EXTENSIONS TO RANDOM POLYGON GENERATION IN SPHERICAL CONFINEMENT

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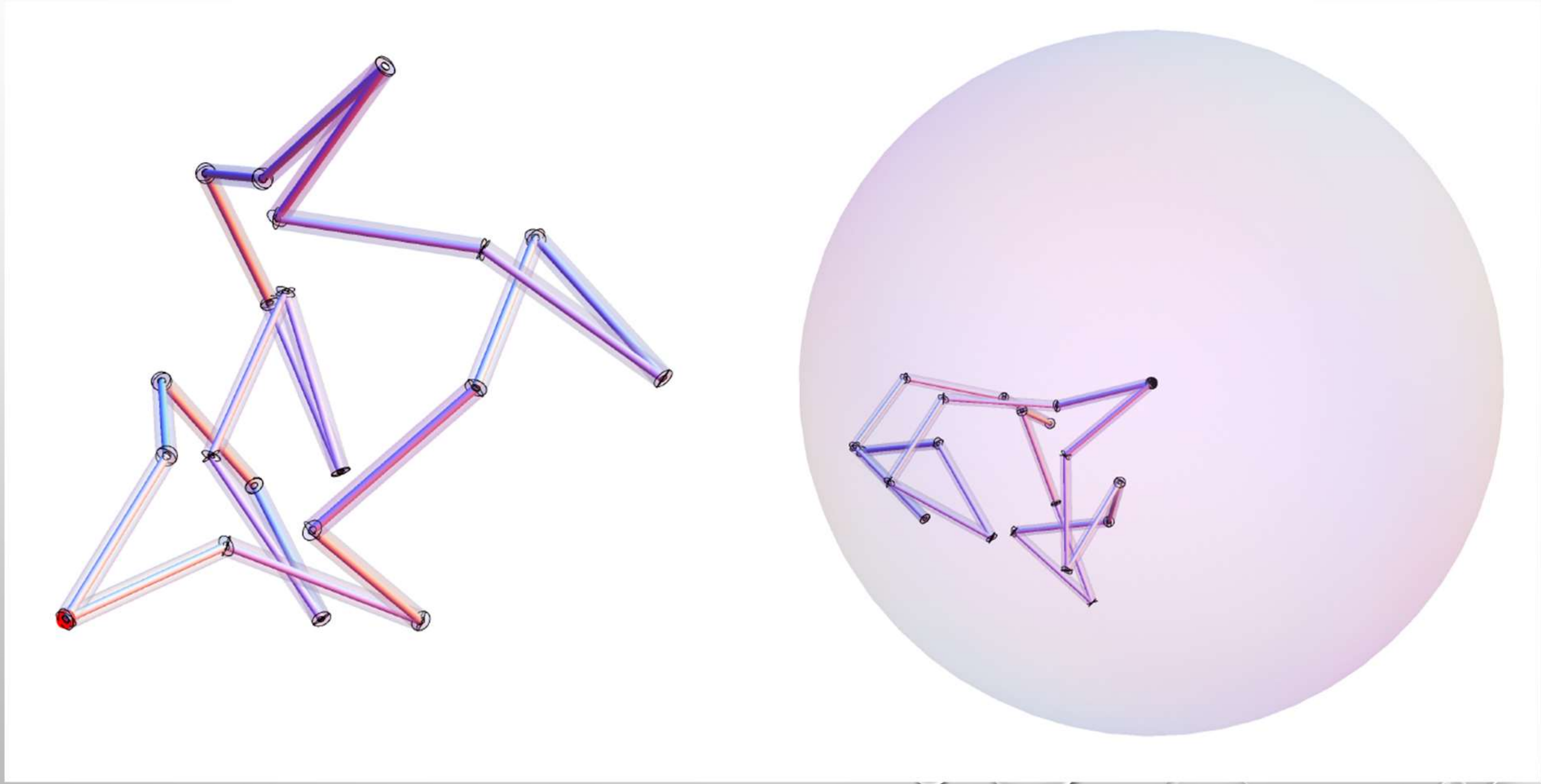
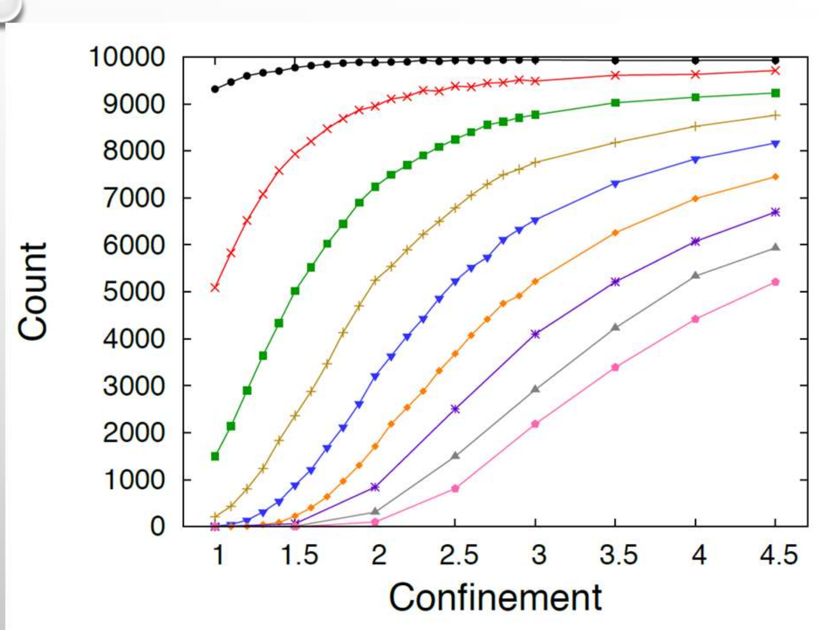
OUTLINE

- SHORT SUMMARY FROM THIS MORNING’S TALK ON RANDOM POLYGONS FROM CLAUS
- EXTENSION 1: WHAT HAPPENS IN SPHERICAL CONFINEMENT FOR $R < 1$?
  - DOES THE MODEL PRODUCE REASONABLE DATA?
  - IS THE DATA CONSISTENT WITH PREVIOUS SPHERICAL CONFINEMENT DATA?
  - CAN WE QUANTIFY THE ‘CONFINEMENT RADIUS’ FOR THE MODEL?
- EXTENSION 2: BIASING POLYGONS IN CONFINEMENT TOWARDS THICKNESS
  - DOES THE MODEL PRODUCE REASONABLE DATA?
  - IS THE DATA CONSISTENT WITH PREVIOUS SPHERICAL CONFINEMENT DATA?
  - CAN WE QUANTIFY THE EFFECT OF THICKNESS

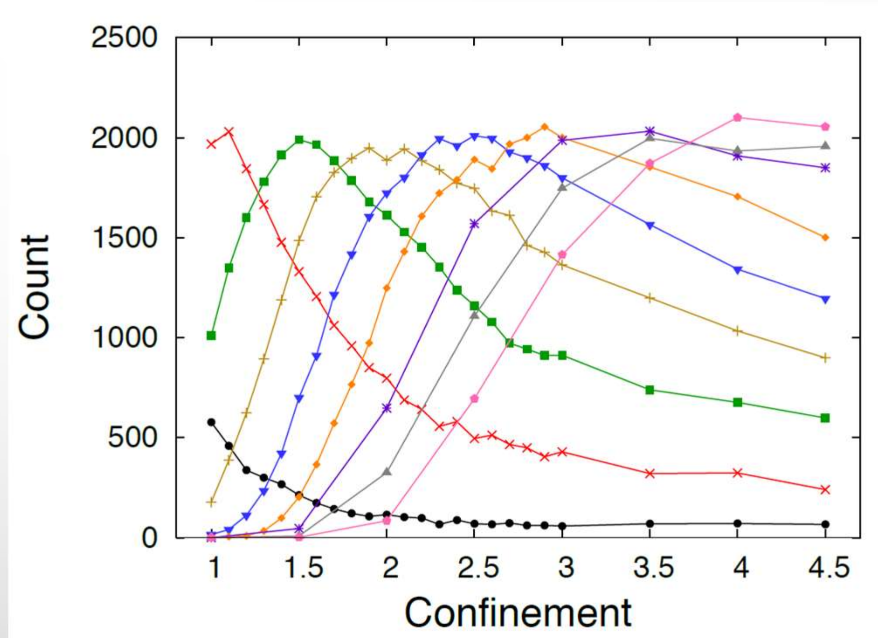
SHORT SUMMARY FROM PRIOR TALK



SHORT SUMMARY FROM PRIOR TALK

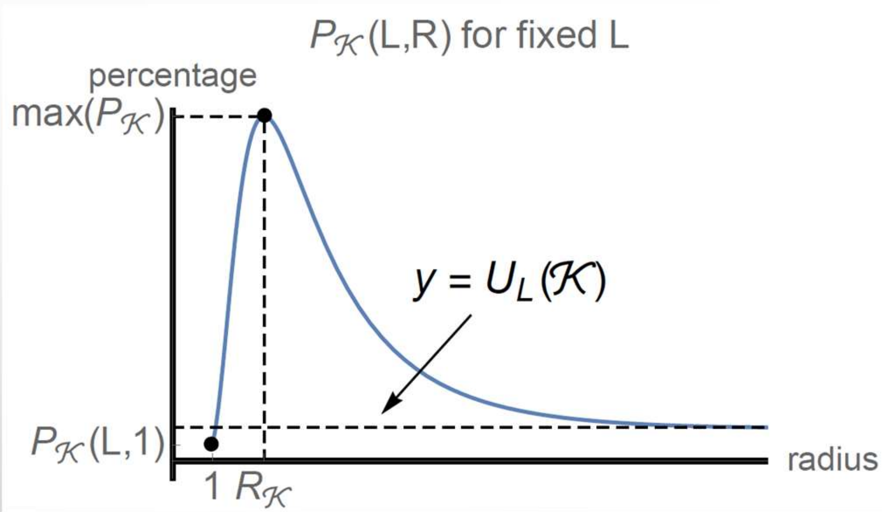


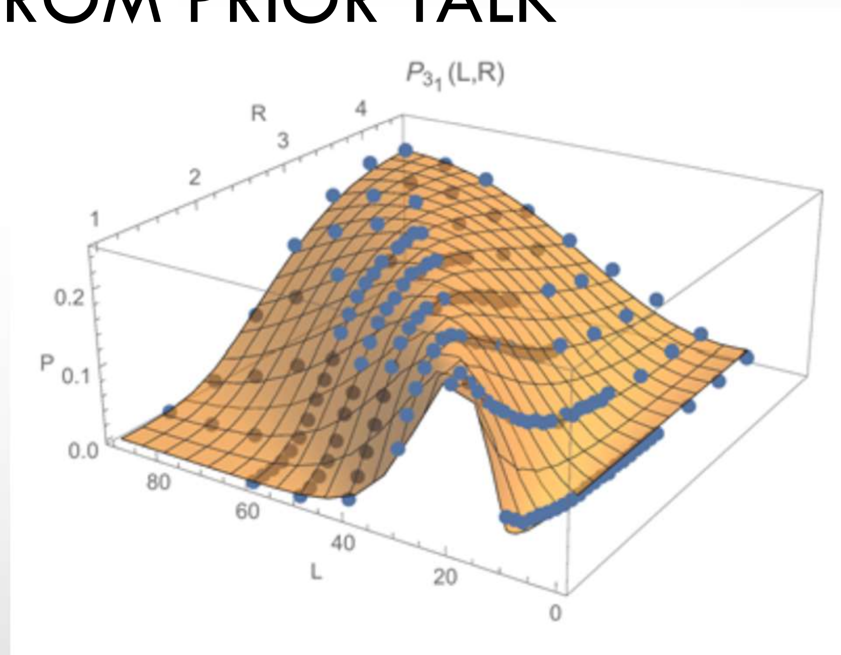
unknots



trefoils

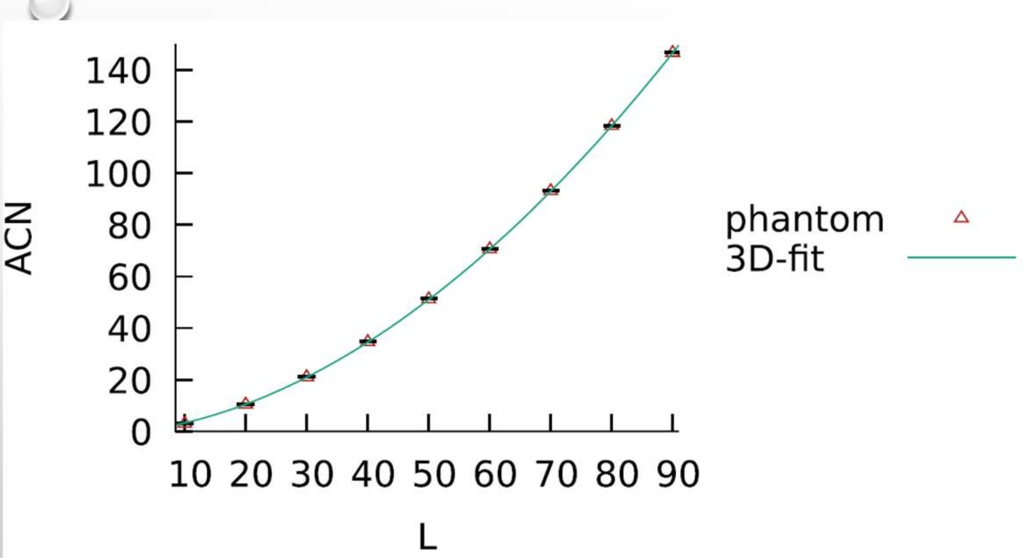
SHORT SUMMARY FROM PRIOR TALK

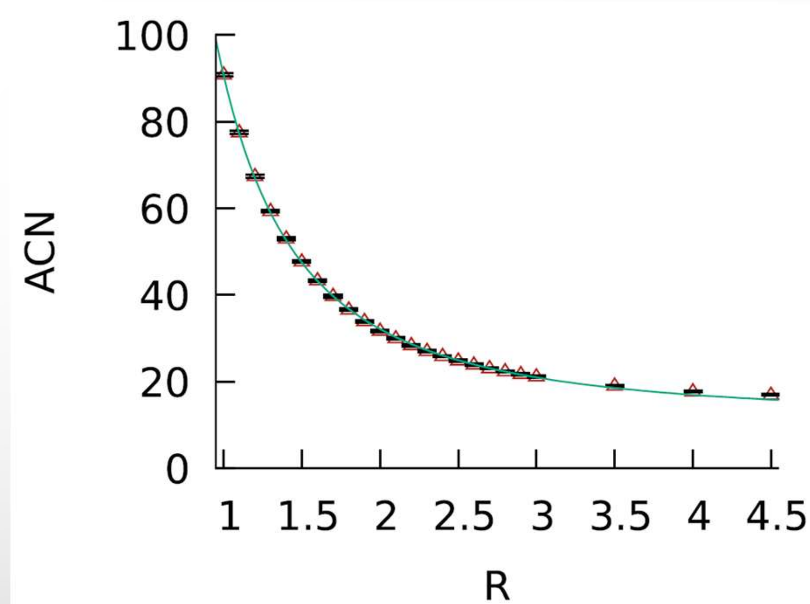




$$P_{\mathcal{K}}(L,R) = a\left(d + \left(\frac{L - L_0(\mathcal{K})}{R - 0.6}\right)^e\right)\exp\left(-\frac{L}{bR - c}\right)$$

