KNOTS IN EXTREME CONFINEMENT

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Joined work with

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Outline

- Motivation
- Approach
- Results
  - Overall distribution
  - Extension to earlier results

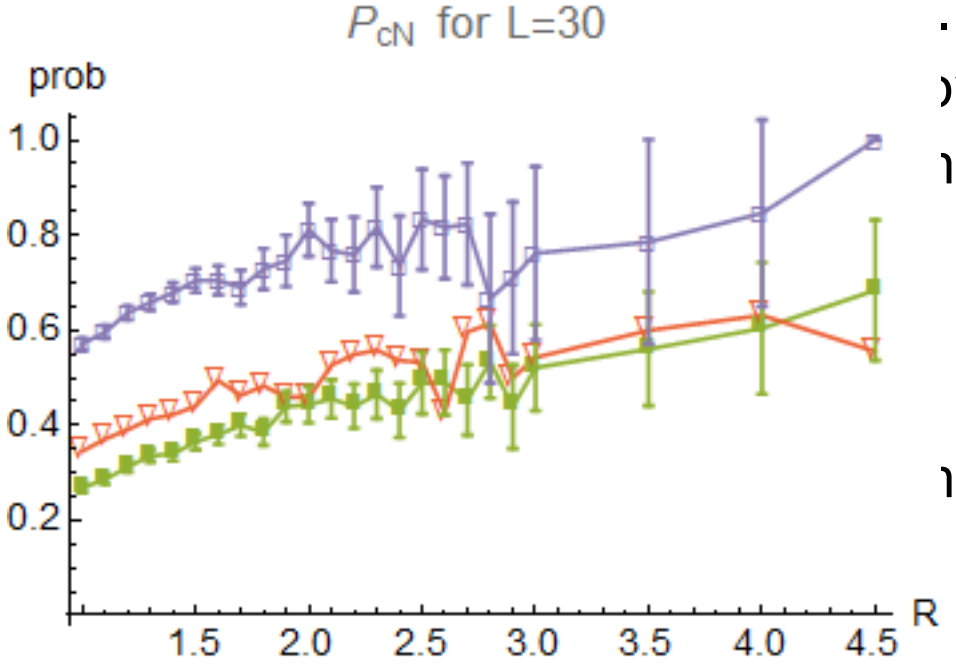
Motivation

- We studied topological and geometric properties of confined polygons.
- Increase confinement pressure by
  - increasing length of polygons
  - decreasing the radius of the confining sphere

Could not make radius smaller than 1, due to the properties of the generation algorithm.

Motivation

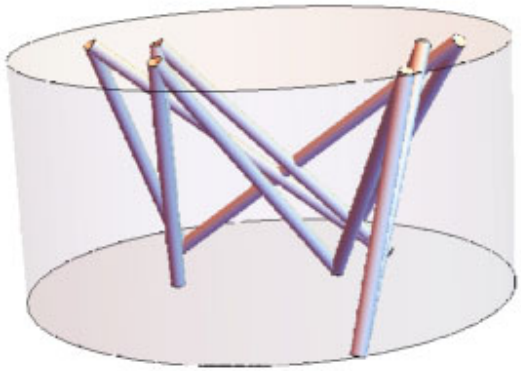
- Studied topological and geometric



Approach

Note: If the confinement radius is close to ½, then the polygon edges would use up the entire diameter at each step

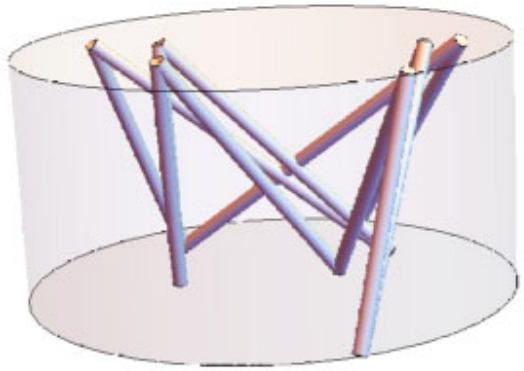
- Uniformly pick points on the top and bottom of a cylinder of height 1 and radius 1.
- Connect the points and then connect the last point to the first point.
- Reduce the radius of the cylinder (or stretch the height).



