, including the hyperbolic volume, grow linearly with  $n$ . Cantarella et al. (2016) and Chapman (2016c) precisely compute knot probabilities for  $n \leq 10$ , and study their behavior for larger  $n$  based on random samples. The methods used in these experiments are implemented into publicly available software packages: *plCurve* (Ashton et al. 2016) and *SnapPy* (Culler et al. 2016).

### 3.8 Random planar curves

Other models generate a random 4-regular plane graph in various ways, and then assign crossing signs uniformly at random. For example, Diao et al. (2010) randomly add  $n$  non-intersecting chords inside and outside an  $n$ -vertex cycle, to make it 4-regular, and then toss a coin to decide each crossing.

In the following random-crossing constructions the underlying graph is generated by sampling polygonal curves in the plane.

- Equilateral closed polygons in  $\mathbb{R}^2$  (Michels and Wiegel 1989).
- Closed SAW in  $\mathbb{Z}^2$  with diagonal crossings: or (Gitter and Orlandini 1999).
- Jumps between uniform points in the square  $[0, 1]^2$  (Arsuaga et al. 2007b; Diao et al. 2010).
- A chain of chords between uniform points around the circle (Cohen 2007).
- The *griddle*: Random grid diagrams with randomized crossings (Even-Zohar et al. 2017b).

There are close connections between the finite type invariants of such knots and those of the underlying curve (Polyak 1998). For example, the expected value of the Casson invariant  $c_2$  is one eighth the *defect*, a first-order invariant of the curve. In the griddle model we calculated  $E[c_2] = E[\text{defect}]/8 = n^2/144 + O(n)$  and  $V[c_2] = n^4/7776 + O(n^3)$ , though  $V[\text{defect}] = 29n^3/4050 + O(n^2)$  (Even-Zohar et al. 2017b).

Finally, we note that given a 4-valent graph in the plane, exactly two sign assignments produce an *alternating link diagram*, where over-crossings and under-crossings alternate as one travels along the link. Diao et al. (2005), Arsuaga et al. (2007b) and Diao et al. (2010) and Obeidin (2016) used this observation to construct models for prime alternating knots and links. Except for the  $(2, n)$ -torus these are hyperbolic links, whose volume can be read off the diagram up to a multiplicative constant (Lackenby 2004). Taking the uniform distribution over

prime alternating link diagrams, the expected hyperbolic volume is linear in the crossing number (Obeidin 2016).

### 3.9 The knot table model

The crossing number is perhaps the most popular measure for knot complexity. Historically, prime knots are tabulated and nomenclated according to their crossing number, as reflected in the widely used Alexander-Briggs–Rolfsen knot notation (Alexander and Briggs 1926; Rolfsen 1976). See also Fig. 9.

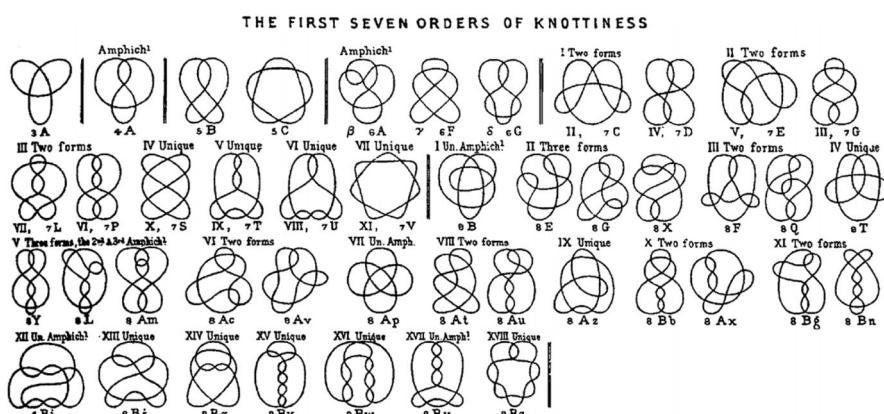
Consequently, many investigators find it quite natural to generate random prime knots by uniformly sampling from knot tables with up to  $n$  crossings. If one cares about chirality and orientation, these can be decided by further coin flips.

It is known that there are exponentially many knots with  $n$  crossings (Ernst and Sumners 1987; Welsh 1991; Carl Sundberg and Morwen Thistlethwaite 1998), but the exact count is known only for small  $n$  (Jim Hoste et al. 1998). The difficulties in recognition and enumeration of  $n$ -crossing knots make this model less suitable for precise computations, though it is known that most knots are not rational (Ernst and Sumners 1987), nor are most links alternating (Thistlethwaite 1998).