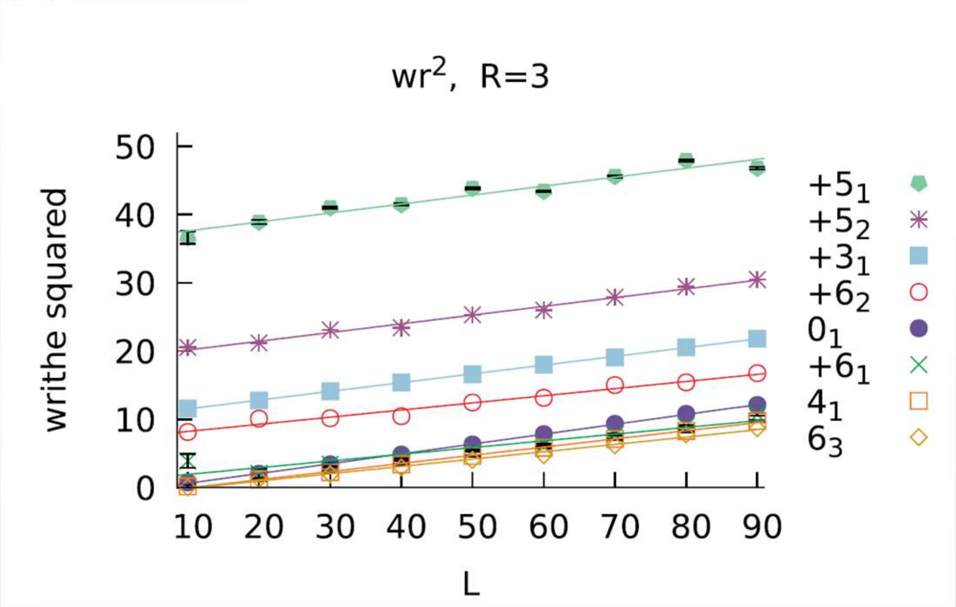
SHORT SUMMARY FROM PRIOR TALK

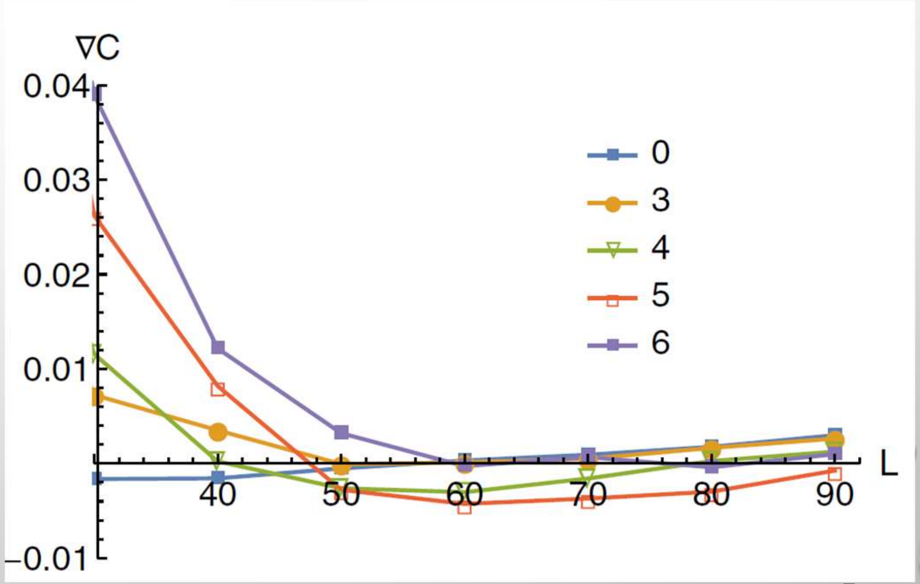




$$A(R,L) = \left(\frac{a}{R} + \frac{b}{R^2}\right)L^2 + \left(c + \frac{d}{R^2}\right)L\ln L$$

SHORT SUMMARY FROM PRIOR TALK





EXTENSION 1: EXTREME CONFINEMENT

OUTLINE

- MOTIVATION
- CYLINDRICAL MODEL & DATA COLLECTED
- QUESTIONS:
  - DO THE CYLINDRICAL POLYGONS SEEM TO BE GENERATED IN CONFINEMENT WITH $R < 1$?
  - ARE THE FEATURES OF THE CYLINDRICAL POLYGONS IN LINE WITH THE FEATURES OF SPHERICAL POLYGONS?
  - CAN THE CONFINEMENT RADIUS BE QUANTIFIED?
- ASYMPTOTIC BEHAVIOR OF RANDOM POLYGONS OF LENGTH 30 FOR $R \rightarrow 0.5^+$

MOTIVATION – EXTREME CONFINEMENT

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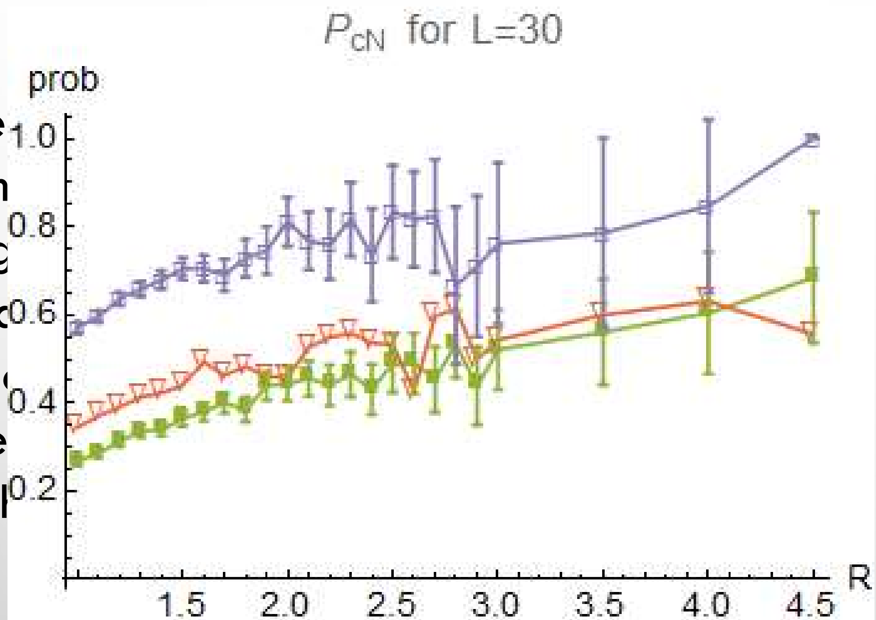
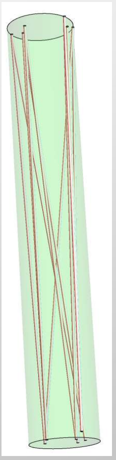


We could only study confinement spheres with a radius larger than 1, due to the properties of the generation algorithm.

APPROACH

Simple model – polygons do not have exact probabilities as in tight spherical confinement

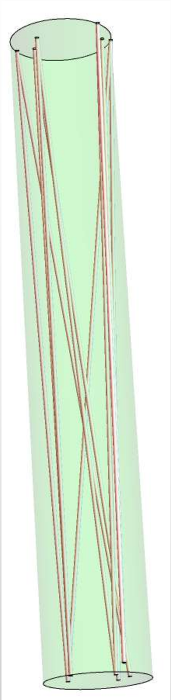
- Generate random, nearly equilateral polygons which lie within a cylinder with flat top and bottom disks.
- Uniformly pick points on the top and bottom of a cylinder of height h and radius r.
- Connect the points and then connect the last point to the first point.



CYLINDRICAL MODEL

- The probability to randomly generate certain knots does not change with a change in the height of the cylinder.

- Geometric quantities may change with the height of the cylinder



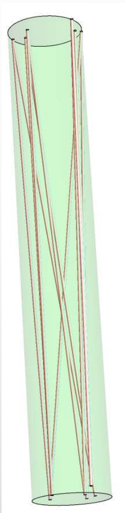
DATA

- Generated cylindrical polygons of length 6 to 30; 1 million for each length

- Comparison: spherical data for R = 1 to 3 in 0.1 increments for lengths 10 to 50

- Identified the knot type of each polygon – or determine an upper bound on the crossing number of the polygon.

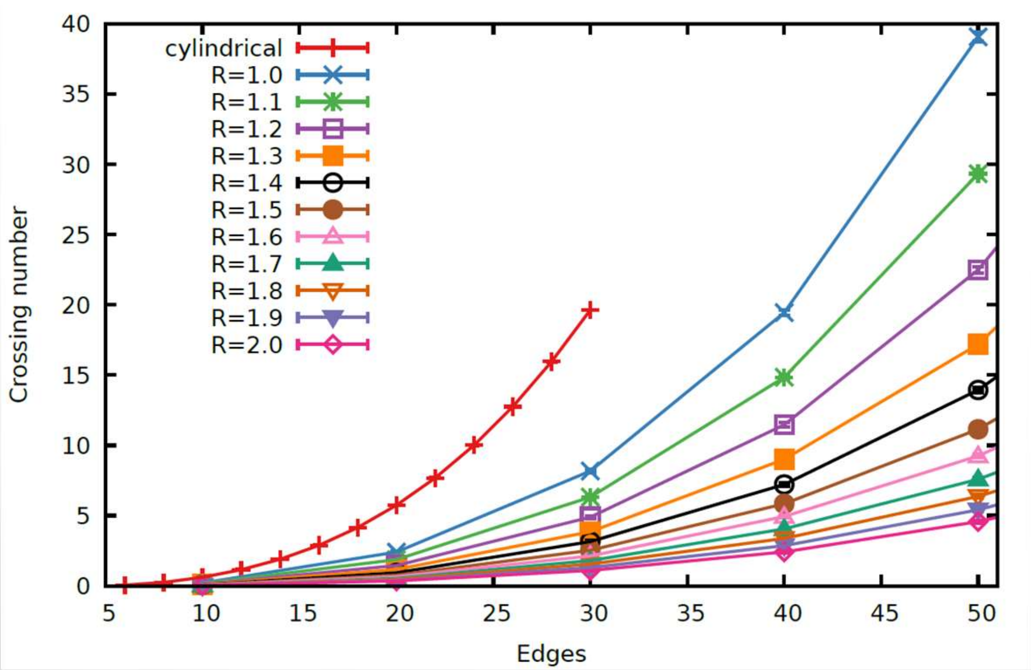
- Compute the ACN, writhe, curvature, and torsion for each polygon.



QUESTION 1:

DO THE CYLINDRICAL POLYGONS SEEM TO BE GENERATED IN CONFINEMENT WITH $R < 1$?

RESULTS - TOPOLOGICAL



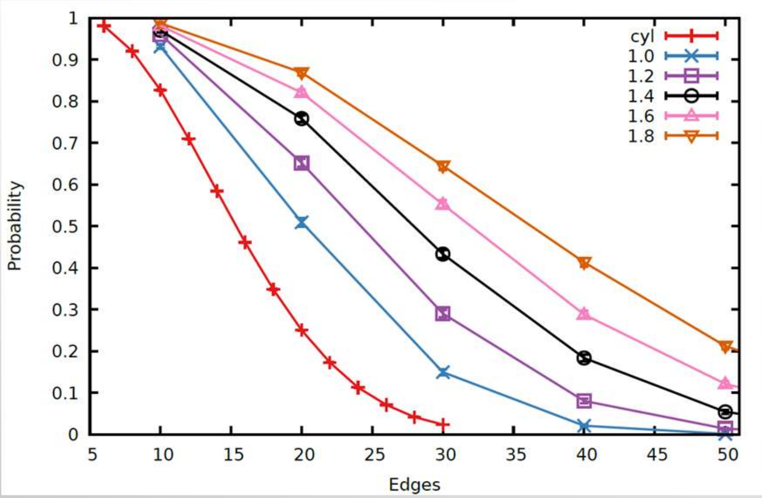
At length 30	%
unclassified	59.16
unknot	2.36
alternating	14.47
non-alternating	20.47
composite	3.54

Mean topological crossing number for spherical and cylindrical confinement

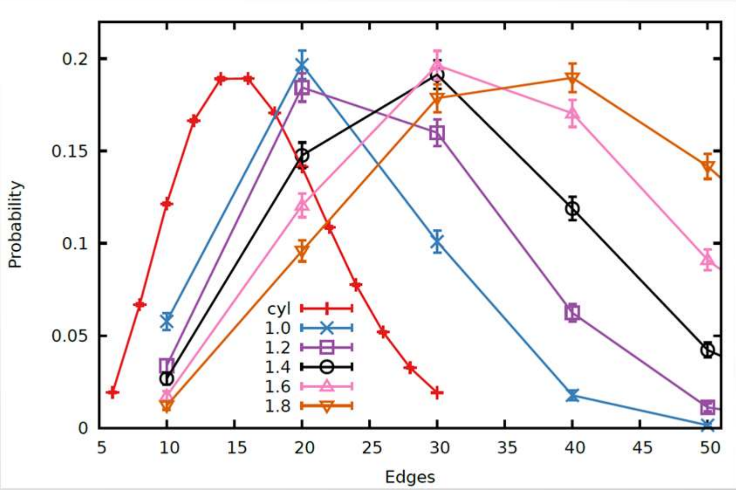
C. Ernst, E.J. Rawdon, and U. Ziegler; Knotting spectrum of polygonal knots in extreme confinement; J. Phys. A Math. Theor. (2021) **54** 235202

RESULTS - TOPOLOGICAL

for unknots



for trefoils



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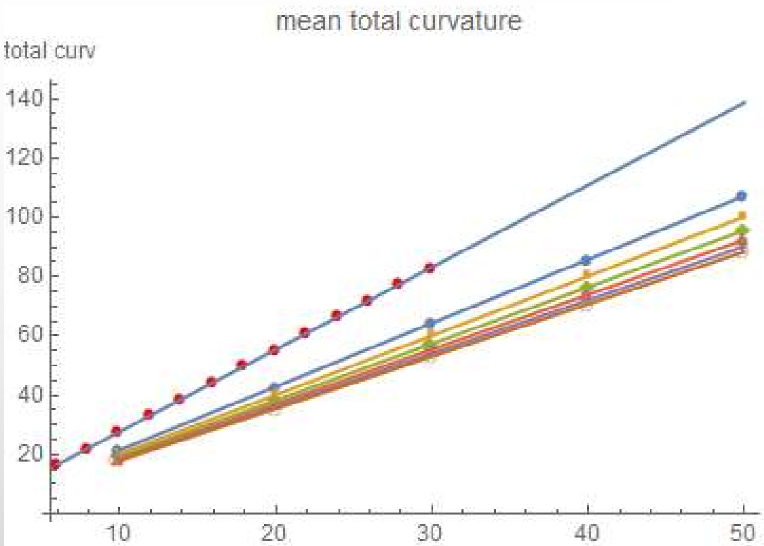
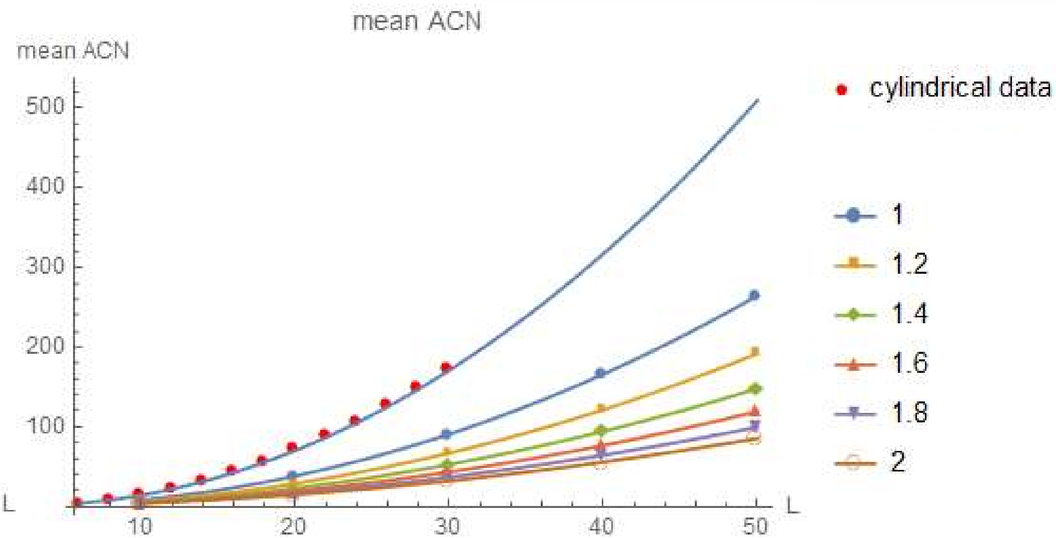
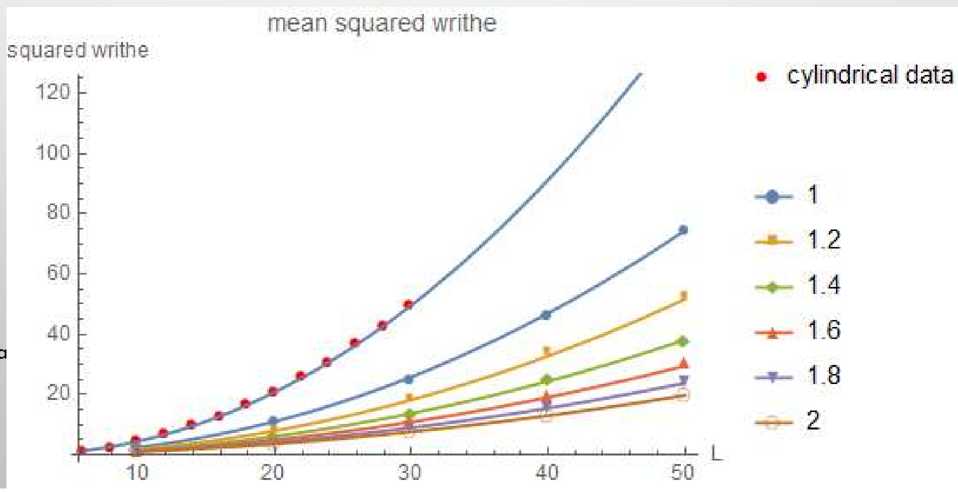
RESULTS - GEOMETRICAL