Approach

Note:

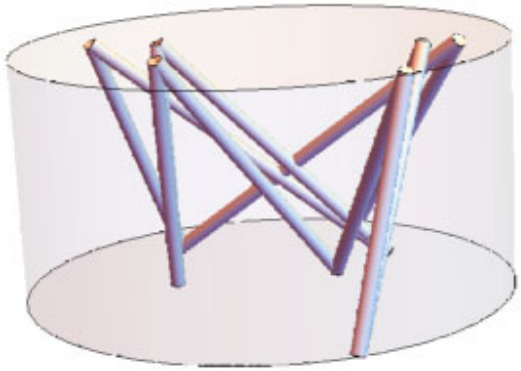
1) Stretching may change the values of geometric quantities.
2) Stretching does NOT change the knot distribution of the generated polygons.



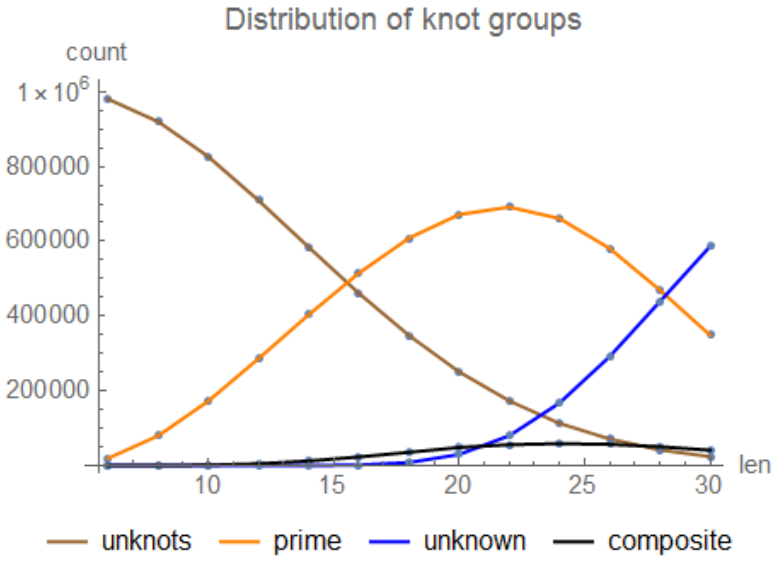
Approach

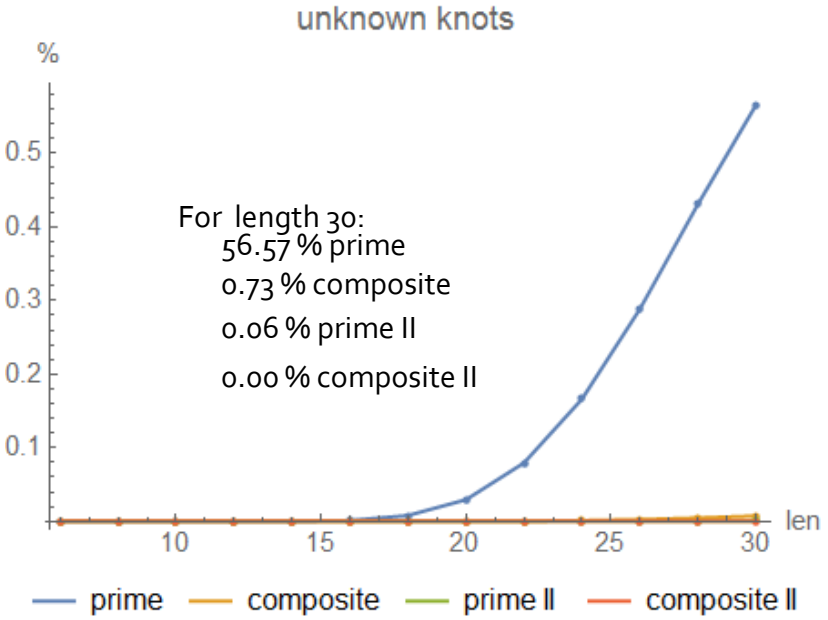
- Generated polygons of lengths 6, 8, 10, …. , 28, 30.
- For each length 1 million polygons were generated

- Identify the knot type of each polygon
- Compute the ACN, writhe, curvature, and torsion for each polygon for various stretch factors between 1 and 100.