The vast majority of knots with up to  $n \leq 16$  are hyperbolic, which may suggest that their asymptotic proportion tends to 1. This is however not likely to be true, in view of a recent surprising result of Malyutin (2016). He assumes the plausible, but still unproven, conjecture that the crossing number is weakly monotone with respect to connected sum. The crux of his proof is the addition of small satellite configurations to existing diagrams.

### 3.10 Random braids

It goes back to Alexander that every knot or link is the closure of some *braid* (Lickorish 1997). Namely, it can be represented by some  $m$  intertwining



**Fig. 9** Excerpt from Tait's original table of knots with up to 8 crossings (Tait 1884). Note that unlike the discussed model it contains only alternating knots, with several equivalent diagrams for some of them

strings that monotonously go from left to right, and close at some canonical way as in Fig. 10. Such braids form a group  $B_m$ , with generators  $\{\sigma_i^{\pm 1}\}_{1 \leq i < m}$  that correspond to swapping strings  $i$  and  $i + 1$ , and appropriate relations.

There is recent interest in generating knots by random walk in the braid group. This parallels well-known constructions of random 3-manifolds (Dunfield and Thurston 2006) and more.

Such a model is defined in terms of a probability distribution on a finite subset of the braid group  $B_m$ , such as the generators  $\sigma_i^{\pm 1}$ . A random knot is obtained by  $n$ -step random walk in these generators, with some standard closure as depicted in Fig. 10. The context of Markov Chains on groups proves useful in the analysis of this model (Nechaev et al. 1996).

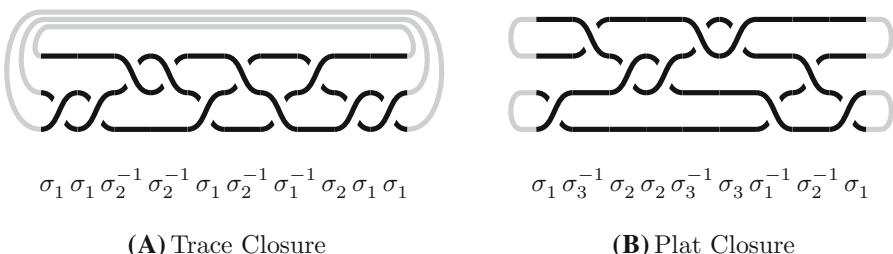
This definition yields random links of a varying number of components. For fixed  $m$  and large  $n$  we obtain knots with probability about  $1/m$ . Additionally, only links of *braid index* or *bridge index* at most  $m$  appear, according to the closure convention. Remarkably, random knots and links in this setting are hyperbolic with high probability (Malyutin 2012; Ma 2013, 2014; Tetsuya Ito 2015; Ichihara and Yoshida 2015; Ichihara and Ma 2016).

### 3.11 Crisscross constructions

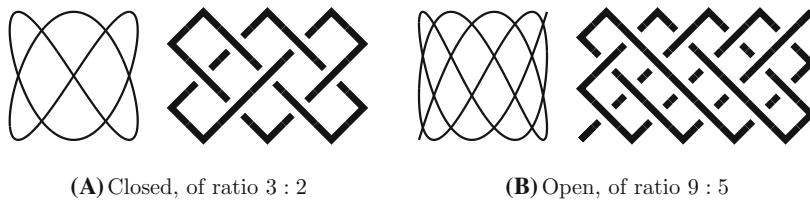
This family of random models includes several constructions in which a planar curve is explicitly specified, and all randomness comes from the choice of crossing signs, sampled independently and uniformly at random.

One source for such models is planar Lissajous curves (Lissajous 1897), illustrated in Fig. 11. These closed curves are parametrized by  $(\cos(at + \phi), \cos bt)$  where  $t \in [0, 2\pi]$  with ratio  $b:a \in \mathbb{Q}$  and a phase shift  $\phi \in \mathbb{R}$ . We also consider the *open* curve  $(\cos at, \cos bt)$  where  $t \in [0, \pi]$ , being closed from the outside. These curves are plane isotopic to the polygonal trajectory of a billiard ball in  $[0, 1]^2$ , fired at slope  $b/a$  (Jones and Przytycki 1998).