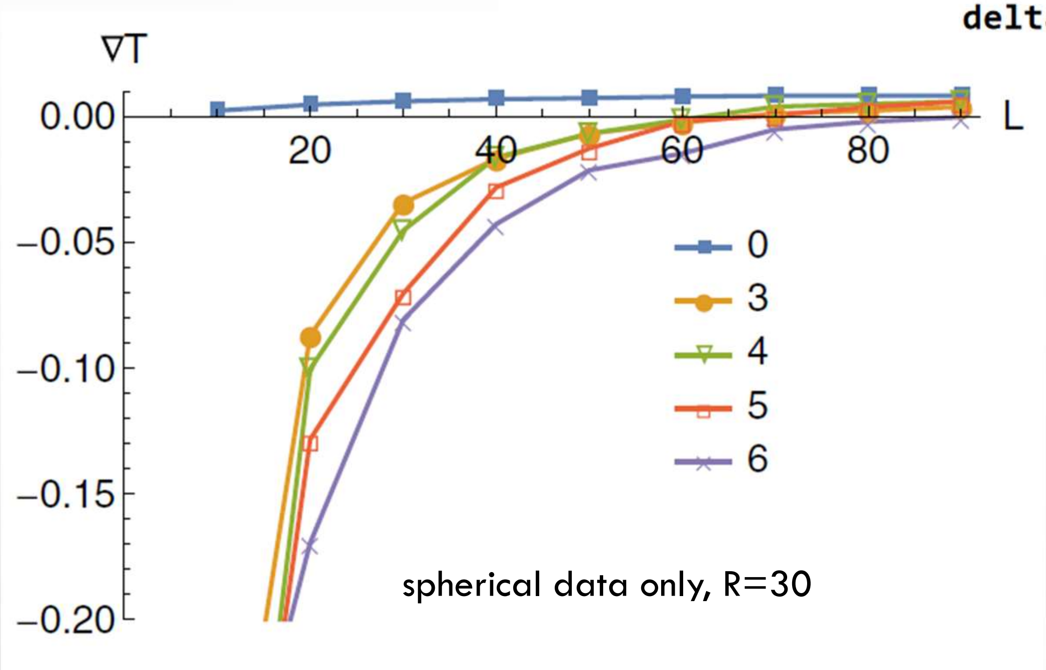


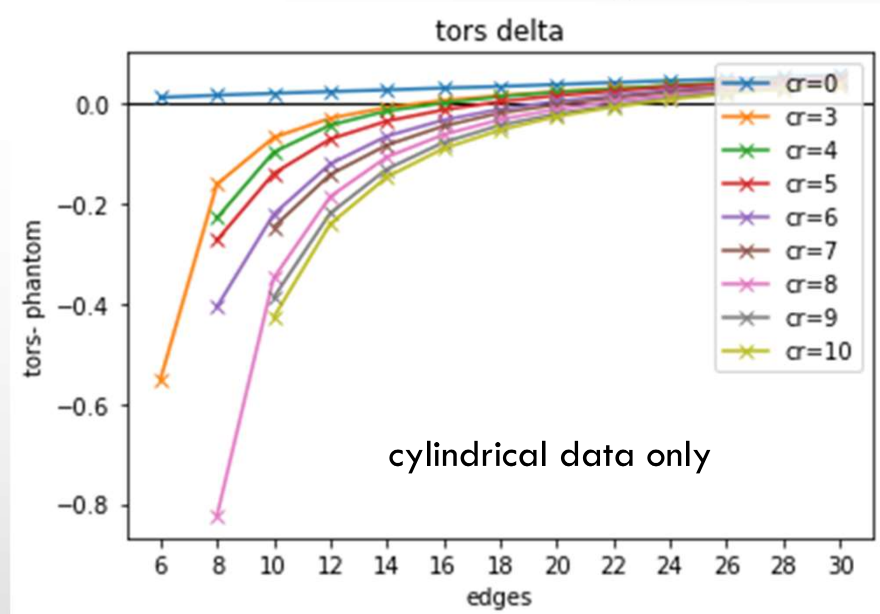
QUESTION 2:

ARE THE FEATURES OF THE CYLINDRICAL POLYGONS CONSISTENT WITH THE FEATURES OF SPHERICAL POLYGONS?

RESULTS - GEOMETRIC – TORSION

$$\mathbf{delta\ tors_{cr}\ (R,\ L)} = \frac{\mathbf{tors_{cr}\ (R,\ L) - tors_{phantom}\ (R,\ L)}}{\mathbf{L}}$$

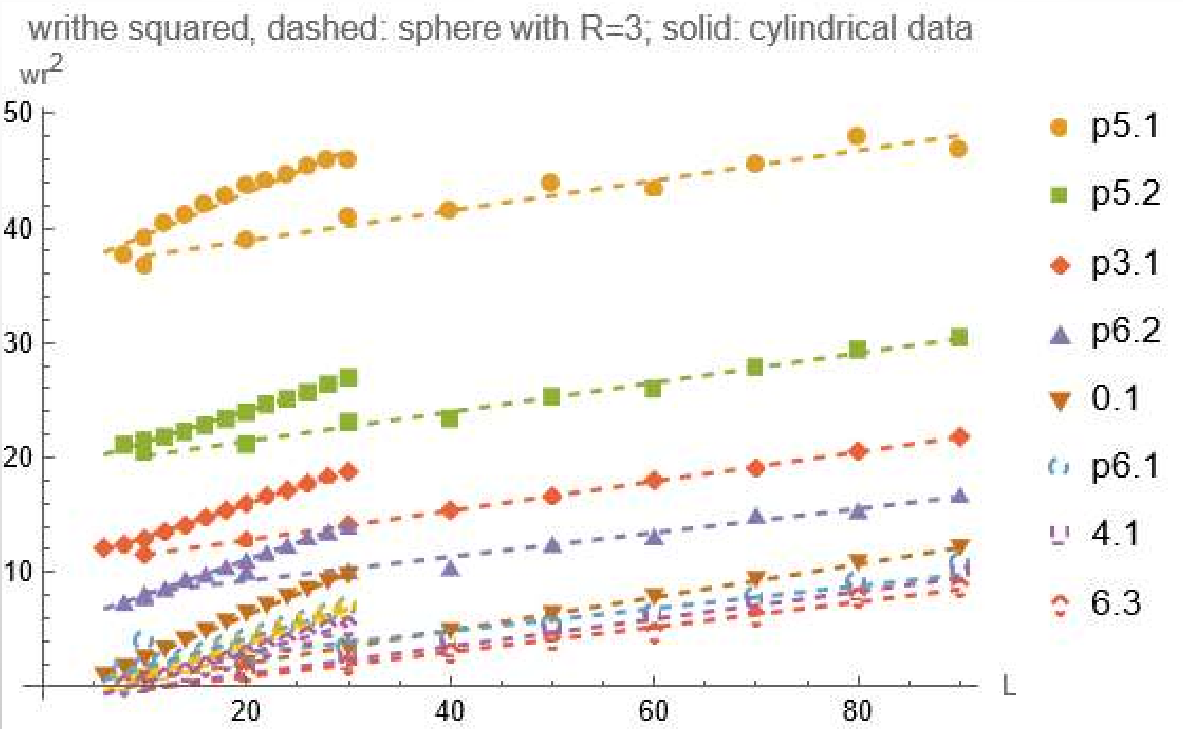




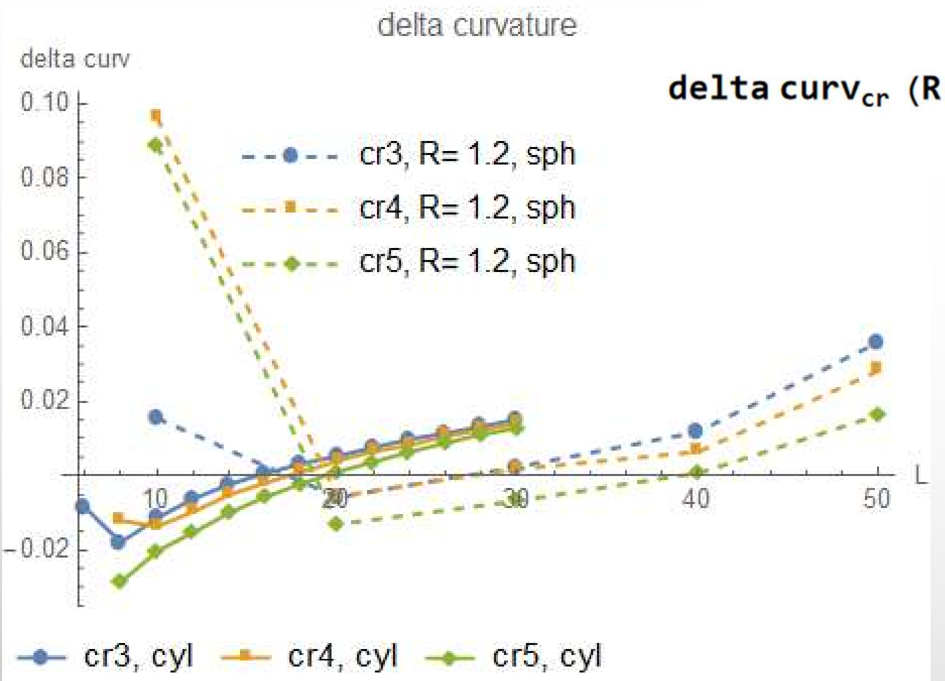
more complex knots have **lower** torsion

Y. Diao, C. Ernst, E.J. Rawdon, U. Ziegler, Total curvature and total torsion of knotted random polygons in confinement, J. Phys. A Math. Theor. 51 (15) (2018), 154002.

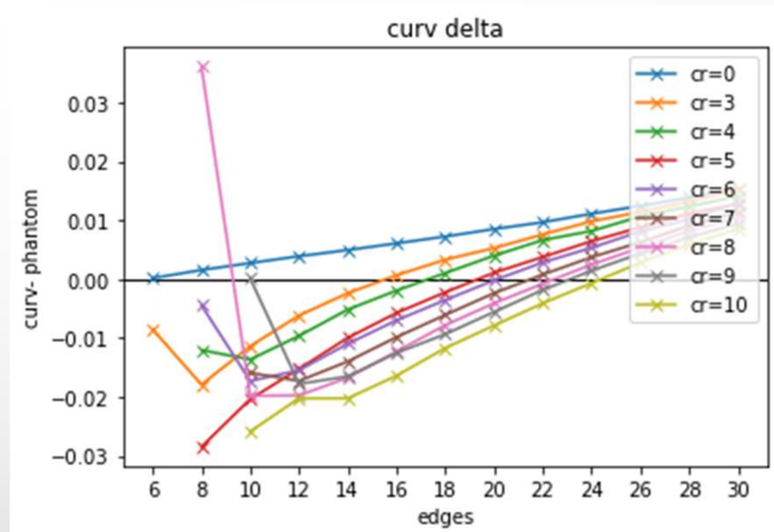
RESULTS - GEOMETRIC – WRITHE^2



RESULTS - GEOMETRIC – CURVATURE



$$\text{delta curv}_{cr}\ (R,\ L) = \frac{\text{curv}_{cr}\ (R,\ L) - \text{curv}_{phantom}\ (R,\ L)}{L}$$



short lengths: more complex knots have **higher** curvature

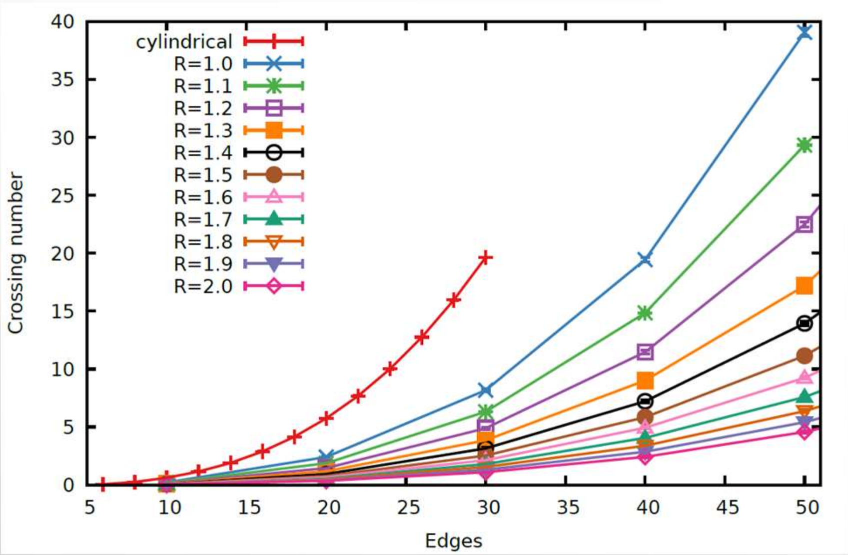
long lengths: more complex knots have **lower** curvature

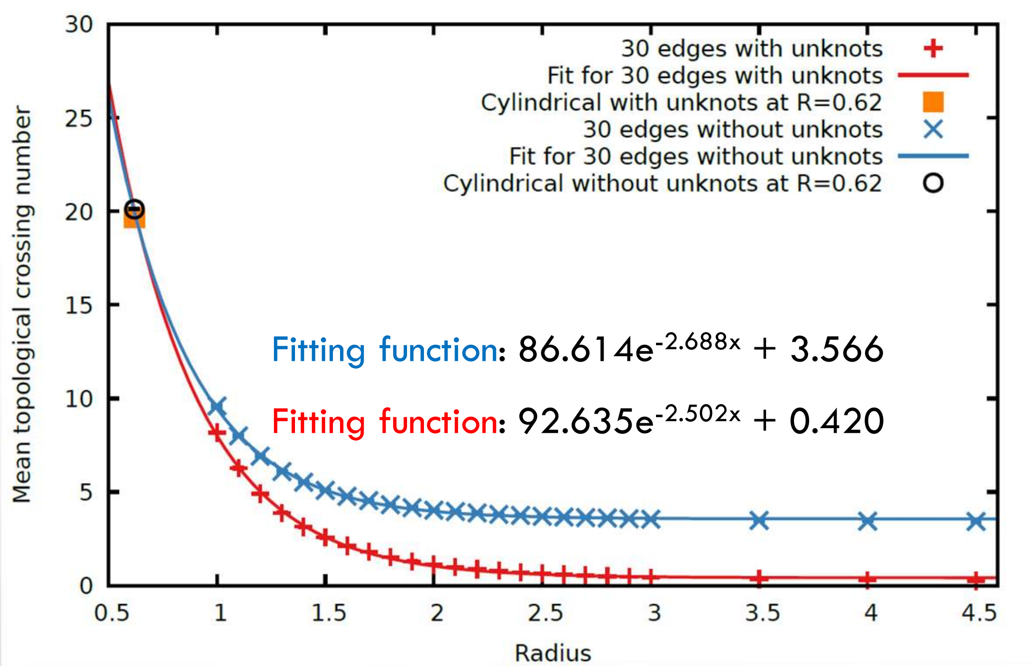
Y. Diao, C. Ernst, E.J. Rawdon, U. Ziegler, Total curvature and total torsion of knotted random polygons in confinement, J. Phys. A Math. Theor. 51 (15) (2018) 154002.