Overall distribution

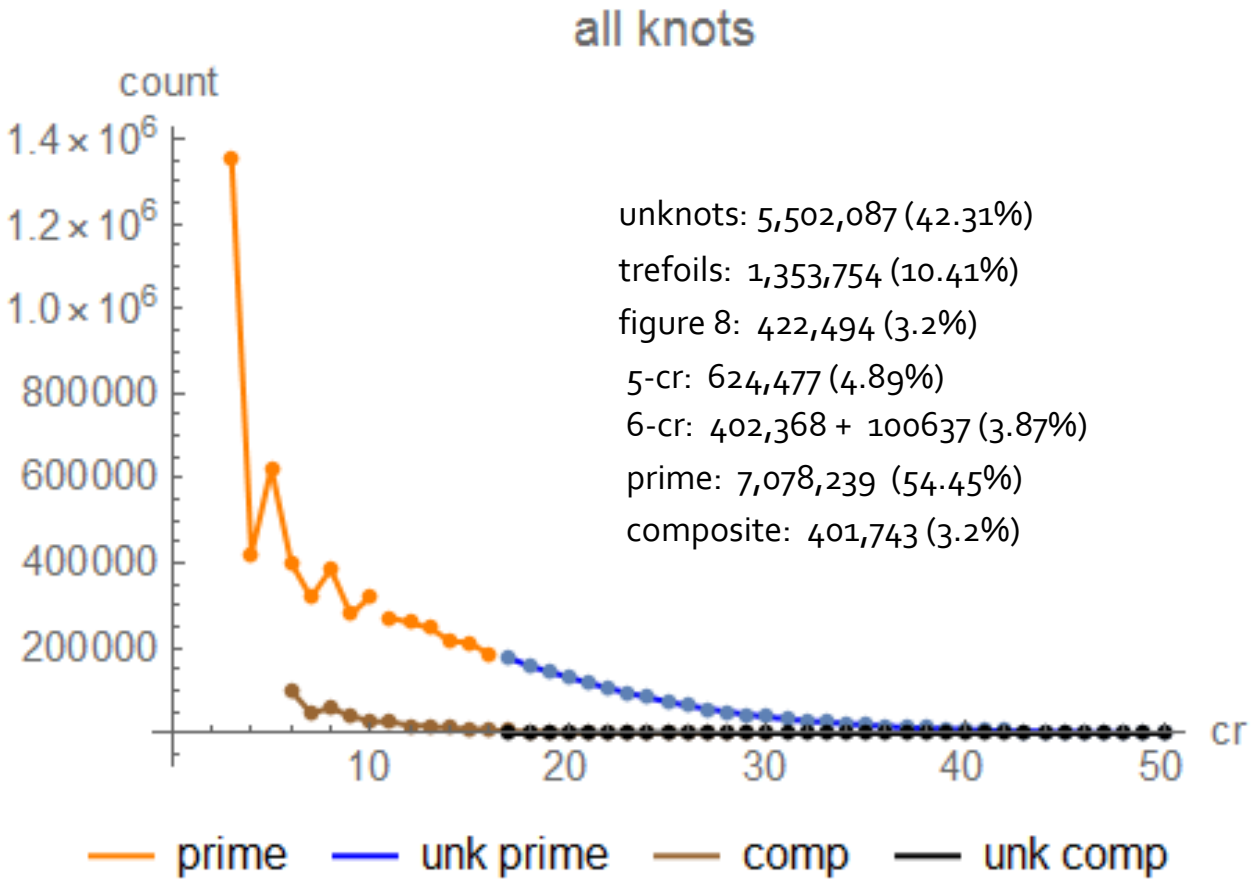




For length 30:
56.57 % prime
0.73 % composite
0.06 % prime II
0.00 % composite II

unknots: 980,802 for len=6
23,609 for len=30

Total number of knots



unknots: 5,502,087 (42.31%)

trefoils: 1,353,754 (10.41%)

figure 8: 422,494 (3.2%)