The three-dimensional analogues of these curves constitute *Lissajous knots* (Bogle et al. 1994; Lamm 1997; Jones and Przytycki 1998) and *Harmonic Knots* (Comstock 1897; Koseleff and Pecker 2011), but these families do not contain all knots. However, planar Lissajous curves with suitable crossing signs do give rise to all knots. This underlies the construction of the above-mentioned



**Fig. 10** Random knots in the braid model



**Fig. 11** Billiard table diagrams from Lissajous curves

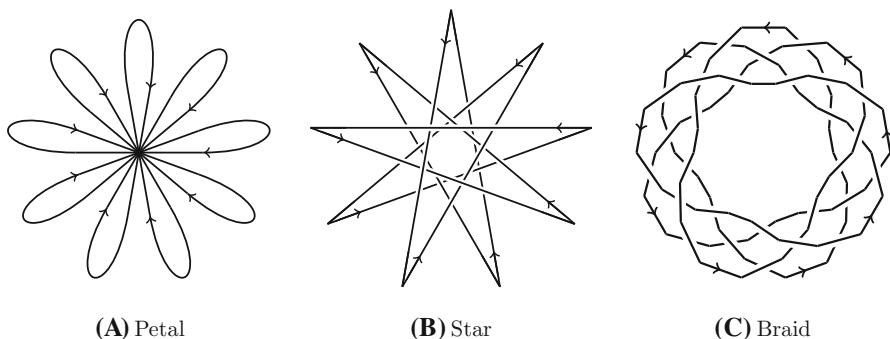
*Fourier Knots* (Buck 1994; Trautwein 1995; Kauffman 1998; Hoste and Zirbel 2006; Lamm 2012; Soret and Ville 2016) and *Chebyshev Knots* (Koseleff and Pecker 2011), as well as the next random construction, the *billiard table model* suggested by Cohen and Krishnan (2015).

A random knot  $K_{b:a}$  is thus obtained by randomizing the crossing signs, as in Fig. 11. It can also be regarded as a special case of the random braid model. For example, the case  $a = 5$  as in Fig. 11b is generated by the 16 elements  $\{\sigma_1^\pm \sigma_3^\pm \sigma_2^\pm \sigma_4^\pm\}$  with the uniform distribution.

In Cohen et al. (2016) we study the asymptotic properties of  $K_{n:3}$ , which yields random two-bridge knots, also known as *rational knots* (Kauffman and Lambropoulou 2004). We show that the probability of obtaining any particular knot is  $(\alpha + o(1))^n$  for  $\alpha = \sqrt[3]{27/32} \approx 0.945$ , and the crossing number is  $(\beta + o(1))n$  in probability, for  $\beta = (\sqrt{5} - 1)/4 \approx 0.309$ .

We remark that, without restricting to fixed diagrams, other random models arise from the highly developed theory of rational knots. In particular, a random braid in  $\{\sigma_1, \sigma_2^{-1}\}^* \subset B_4$  yields a rational knot by its Conway symbol (Conway 1970). See Ernst and Sumners (1987) and Diao et al. (2010) for corresponding results.

Star diagrams are obtained from  $(2n + 1)$ -petal diagrams by straightening the segments between petal tips. See Fig. 12a, b. A random knot in the *star model* is generated by randomizing the  $(n - 1)(2n + 1)$  crossings. Star diagrams are plane isotopic to closed  $n$ -braids (Adams et al. 2015a), as demonstrated in Fig. 12b, c.



**Fig. 12** From petal diagrams to regular knot diagrams

The star model yields all knots, since the Petaluma model does, but with quite different distribution. We show in Even-Zohar et al. (2016) that its expected Casson invariant is  $E[c_2] = n^3/12 + O(n^2)$  with a standard deviation of  $n^2/\sqrt{24} + O(n^{3/2})$ . This means that  $c_2$  drifts away from zero.

Chang and Erickson (2015) consider a generalization of the star model. They define the *flat torus* diagram  $T(p, q)$  as the closed braid  $(\sigma_1 \sigma_2 \cdots \sigma_{p-1})^q$ , and assign crossing signs at random. The star model is  $T(n, 2n+1)$ , as shown in Fig. 12c for  $n=4$ . Following Hayashi et al. (2012), they show that the expected Casson invariant of  $T(n+1, n)$  is  $\Theta(-n^3)$ . It is conceivable that this latter model contains all knots as well.

The probability space in such crisscross models consists of  $2^c$  crossing states. Some invariants are more accessible in this simple setting, as they are computable by summation over  $2^c$  local configurations at the  $c$  crossings. One important example is the Kauffman Bracket (1987), and its connections to statistical physics (Kauffman 1988; Jones 1989; Wu 1992).