QUESTION 3:

- CAN THE ‘EQUIVALENT’ CONFINEMENT RADIUS BE QUANTIFIED?

RESULTS – TOPOLOGICAL

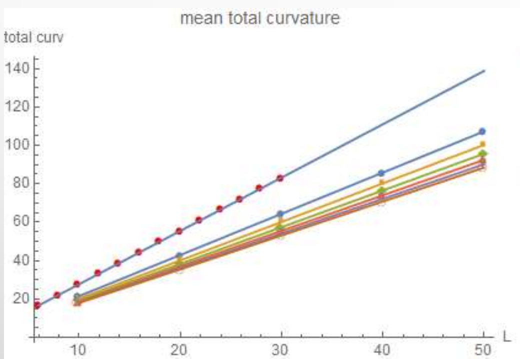


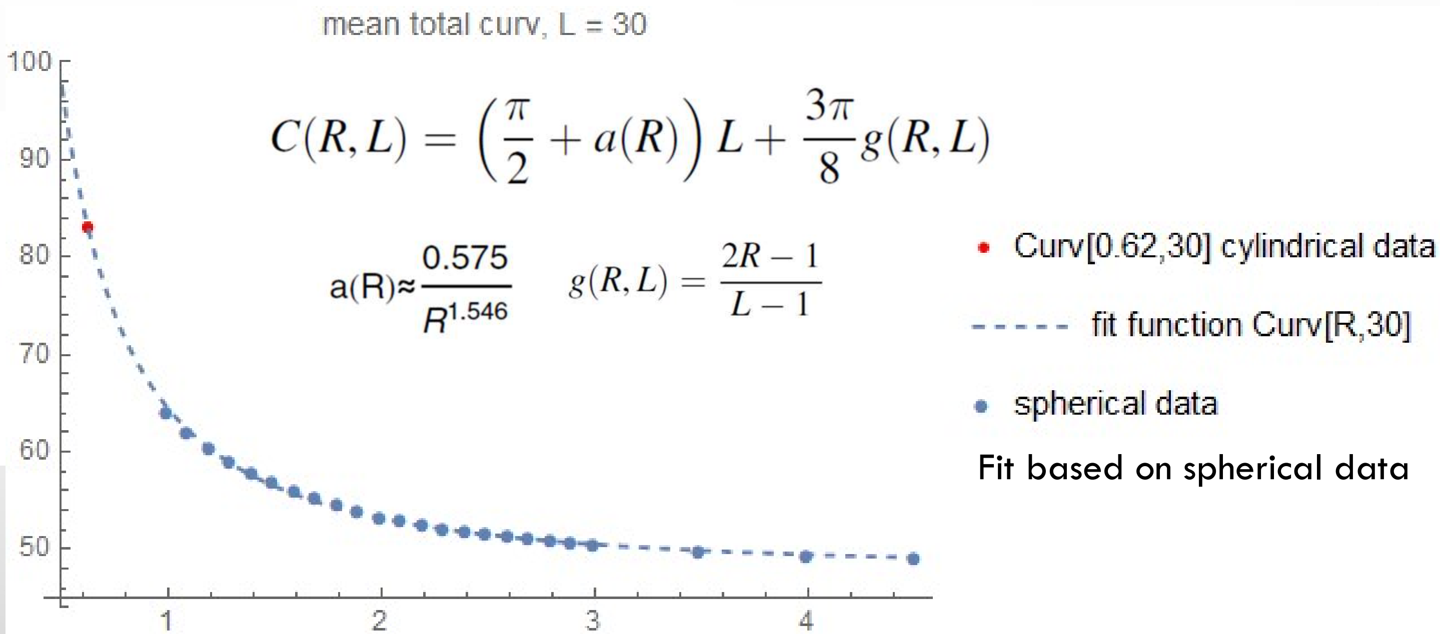


Mean topological crossing number for cylindrical data for polygons of length 30 is a good match for R= 0.62 of the spherical data line

C. Ernst, E.J. Rawdon, and U. Ziegler; Knotting spectrum of polygonal knots in extreme confinement; J. Phys. A Math. Theor. (2021) **54** 235202

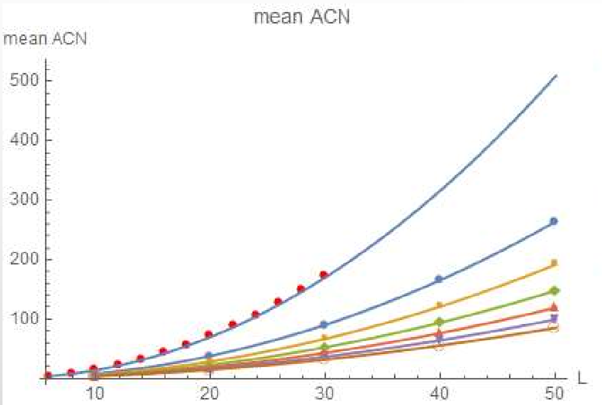
RESULTS - GEOMETRIC – CURVATURE PHANTOM

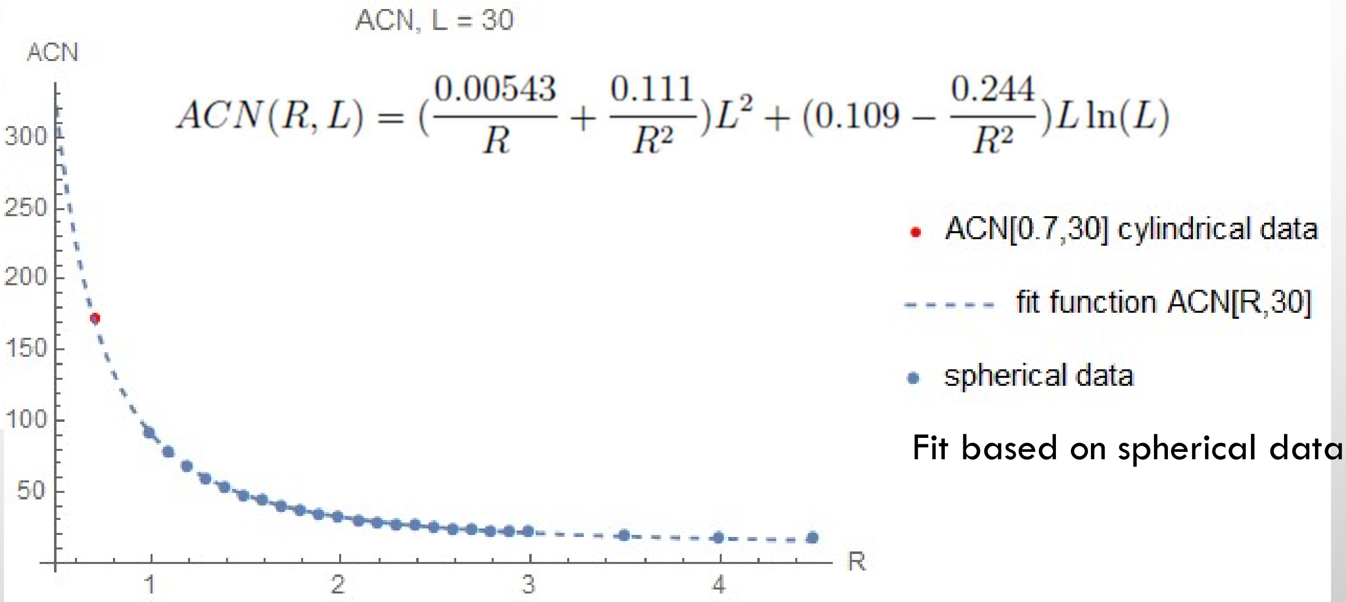




Y. Diao, C. Ernst, E.J. Rawdon, U. Ziegler, Total curvature and total torsion of knotted random polygons in confinement, J. Phys. A Math. Theor. 51 (15) (2018) 154002.

RESULTS - GEOMETRIC – ACN PHANTOM



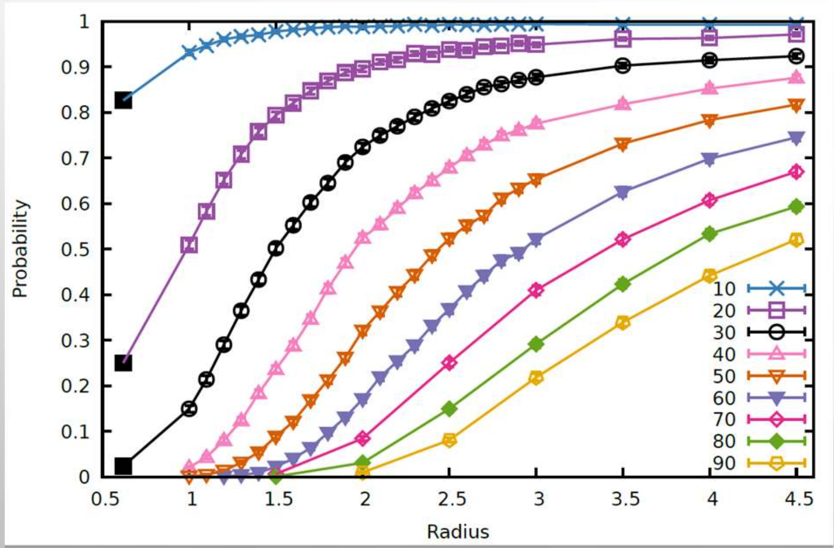


Fit based on spherical data

Yuanan Diao, Claus Ernst, Eric J Rawdon, and Uta Ziegler. Average crossing number and writhe of knotted random polygons in confinement. Reactive and Functional Polymers, 131:430-444,2018.

RESULTS - TOPOLOGICAL

for unknots



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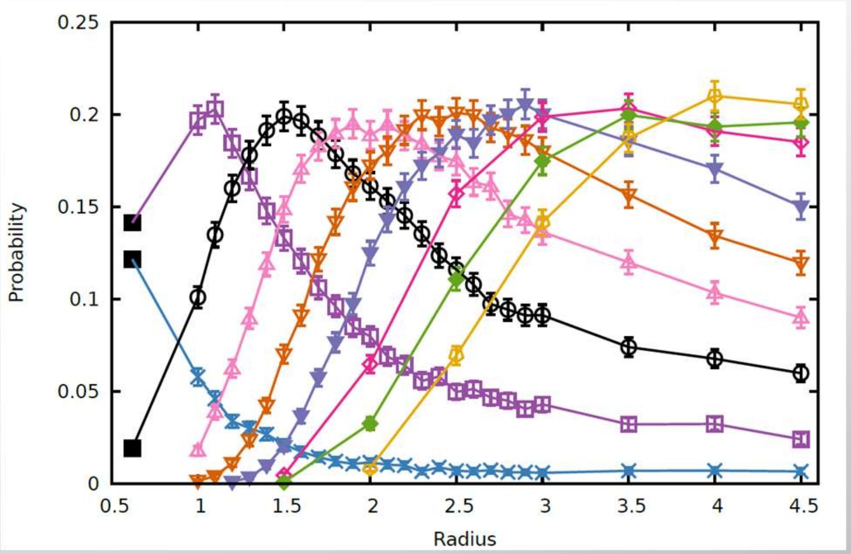

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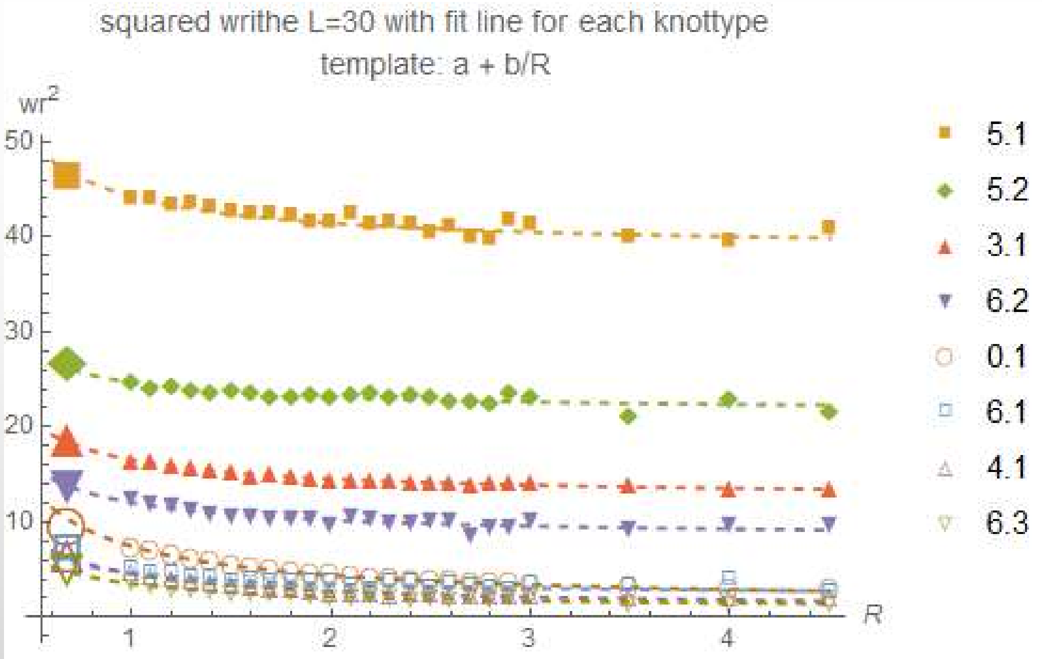
RESULTS - GEOMETRIC – WRITHE^2