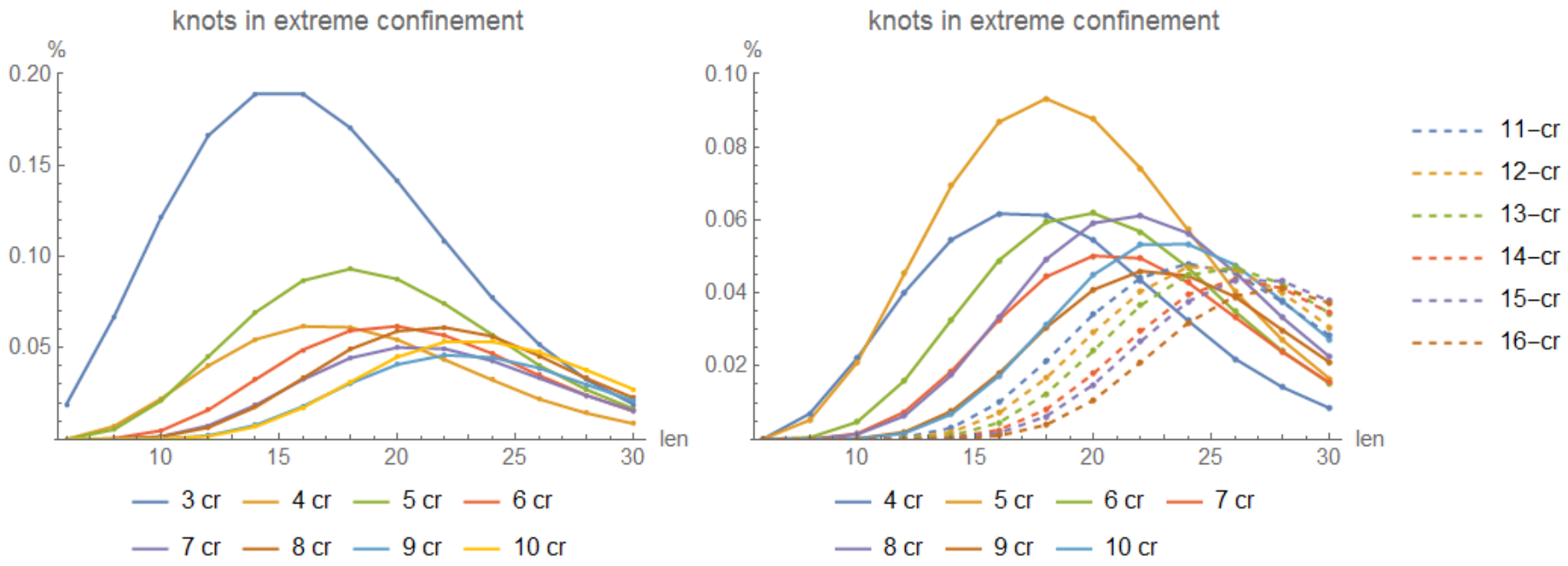
5-cr: 624,477 (4.89%)

6-cr: 402,368 + 100637 (3.87%)

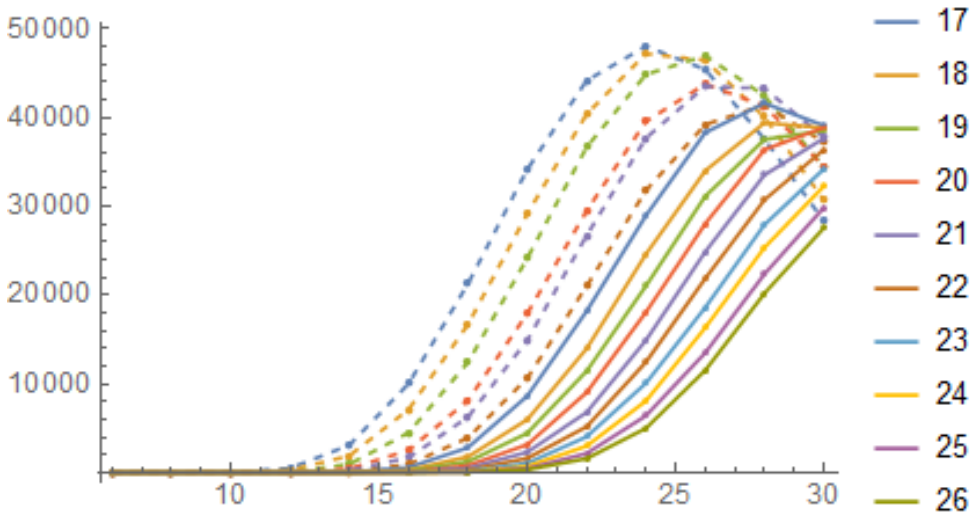
prime: 7,078,239 (54.45%)

composite: 401,743 (3.2%)