For crisscross diagrams on the 2-dimensional lattice, rather similar to the above ones, the degree distribution of the Jones polynomial is analyzed in terms of the Potts model from statistical mechanics (Grosberg and Nechaev 1992; Nechaev 1996; Vasilyev and Nechaev 2001).

### 3.12 Miscellanea

We have attempted to cover the main themes of random knot models. Of course, our list of models and results is not completely exhaustive, neither historical, and to some extent reflects our own viewpoint. To conclude, we mention some random ideas in further directions.

Various models from the natural sciences seek to emulate dynamical processes of knot formation in real life scenarios. Some studies describe numerical simulations of a polygonal DNA chain that folds, coils and spools within a cavity, before its two ends anneal and produce a knot (Aruaga and Diao 2008; Marenduzzo et al. 2009, for example). Such dynamical models are important for understanding biological processes by comparing simulated and observed data, but usually they don't lend themselves easily to mathematical analysis.

Other studies (Flammini et al. 2004; Hua et al. 2007; Liu and Chan 2008; Szafron and Soteros 2011; Cheston et al. 2014) are inspired by the interaction between DNA and *topoisomerase*, a specific enzyme that cuts and rejoins strands, and thus modifies their topological state. Such strand-passage models induce transition probabilities between knot types, which can be estimated by numerical simulations, and these lead to a stationary equilibrium distribution over knots.

Finally, Babson and Westenberger study knots obtained from a curve in  $\mathbb{R}^n$  by projecting to  $\mathbb{R}^3$  in a random direction. They relate several of the above constructions to this original framework (Westenberger 2016).

In principle, any reasonable way to construct or represent knots could be turned into a random model. Another case in point are trajectories of dynamical systems, such as three-dimensional billiard (Jones and Przytycki 1998).

## 4 A closer look at the Petaluma model

We now focus on random knots and links in the Petaluma model (3.5), and discuss the distribution of their finite type invariants and hyperbolic volume. First we recall the definition of finite type invariants, given in terms of singular knots and links (Birman and Lin 1993).

### 4.1 Finite type invariants

Unlike a regular knot, which is a smooth embedding of  $S^1$  into  $\mathbb{R}^3$  up to isotopy, a *singular* knot is allowed to have finitely many double points of transversal self intersection. Each of these points can be locally *resolved* in two well-defined ways: positive  and negative .

Let  $v$  be a knot invariant taking values in some abelian group, usually in  $\mathbb{Z}$ . The extension of  $v$  to singular knots is given by  $v(K) = v(K_p^+) - v(K_p^-)$ , where  $K_p^\pm$  are the two resolutions of the singular knot  $K$  at the double point  $p$ . By recursion, the value of  $v$  on a singular knot with  $m$  double points is given by a signed sum of its value on  $2^m$  regular knots. We say that  $v$  is a *finite type* knot invariant of *order*  $m$  if it vanishes on all singular knots with  $m + 1$  double points.

This condition is satisfied by several well-studied knot invariants, such as coefficients of knot polynomials (Bar-Natan 1995a; Chmutov et al. 2012) and the Kontsevich integral (Bar-Natan 1995b; Chmutov and Duzhin 2001). There is only one knot invariant of order two, up to affine equivalence—the *Casson invariant*  $c_2(K)$ , which is the coefficient of  $x^2$  in the Alexander-Conway polynomial  $C_K(x)$ . It similarly appears in the modified Jones polynomial,  $V_K(e^x)$  considered as a power series in  $x$ , which also yields an invariant  $v_3(K)$  of order three. The number of new independent finite type invariants grows with the order: 3 invariants of order four, 4 of order five, 9 of order six, etc. Bar-Natan (1995b).

No invariant of knots has order one. However, the Gauss *linking number*  $lk(L)$  is a classical first order invariant of two-component links. Also the framing number, or *writhe*  $w(K)$  as in Even-Zohar (2017), is a first order invariant of framed knots.

### 4.2 Asymptotic distributions

Finite type invariants of random knots and links in the Petaluma model (3.5) have been studied by Hass, Linial, Nowik, and the author (Even-Zohar et al. 2016; Even-Zohar 2017). In particular, we have investigated how these invariants scale and distribute for knots with a large number of petals.