Fit R = .62 to 0.77

ASYMPTOTIC BEHAVIOR OF RANDOM POLYGONS OF LENGTH 30 FOR R → 0.5+

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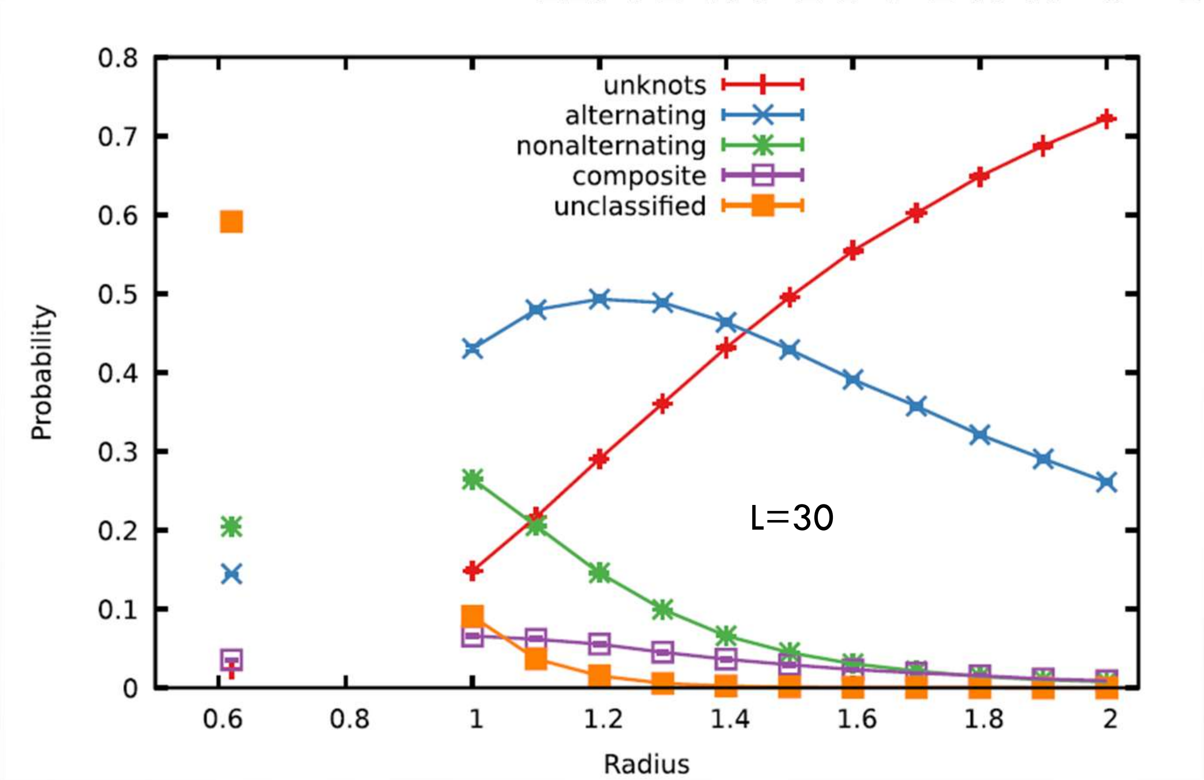


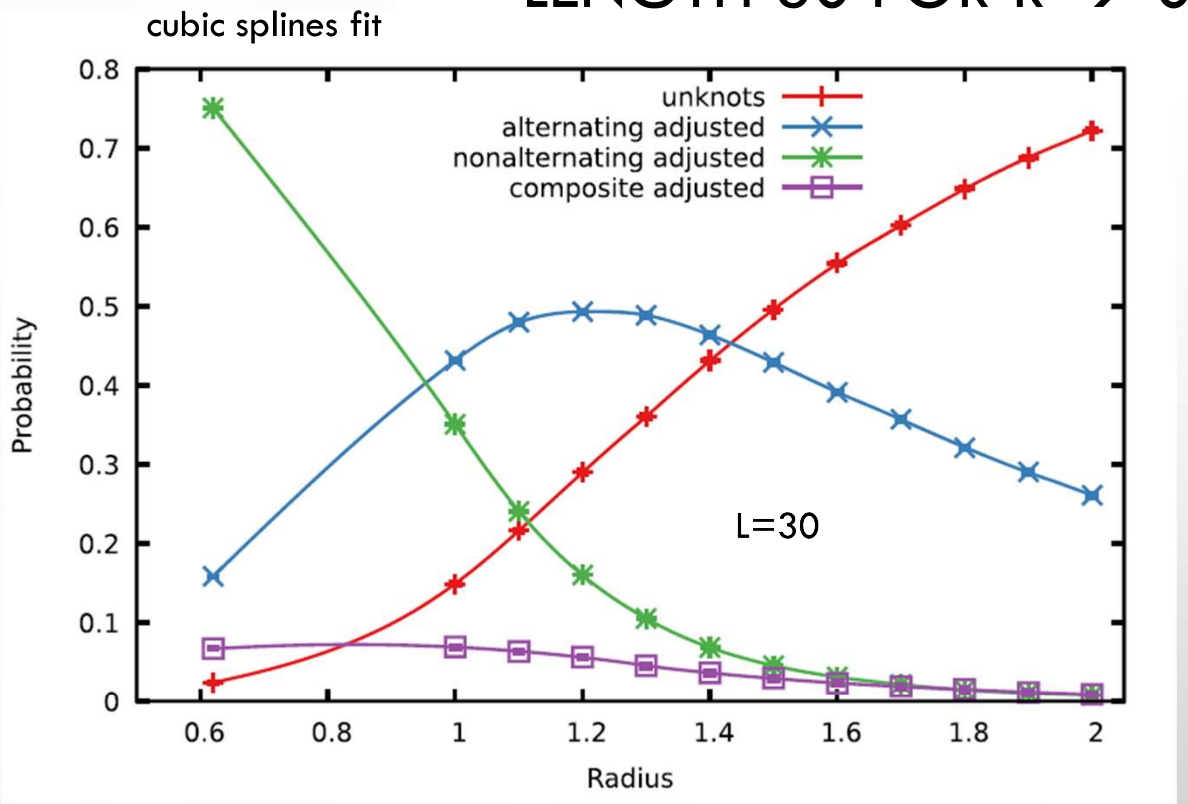
- TOO MANY UNCLASSIFIED POLYGONS

→ADJUST THE % FOR EACH OF THE CATEGORIES BASED ON THE % IN EACH CATEGORY FOR 16-CROSSING KNOTS;

E.G. R = 1.1: 3.67 % UNCLASS.

	unknt	Alt	NonAlt	comp
data	21.65	47.96	20.57	6.17
16-cr	0.00	0.60	95.18	4.22
adjstd	21.65	47.98	24.05	6.32

ASYMPTOTIC BEHAVIOR OF RANDOM POLYGONS OF LENGTH 30 FOR R → 0.5+



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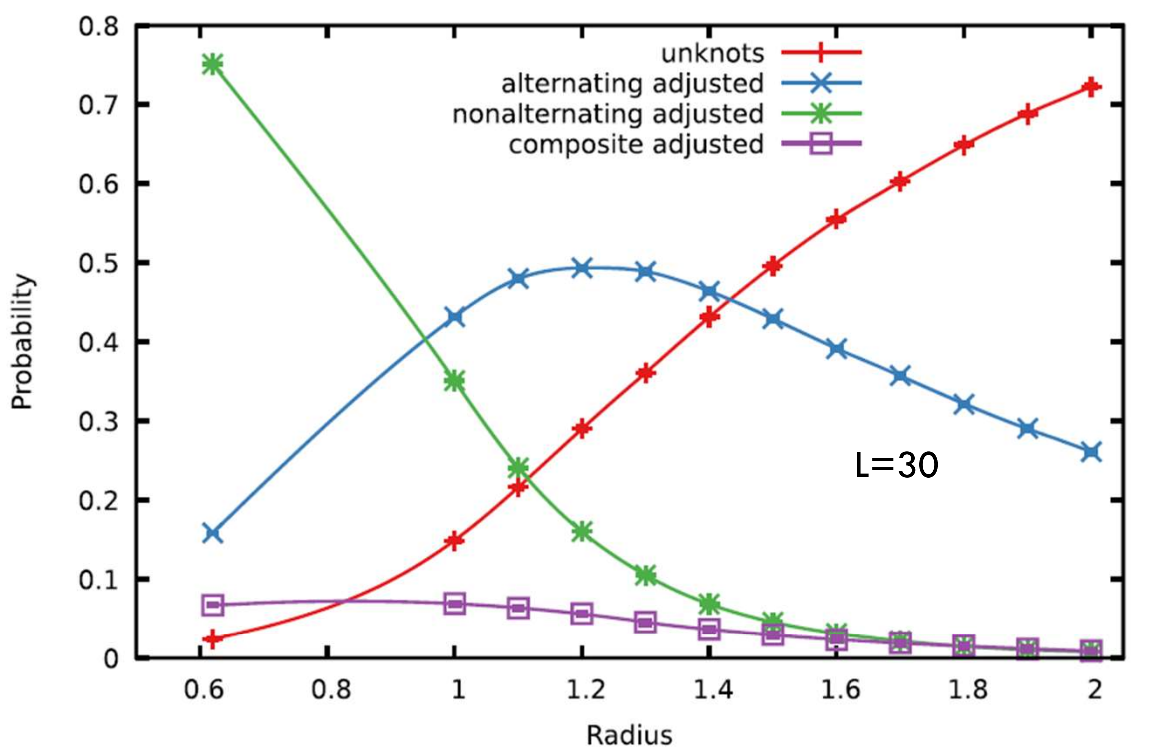
ASYMPTOTIC BEHAVIOR OF RANDOM POLYGONS OF LENGTH 30 FOR R → 0.5+

cubic splines fit



CONJECTURE:

UNKNOTS: → 0

NONALTERNATING: → ~80%

ALTERNATING: → ~ 12%

COMPOSITE: → ~ 6.5%

EXTENSION 2

OUTLINE

- MOTIVATION
- BIAS MODEL & DATA COLLECTED
- QUESTIONS:
    - ARE THE GENERATED POLYGONS 'THICKER' ON AVERAGE?
    - ARE THE FEATURES OF THE BIASED POLYGONS IN LINE WITH THE FEATURES OF UNBIASED POLYGONS?
    - CAN THE EFFECT OF THICKNESS BE QUANTIFIED?

MOTIVATION – BIAS TO THICKNESS

- THE RANDOM POLYGONS GENERATED WITH THE MODELS DISCUSSED FOR FAR HAVE NO VOLUME
- WHAT WOULD BE THE EFFECT OF ADDING SOME VOLUME?
- DON'T KNOW HOW TO GENERATE RANDOM POLYGONS WITH A FIXED THICKNESS.
- INSTEAD OF FORCING THICKNESS, WE BIAS THE GENERATION PROCESS TOWARDS GENERATING POLYGONS WITH THICKER SEGMENTS.

BIASED THICKNESS MODEL

- GENERATE ROOTED RANDOM POLYGONS IN SPHERICAL CONFINEMENT
- BIAS EACH SEGMENT TOWARDS THICKNESS RIGHT AFTER ITS GENERATION
- USE ACCEPT/REJECT APPROACH BASED ON MAXIMAL SEGMENT THICKNESS
- CONSECUTIVE SEGMENTS ARE NOT SELF-AVOIDING

Definitions

A **thick segment** S_i of thickness r_i is the set of all points which are at a distance d less than or equal to r_i from the segment S_i. r_i is called the radius of the thick segment S_i.

The **maximal thickness** r_i^t of a thick **segment** S_i is the largest value for the radius r_i of the thick segment S_i, such that the thick segment S_i of radius r_i does not intersect with any other non-adjacent thick segment S_j with radius r_i.

The maximal thickness r_p of a polygon is the minimum over all r_i^t values.

ALGORITHM

Algorithm to generate biased polygon of length n

$X_0 \leftarrow$ origin
$X_1 \leftarrow$ random point on unit sphere around origin
i $\leftarrow$ 2 to n-1
        determine next vertex X_i
    until segment $X_{i-1}X_i$ is accepted*
next i
$X_n \leftarrow X_0$

* segment $X_{i-1}X_i$ is accepted if its maximal segment thickness is larger than a thickness chosen randomly based on the bias function

DATA COLLECTED

- GENERATED RANDOM POLYGONS FOR R = 1 TO 2 IN INCREMENTS OF 0.1 AND R= 2.5, R=3.0
  - 50K POLYGONS FOR L=30
  - 10K POLYGONS FOR L = 10, 20, 40, AND 50
- FOR BIASED AND FOR UNBIASED RANDOM POLYGONS FOR DIRECT COMPARISON
- DETERMINED KNOT TYPE FOR EACH POLYGON (UP TO 16 CR)

SHOUTOUT FOR ERIC RAWDON & ROB SHAREIN

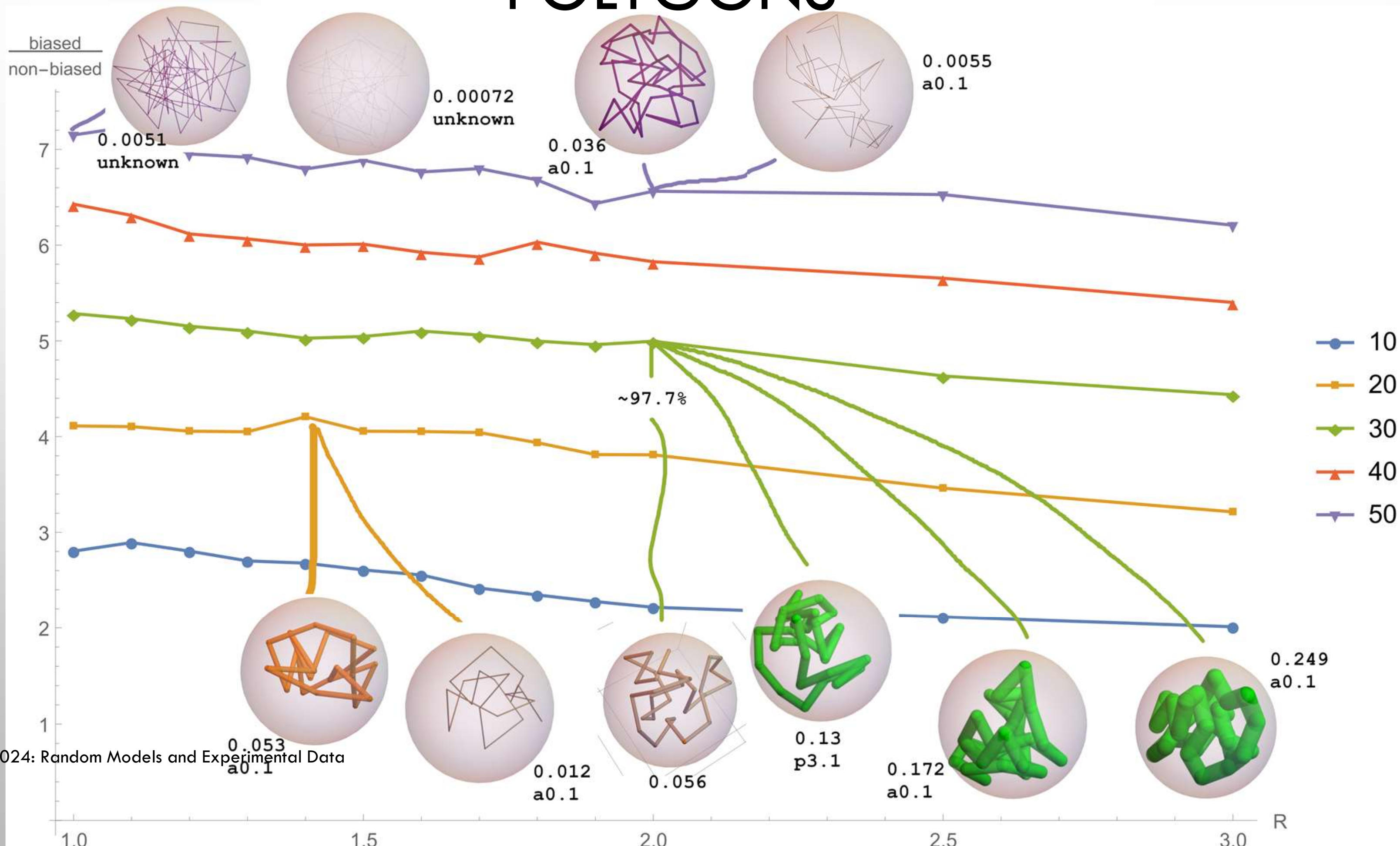
- USING THE HOMFLY-PT POLYNOMIAL TO COMPUTE KNOT TYPES

QUESTION 1:

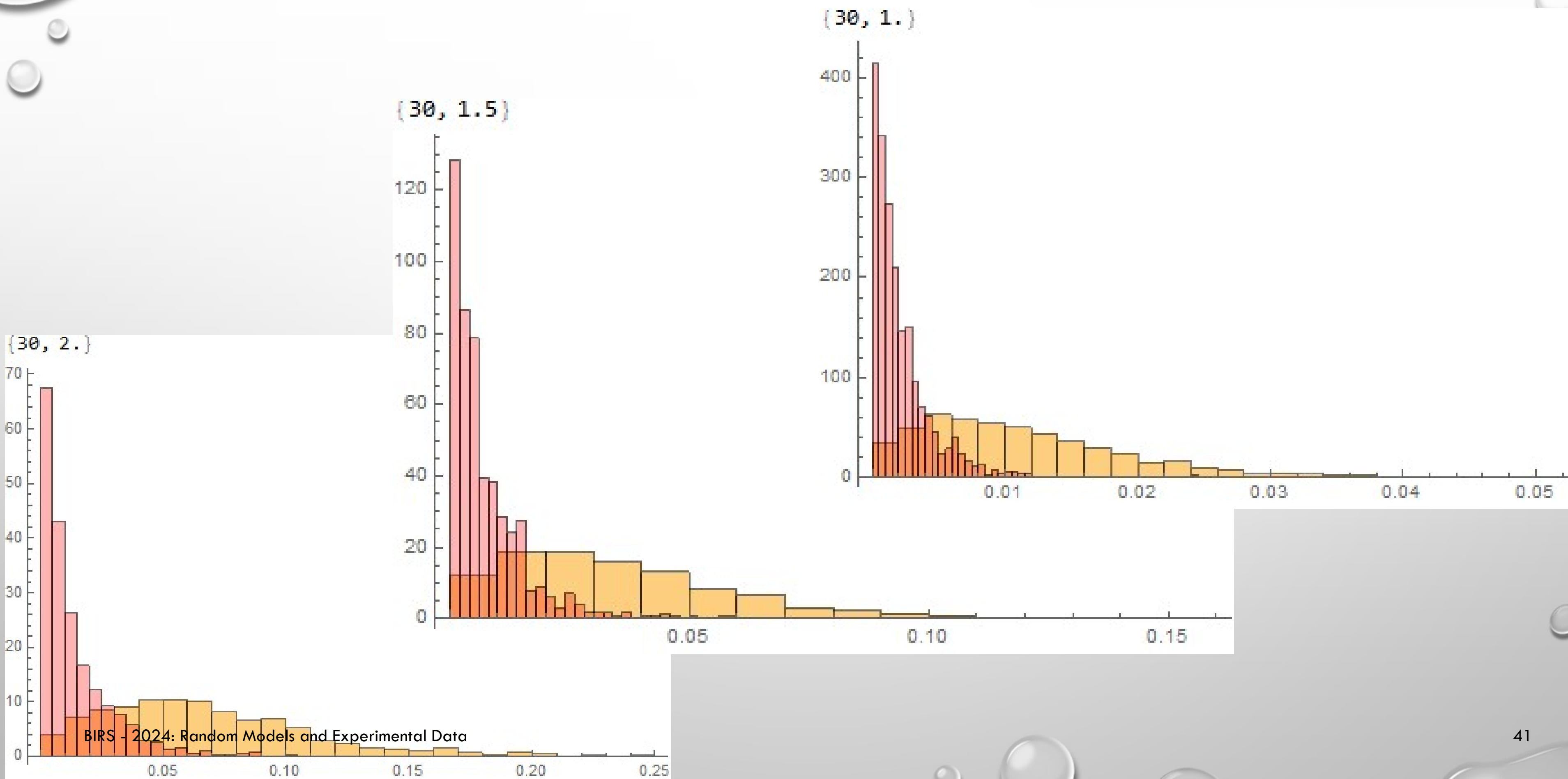
ARE THE GENERATED POLYGONS ‘THICKER’ ON AVERAGE?

THAT MEANS DO THEY HAVE A LARGER AVERAGE MAXIMAL THICKNESS?

AVERAGE MAX THICKNESS OF BIASED VS UNBIASED POLYGONS



DISTRIBUTION OF THICKNESS IN BIASED POLYGONS



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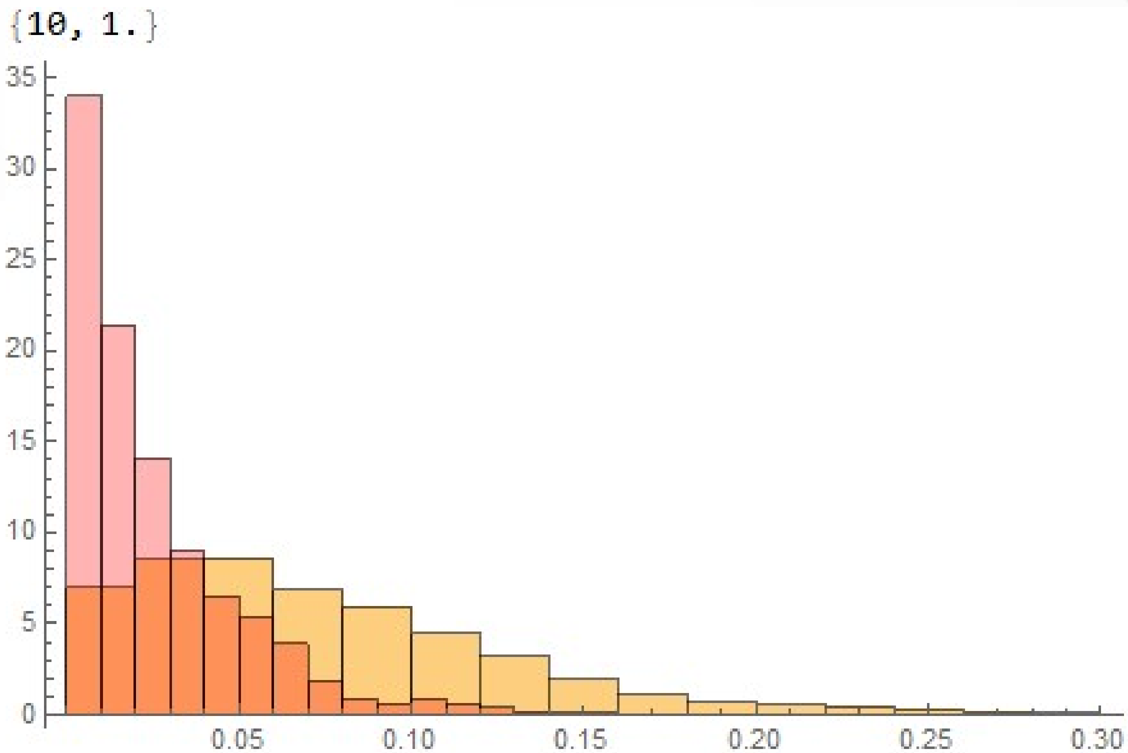
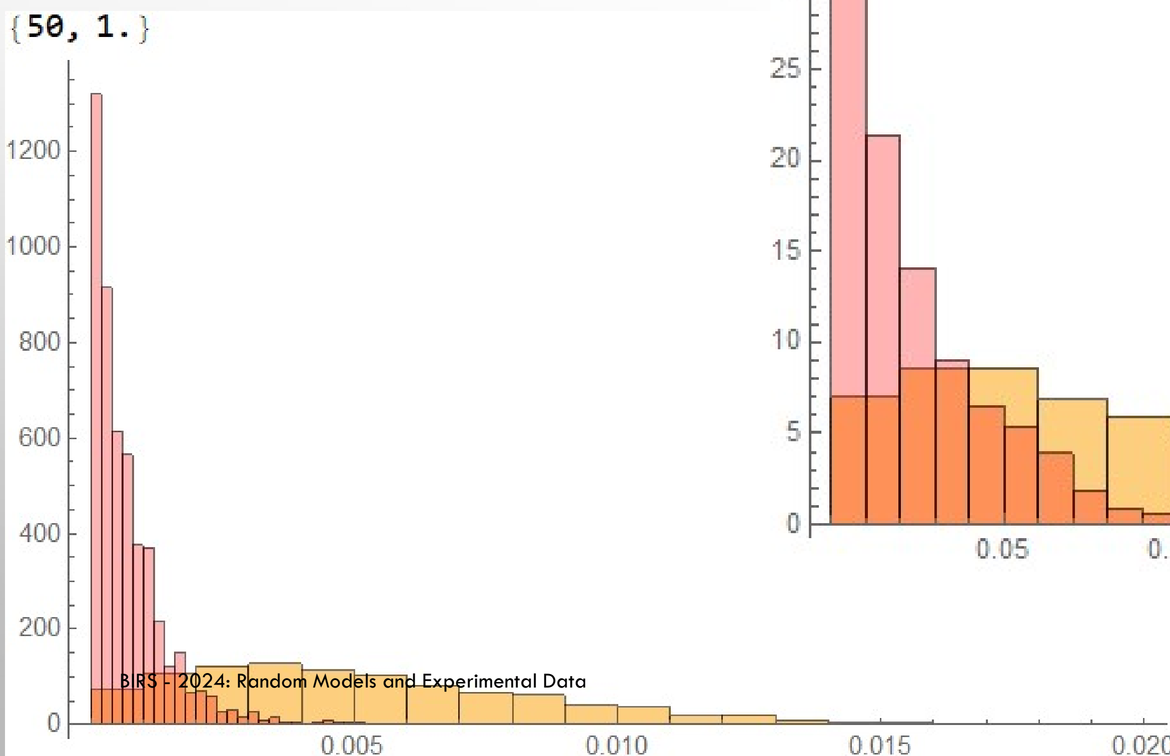
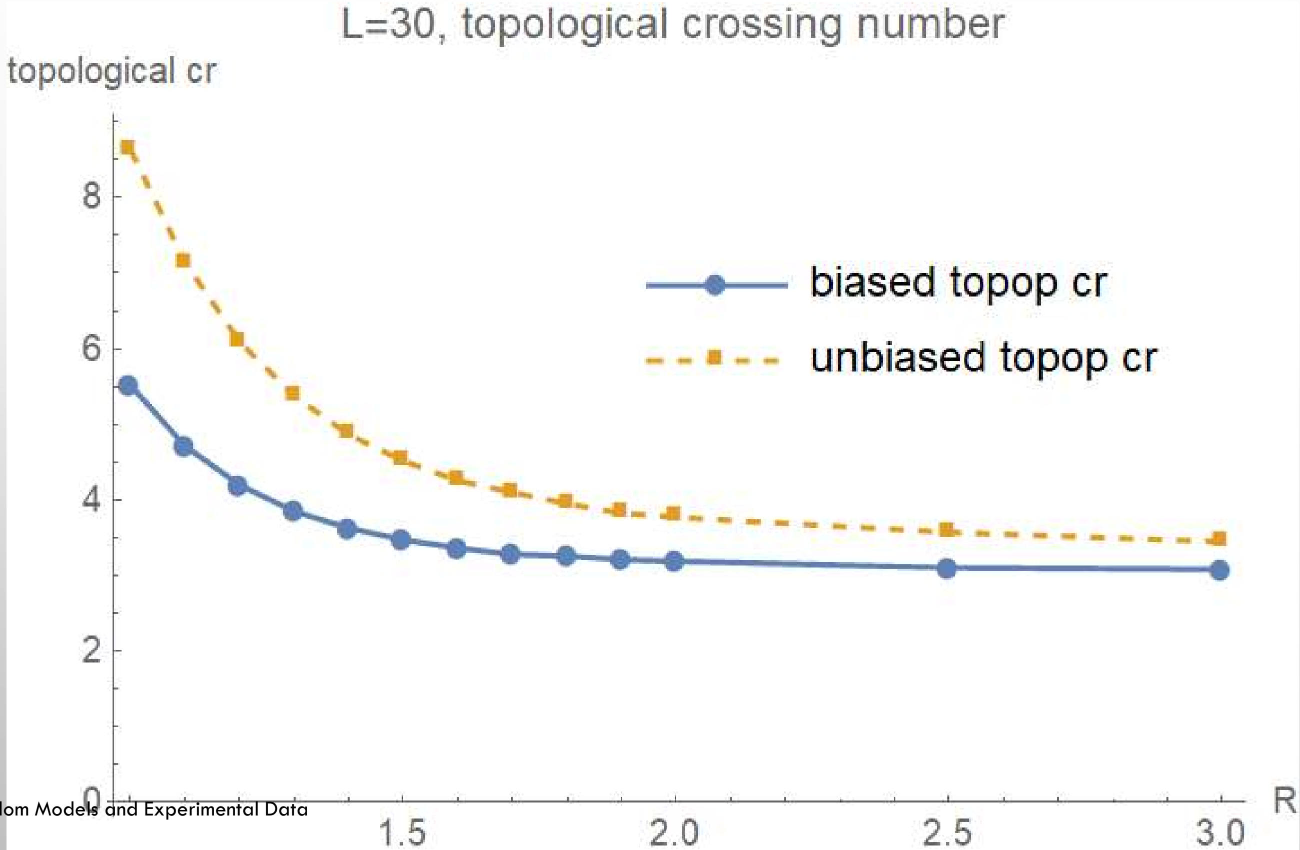




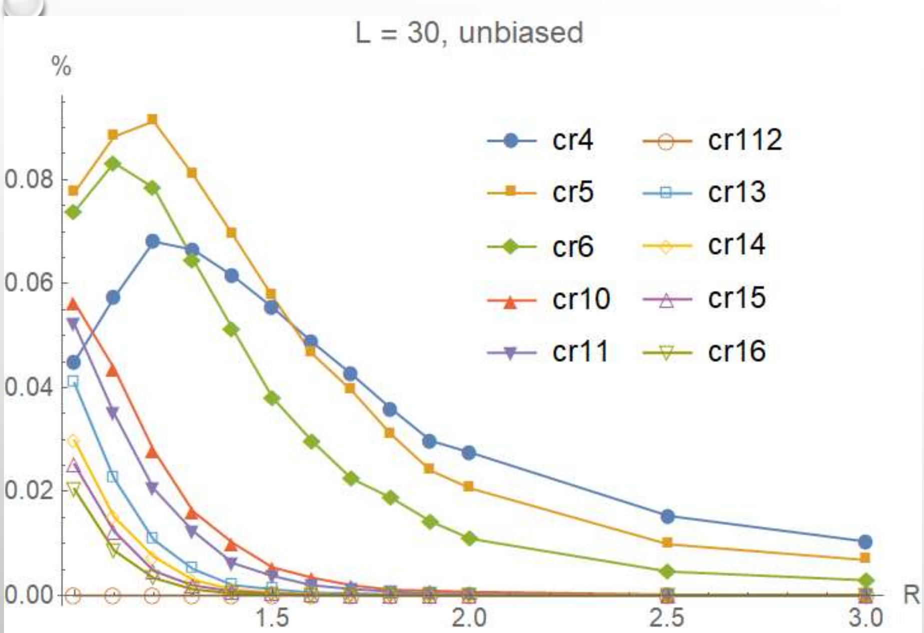
QUESTION 2:

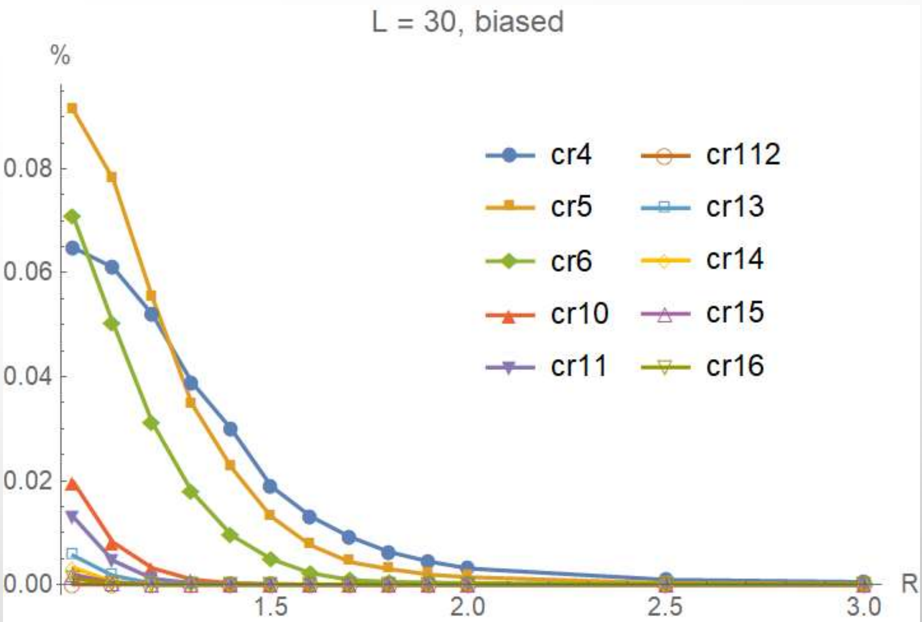
ARE THE FEATURES OF THE BIASED POLYGONS IN LINE WITH THE FEATURES OF UNBIASED POLYGONS?