Consider the Casson invariant of a random knot with  $2n + 1$  petals. It is not hard to observe that  $c_2(K_{2n+1}) = O(\pm n^4)$ , which is shown to be sharp for torus knots and other explicit constructions. However, we have found that the typical order of magnitude of the Casson invariant is actually  $n^2$ . Indeed, its expectation is  $E[c_2] = n(n - 1)/24$ , its variance is  $V[c_2] = 7/960 \cdot n^4 + O(n^3)$ , and such formulas have been given for all moments, yielding  $E[c_2^k] = \Theta(n^{2k})$ . We find it intriguing that

the distribution of the properly normalized Casson invariant  $c_2/n^2$  is asymmetric and not centered at zero, asymptotically as  $n \rightarrow \infty$ .

The third order invariant  $v_3(K_{2n+1})$  is antisymmetric with respect to reflection, hence its distribution is symmetric around zero. As for its even-order moments, we have similarly shown  $E[v_3^k] = O(n^{3k})$ , e.g.,  $V[v_3] = 9298/5443200 \cdot n^6 + O(n^5)$ .

In terms of their moments,  $c_2$  grows as  $n^2$  and  $v_3$  as  $n^3$ . This naturally suggests that an  $m$ th order invariant of random knots with  $n$  petals asymptotically scales as  $n^m$ . In Even-Zohar et al. (2016) we conjecture that  $v_m(K_{2n+1})/n^m$  weakly converges to a limiting distribution as  $n \rightarrow \infty$  for every finite type invariant  $v_m$  of order  $m$ . The existence of continuous limit distributions for  $c_2$  and  $v_3$  is supported by computational evidence, as discussed below.

We have established such a limiting distribution in two cases: the linking number of a random two component link with  $2n$  petals in each component, and the writhe of a random framed knot with  $2n+1$  petals. Both are first order invariants, and obtain integer values sharply between  $\pm n^2$ . In Even-Zohar et al. (2016) we prove that  $lk(L_{2n,2n})/4n$  converges to the *logistic distribution*, with density function  $f(t) = \pi/\cosh^2(2\pi t)$ . The normalized writhe  $w(K_{2n+1})/n$  converges to another non Gaussian limiting distribution, established and described in Even-Zohar (2017).

Our proofs combine the method of moments with careful combinatorial analysis of the limiting moments of these invariants, expressed via Gauss diagram formulas.

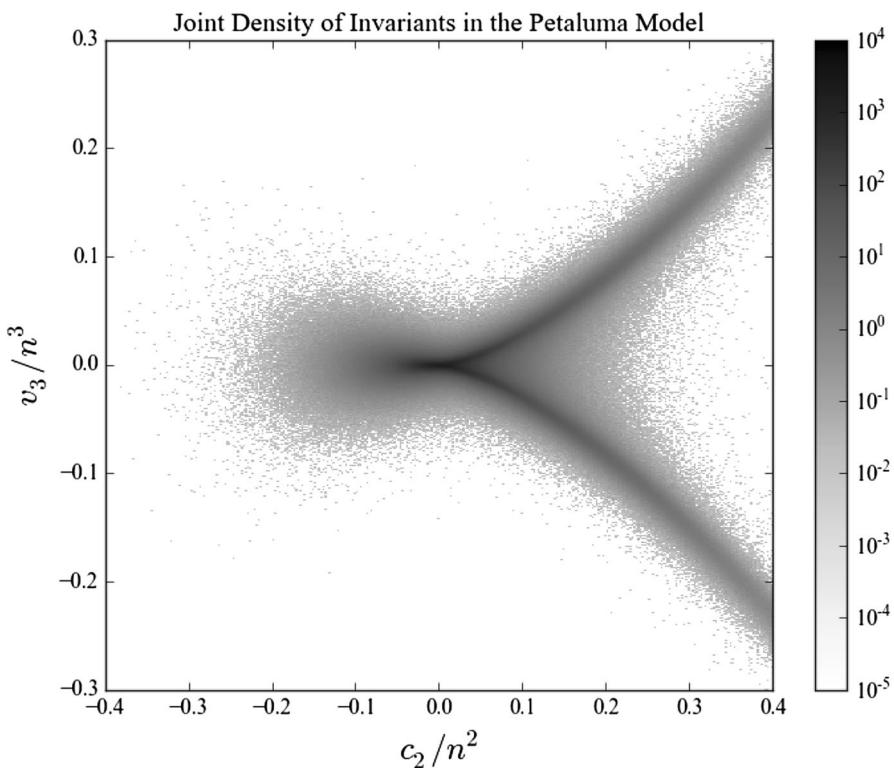
### 4.3 Numerical experiments

We study the invariants  $c_2(K_n)$  and  $v_3(K_n)$  in the Petaluma model, by computing their values for a random sample of permutations in  $S_n$ . Comparing the results for various values of  $n$ , we observe that as  $n$  grows the joint distribution of  $c_2/n^2$  and  $v_3/n^3$  seems to converge to a continuous bivariate distribution of a certain shape. The heat map in Fig. 13 shows the resulting density function of this distribution for  $n = 41$ , which seems to be a good approximation of the conjectured limiting distribution.