MEAN TOPOLOGICAL CROSSING NUMBER

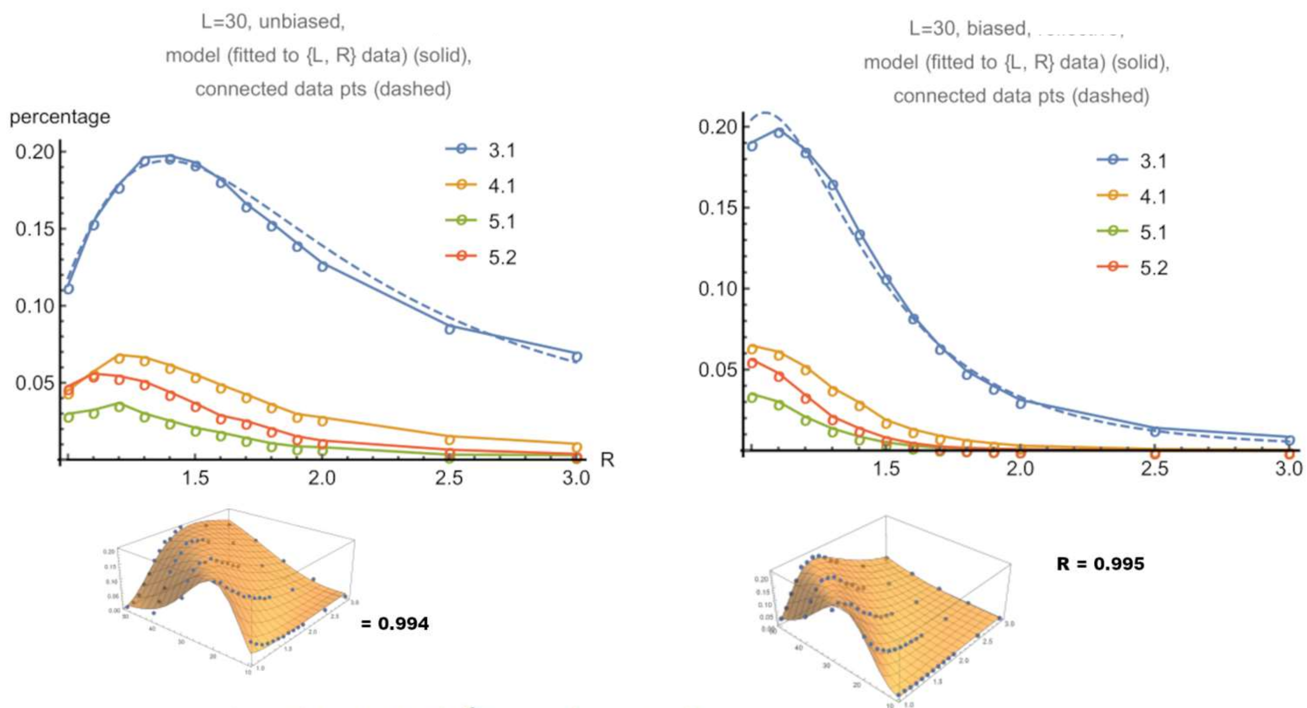


KNOT SPECTRUM FOR CR UP TO 16



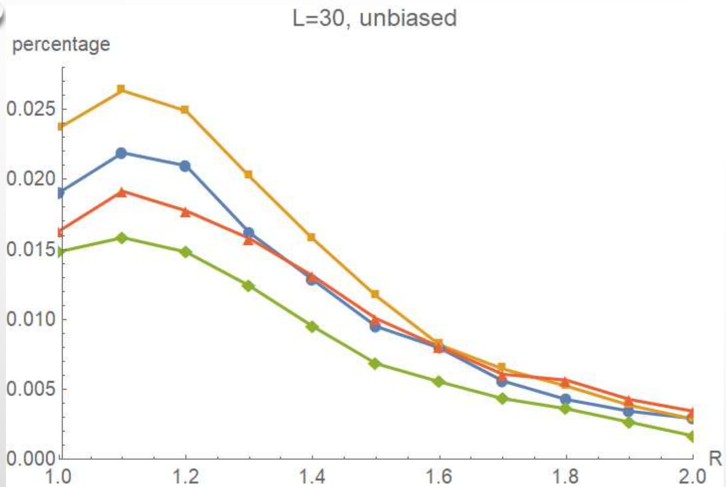


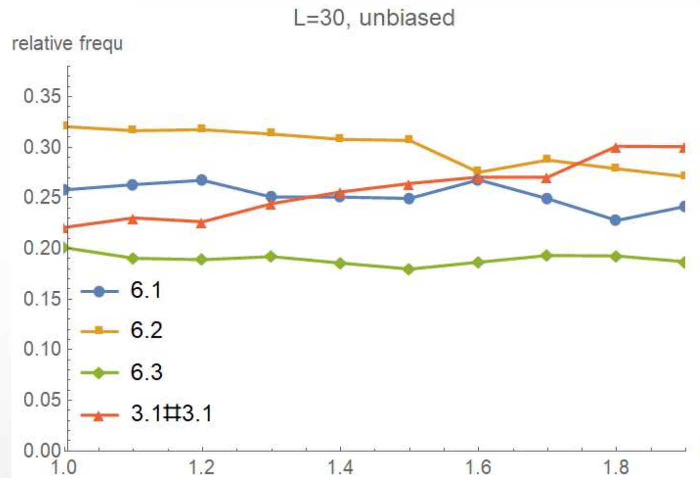
KNOT SPECTRUM FOR KNOTS WITH SMALL CR

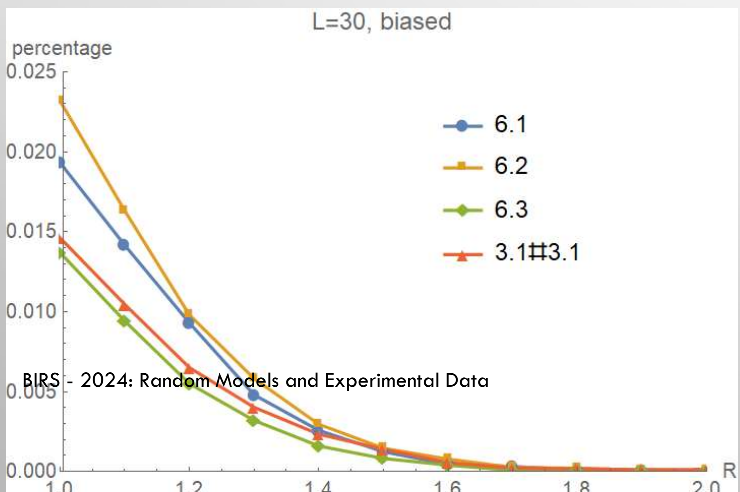


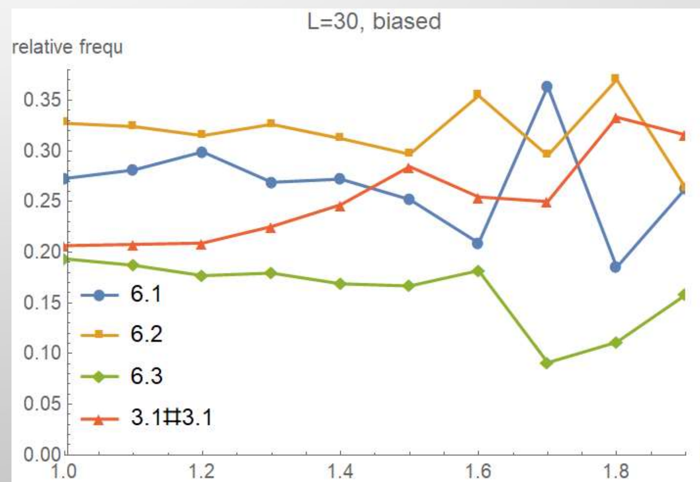
$$P_{\mathcal{K}}(L,R) = a\left(d + \left(\frac{L - L_0(\mathcal{K})}{R - 0.6}\right)^e\right)\exp\left(-\frac{L}{bR - c}\right)$$

KNOT SPECTRUM FOR 6-CR KNOTS

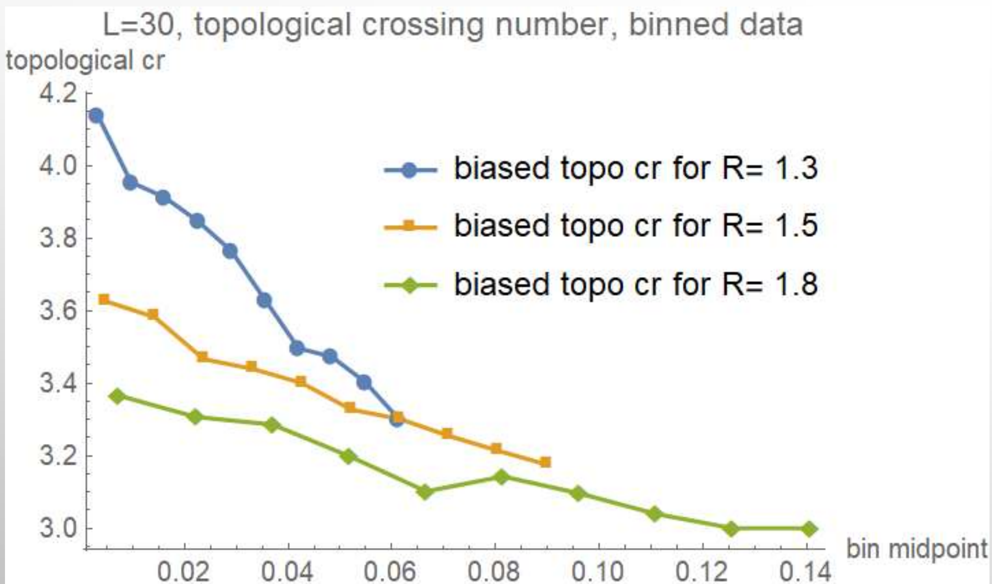


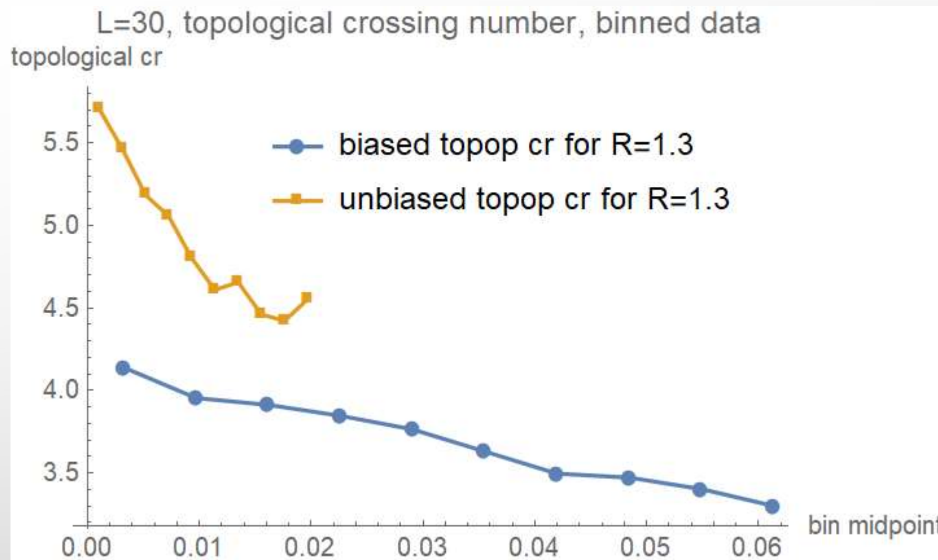




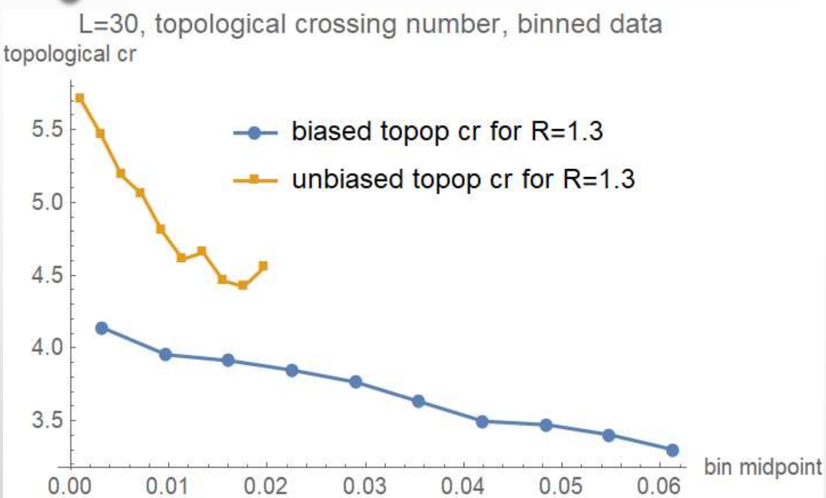


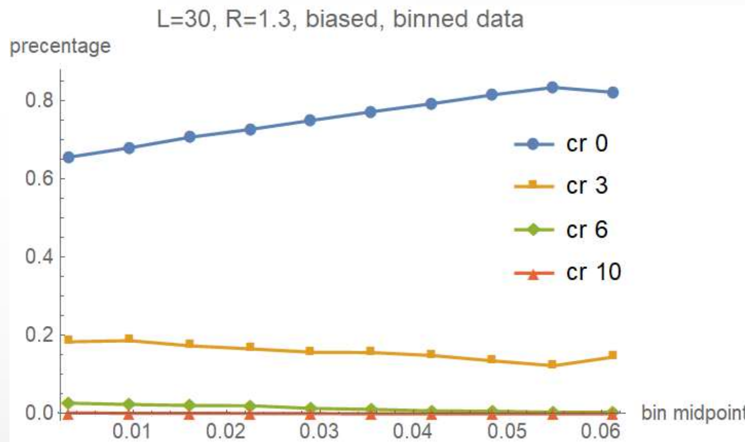
BINNED BY MAX THICKNESS – MEAN TOPOLOGICAL CR

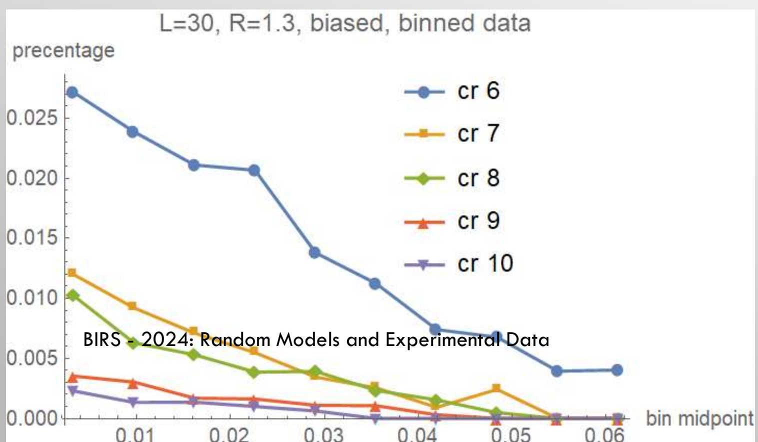




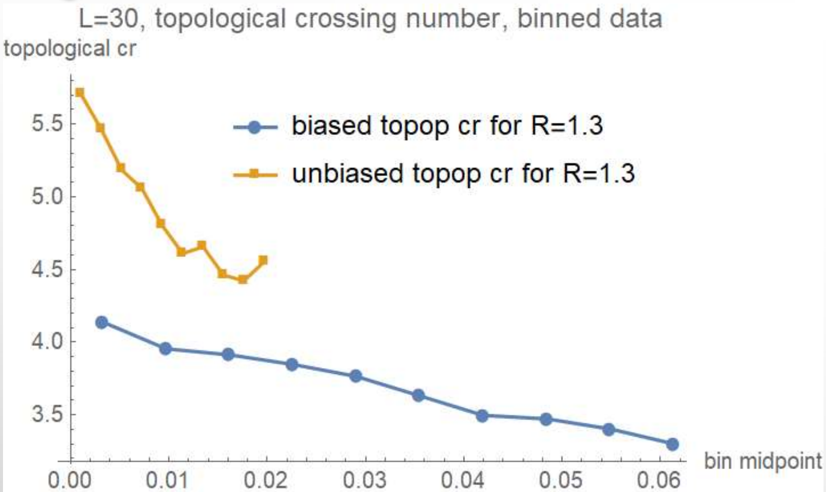
BINNED BY MAX THICKNESS – KNOT TYPES WITH CR

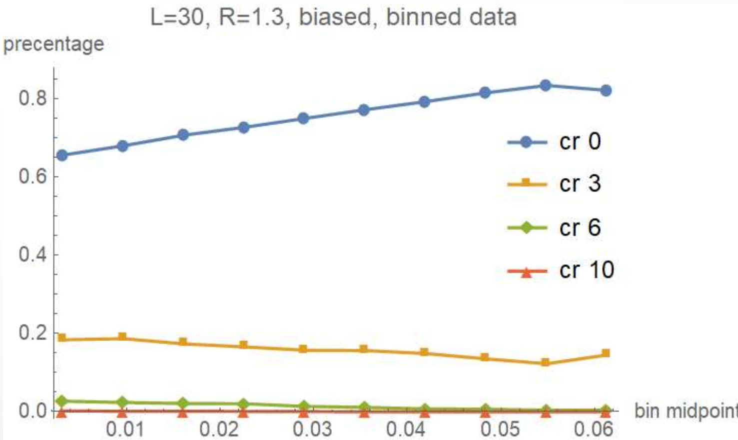


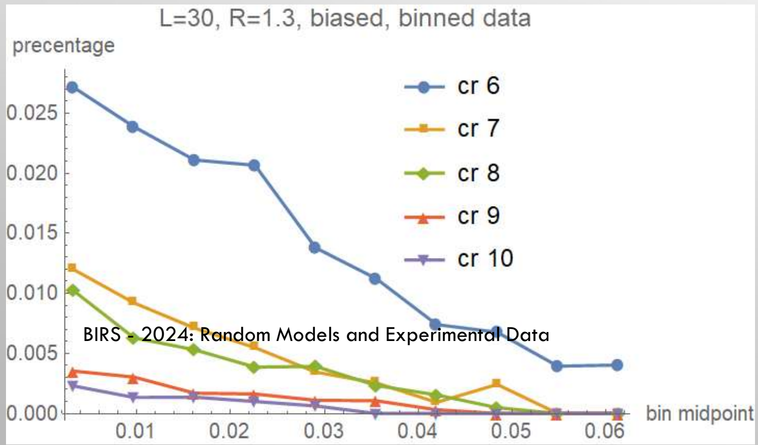


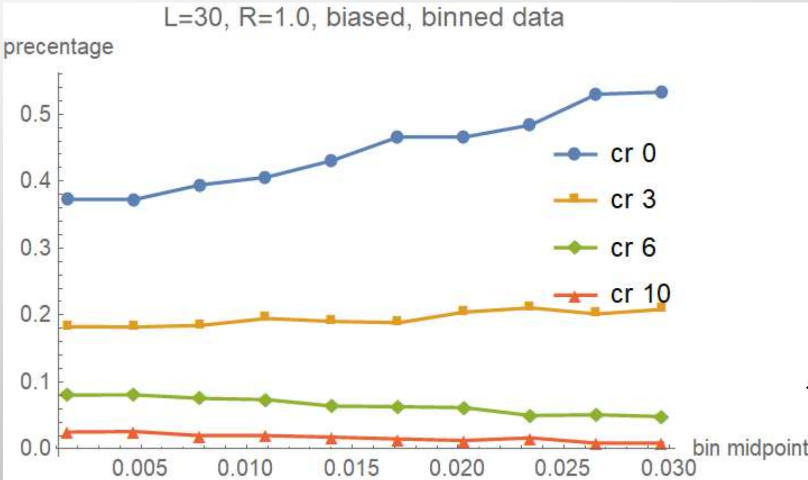


BINNED BY MAX THICKNESS – KNOT TYPES WITH CR





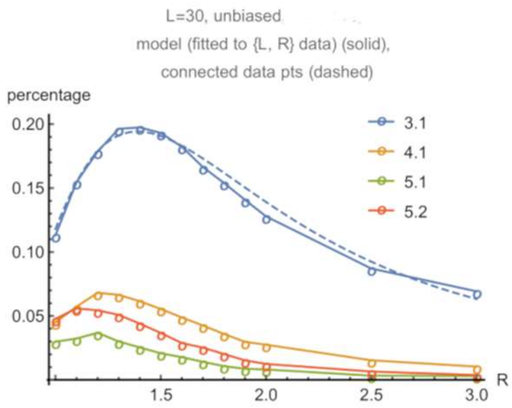


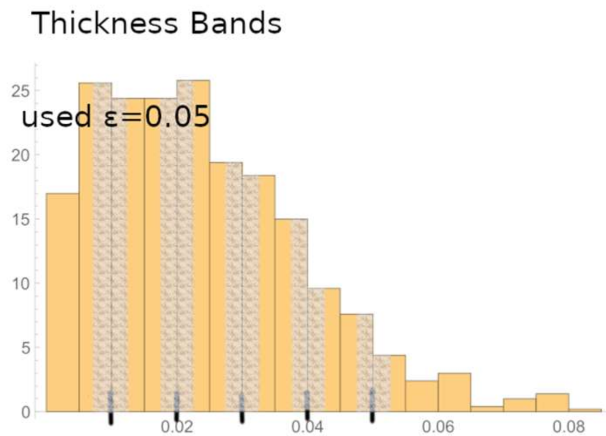


QUESTION 3:

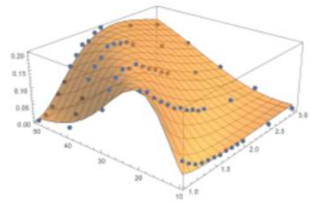
CAN THE EFFECT OF THICKNESS BE QUANTIFIED?

Effect of thickness on $P_{3.1}(L,R)$





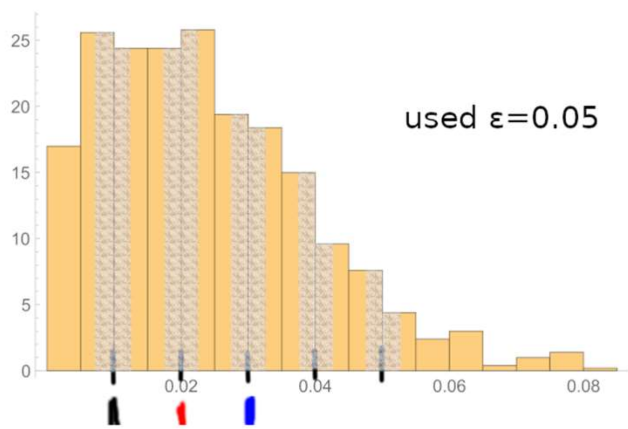
R = 0.994

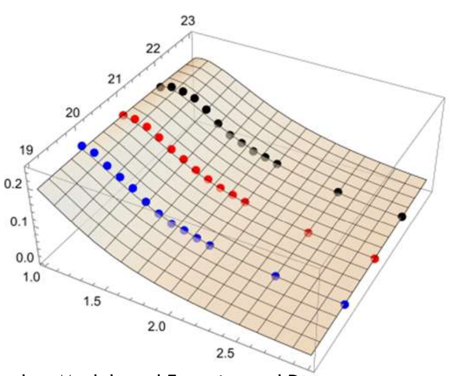


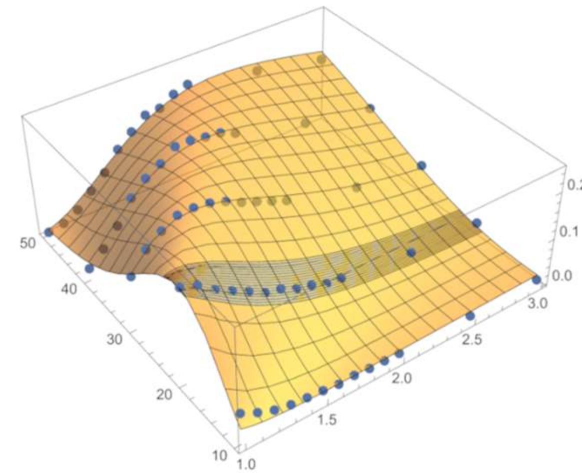
$$P_{\mathcal{K}}(L,R) = a\left(d + \left(\frac{L - L_0(\mathcal{K})}{R - 0.6}\right)^e\right)\exp\left(-\frac{L}{bR - c}\right)$$

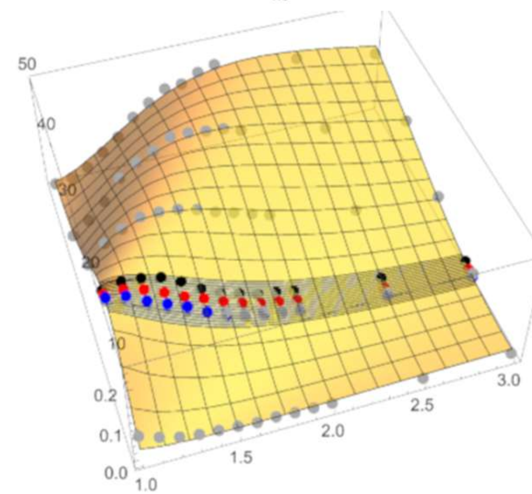
Effect of thickness on $P_{3.1}(L,R)$

Thickness Bands



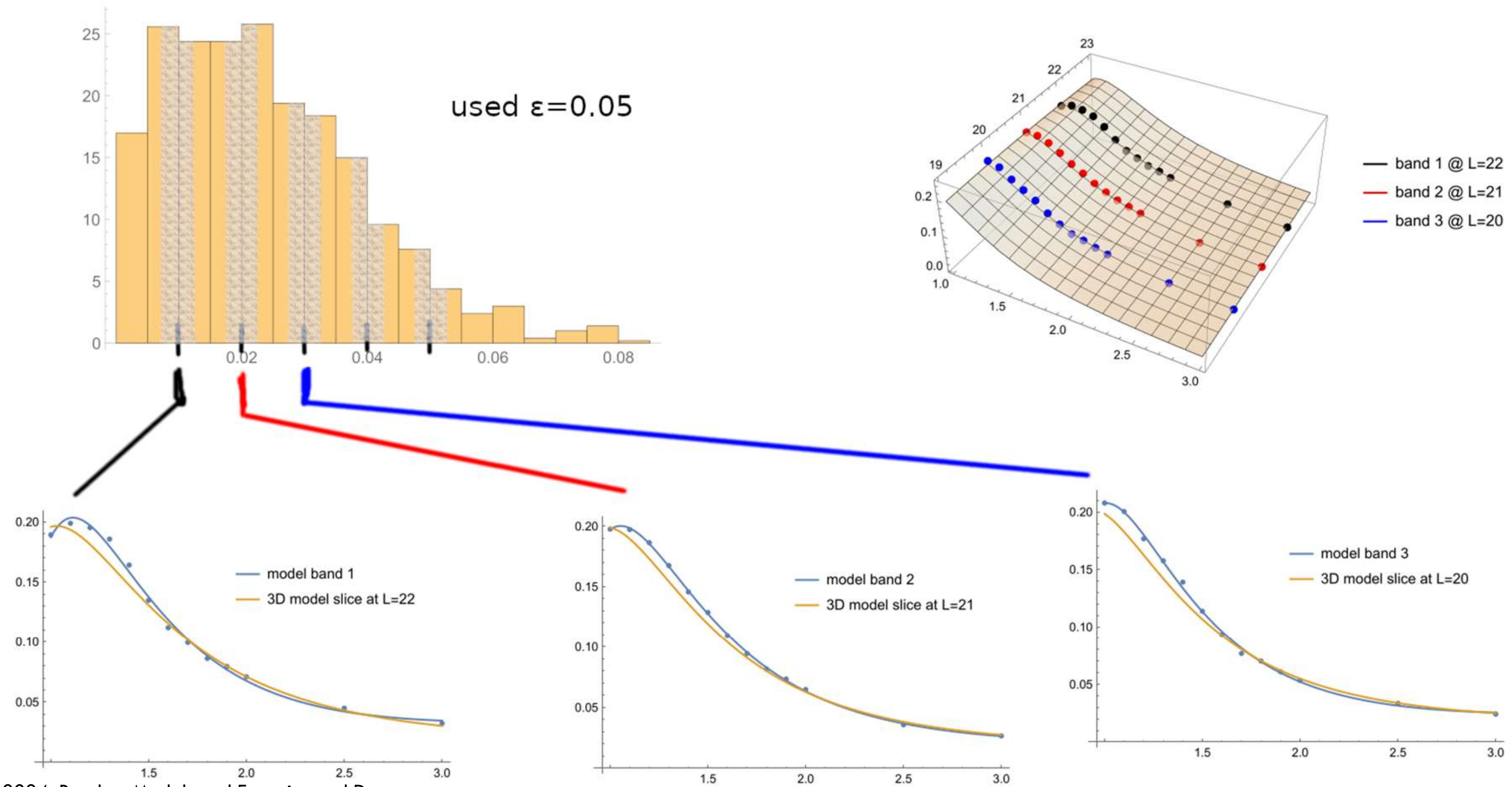






Effect of thickness on $P_{3.1}(L,R)$

Thickness Bands



SUMMARY

- DISCUSSED 2 MODELS FOR EXTENSIONS TO RANDOM POLYGONS IN SPHERICAL CONFINEMENT RELATED TO IMPORTANT QUESTIONS

  - WHAT HAPPENS IN RANDOM POLYGONS IN SPHERICAL CONFINEMENT FOR $R < 1$?
    - CYLINDRICAL POLYGONS ALIGN WELL WITH MANY ASPECTS OF SPHERICAL POLYGONS IN CONFINEMENT WITH $R=0.62$
    - CONJECTURES FOR ASYMPTOTIC BEHAVIOR FOR $L=30$ FOR $R \rightarrow 0.5+$

  - WHAT HAPPENS WHEN RANDOM POLYGONS IN SPHERICAL CONFINEMENT HAVE SOME VOLUME?
    - POLYGONS BIASED TOWARDS THICKNESS SHARED MANY FEATURES WITH UNBIASED POLYGONS
    - THICKER RANDOM POLYGONS CAN BE MODELED AS SHORTER RANDOM POLYGONS FOR P_3.1 (L, R)

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THANK YOU…

QUESTION?