The planar representation of these two invariants follows previous work by Willerton (2002); Chmutov et al. (2012) and Ohtsuki et al. (2002), who generated scatter plots of  $(c_2, v_3)$  for all prime knots with up to  $n$  crossings. They similarly obtained fish-shaped figures, although it is unclear how these should scale as the crossing number grows. The Petaluma model may provide a more concrete way to catch this fish, in the form of a limit density function defined on  $\mathbb{R}^2$ .

Besides representing the first two finite type invariants of knots, the planar map  $\varphi : K \mapsto (c_2(K), v_3(K))$  has some interesting properties. As observed by Dasbach et al. (2001), the evaluation of the Jones polynomial at roots of unity near 1 can be approximated by  $V_K(e^{ih}) = 1 + 3c_2h^2 + 6v_3h^3i + O(h^4)$ , and this yields similar fish graphs for  $V_K(e^{2\pi i/N})$  in the complex plane, for  $N \gg n$ .

Note that by the multiplicativity of the Jones polynomial, the map  $\varphi$  is additive with respect to connected sum:  $\varphi(K \# K') = \varphi(K) + \varphi(K')$  in  $\mathbb{Z}^2$ . Using this fact and some known constructions one can show that as  $n$  grows the resulting point set



**Fig. 13** The normalized distribution of  $c_2$  and  $v_3$  for a random knot  $K_{41}$ , based on  $10^8$  random samples

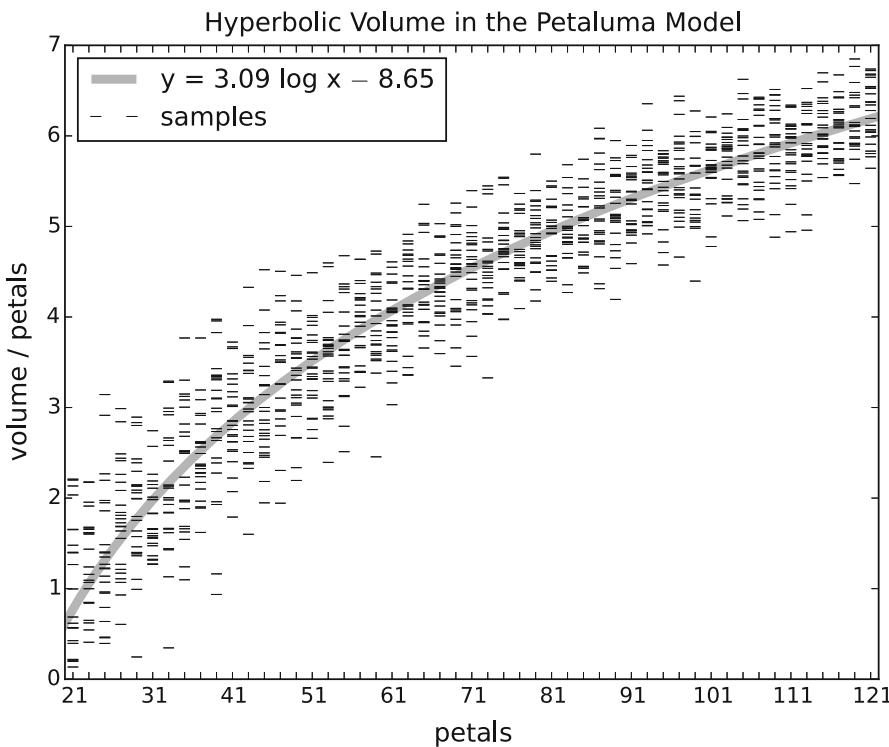
of all  $(c_2/n^2, v_3/n^3)$  is dense in  $\mathbb{R}^2$ . We actually conjecture that the limiting bivariate distribution has positive density everywhere in the plane.

#### 4.4 Hyperbolic volume

We conclude this section with further numerical experiments, concerning the distribution of the hyperbolic volume in the Petaluma model, as approximated by the *Sage* package *SnapPy* (Culler et al. 2016).

As mentioned in Sect. 3.5, our simulations show that randomly sampled knots with up to 200 petals are mostly hyperbolic. This trend seems to strengthen with increasing number of petals, although one must be careful drawing conclusions from small cases, cf. Malyutin (2016) mentioned in Sect. 3.9.

Figure 14 shows how the empirical hyperbolic volume grows super-linearly with the number of petals. More speculatively, the volume of an  $n$ -petal knot appears to be concentrated around a curve of the form  $An \log Bn$ , which seemed to fit better than a linear function, or one of order  $n^{3/2}$ . These experiments have been repeated by Kehne (2016). They have also proved that the expected volume is at most  $4\pi n \log n$ , by constructing a pyramid decomposition of the petal knot



**Fig. 14** The hyperbolic volume per petal grows with the number of petals. This is based on random samples of 25 knots with 21 to 121 petals. Non-hyperbolic knots (< 2.5%) were omitted

complement (Adams 2017; Adams and Kehne 2016). Any such lower bound would be of great interest.

## 5 Discussion

This great variety of approaches for random knot models suggests that we ask how they differ. Do they exhibit some kind of common properties? By what means should we compare models? What do they teach us about knot invariants and knot theory? Below we record some thoughts concerning these questions.

### 5.1 Local knotting

The Delbrück–Frisch–Wasserman conjecture, that a typical random knot is non-trivial, has been proved by now in several models. Some insight on their properties can be gained by comparing the arguments involved in these proofs.

The knottedness of random polygonal and grid walks (3.1, 3.2) is based on the fact that such knots tend to have many spatially *localized* connected summands. This phenomenon can be attributed to the small steps taken in these

models (Sumners and Whittington 1988; Pippenger 1989; Diao et al. 1994; Diao 1995). We do know, however, that large scale knotting occurs as well (Jungreis 1994; Diao et al. 2001). Also for planar diagrams (3.7), knottedness follows from the existence of small prime summands in random knot and link diagrams (Chapman 2016c). Even for prime knots in the knot table model (3.9), local configurations of a double figure-eight knot provide a satellite decomposition (Malyutin 2016).

In contrast to the highly composite knots produced by small-steps models, we believe that models of *non-local* nature yield knots with much simpler factorization. By non-local we mean that the typical step length is comparable to the diameter of the whole curve.

For example, local entanglements yield only a vanishing probability of order  $1/n^3$  for a trefoil summand in the Petaluma model (3.5). Indeed, its knottedness with high probability was shown by other means, a coupling argument based on the effect of random crossing changes on finite type invariants (Even-Zohar et al. 2017a). As mentioned above, numerical experiments indicate that these knots are mostly hyperbolic, so that any connected sum or satellite-type decomposition might become rare.

## 5.2 Dimension

It would be interesting to further distinguish knot models from each other by their asymptotic topological features. On the other hand, it would be very interesting to discover *universal* phenomena and parameters that hold for a variety of different models.

We shall venture some speculations along these lines. As a first step, consider the following three classes of random models.

- 1D** Grid walks (3.1), polygonal walks (3.2), and smoothed Brownian motion (3.3).
- 2D** Random planar diagrams (3.7), the griddle (3.8), knot table (3.9), and star (3.11).
- 3D** Random jumps (3.4), the Petaluma (3.5), and grid diagrams (3.6).

This classification attempts to grasp the “dimension”, or general shape, of the actual spatial curves constructed by the different models, in some loose and undefined sense. It is a fundamental challenge to characterize such a classification precisely.

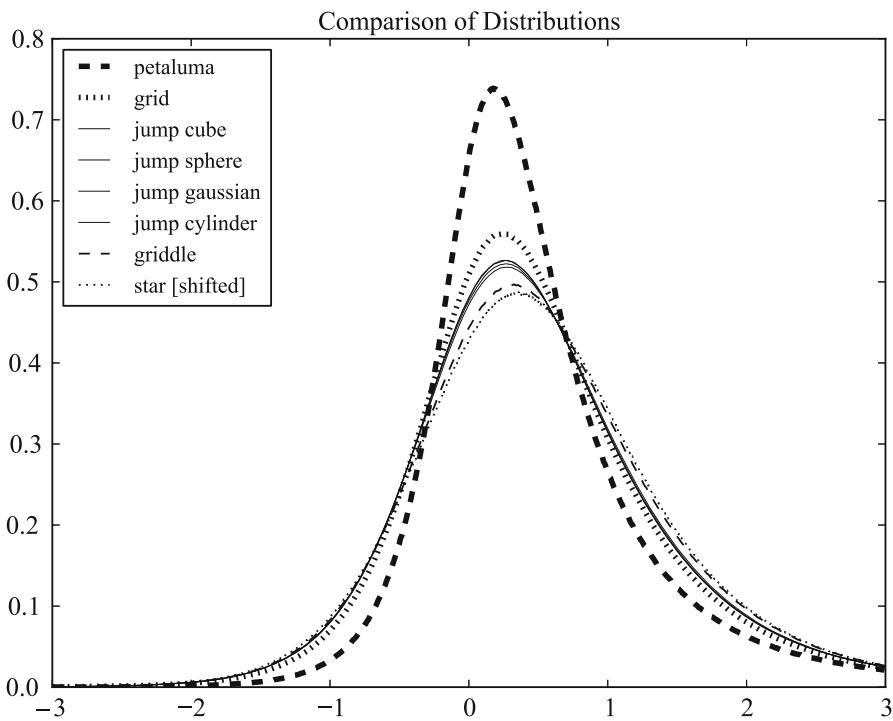
Would it be possible to reconstruct the class to which some random model belongs, by looking only at the asymptotics of the topological invariants of the resulting knots?

### 5.3 Comparing invariants

Our computations and experiments (Even-Zohar et al. 2016, 2017b) show that the asymptotic distributions of the Casson invariant in models of the third class share several important features. In Fig. 15, we exhibit numerically generated histograms of the Casson invariant for three models: Petaluma (3.5), grid (3.6), and several random jump models (3.4). They all seem to converge to continuous unimodal limit distributions on  $\mathbb{R}$ , with two-sided exponentially decaying tails, strictly positive expectations and similarly asymmetric shapes.

Even though models of the second class also seem to converge to distributions of similar shapes around their expectations, their main terms are inconsistent. In the griddle (3.8) model  $E[c_2]/\sqrt{V[c_2]} = \Theta(1)$ , while in the star (3.11) model  $E[c_2]/\sqrt{V[c_2]} = \Theta(n)$ .

We hope that extending such comparisons to other invariants would shed more light on the above questions of classification and universality.



**Fig. 15** The distribution of  $c_2(K_n)/n^2$  in several random knot models, for  $n = 80$  or  $81$ , based on  $10^8$  random samples each, and normalized to have variance one. Only the star histogram was shifted to compensate for its rightward drift

## 5.4 Open problems

Models of the third class outlined above seem especially interesting from a knot-theoretic point of view. They presumably avoid phenomena of local knotting or “flatness”, and their finite type invariants seem to follow well-behaved distributions.

We close our review by listing some of the desired features of these random models, which are yet to be established.

**Conjecture** Let  $K_n$  be a random knot, sampled from any of the following models: Random Jump (3.4), Petaluma (3.5), Grid (3.6). Then,

- With high probability  $K_n$  is prime, and even hyperbolic.
- With high probability  $K_n$  is non-alternating.
- The typical crossing number is super-linear:  $E[c(K_n)] = \omega(n)$ .
- The probability of every knot  $K$  is sub-exponential:  $P[K_n = K] = e^{-\omega(n)}$ .
- Any finite type invariant of order  $m$  has typical order of magnitude  $n^m$ .

## 5.5 Implementation details

We include here some information about the numerical results that are firstly reported in this paper.

The generation of random knots in various models was performed by a *C++* program, available at Even-Zohar (2016b). The computation of finite type invariants, as in Sects. 4.3 and 5.3, was carried out using *Gauss diagram formulas* (Chmutov et al. 2012), which can be evaluated in polynomial time. The computations were distributed on up to 168 processors in the computing facilities of the School of Computer Science and Engineering at HUJI. They were supported by ERC 339096.

The formulas for invariants of random grid and griddle knots with  $2n$  segments in Sects. 3.6 and 3.8, were derived by automated case analysis of the many possible configurations of the involved crossings. It was implemented in a *Python* program, available at Even-Zohar (2016a). These computations took several hours on a PC.

The data in Fig. 14 was obtained from the *Sage* software *SnapPy* (Culler et al. 2016), that approximates the hyperbolic volume of a link by finding a triangulation of its complement with compatible hyperbolic structure. In order to make the random samples suitable as input for the program, we first converted them from petal diagrams to braids, as shown in Fig. 12. Some concerns regarding the verification of hyperbolicity and the stability of the computed volume are discussed by Kehne (2016). Our results are available, together with the source code that generated them, at Even-Zohar (2016c). The computation took several days on a PC.

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### Compliance with ethical standards

**Conflict of interest** The author states that there is no conflict of interest.

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