Knot complexity distributions – prime knots



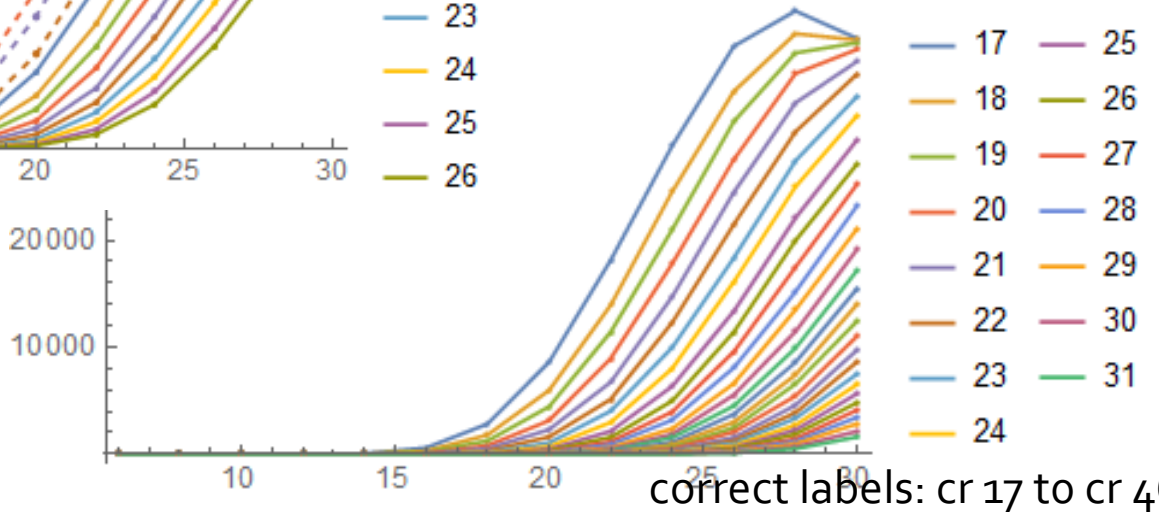
Unknown primes -



correct labels:

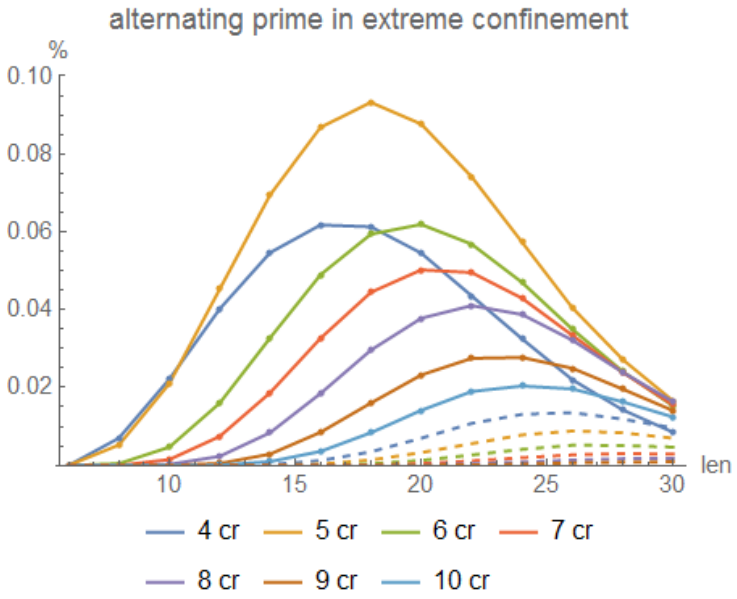
cr 11 to cr 16: dashed

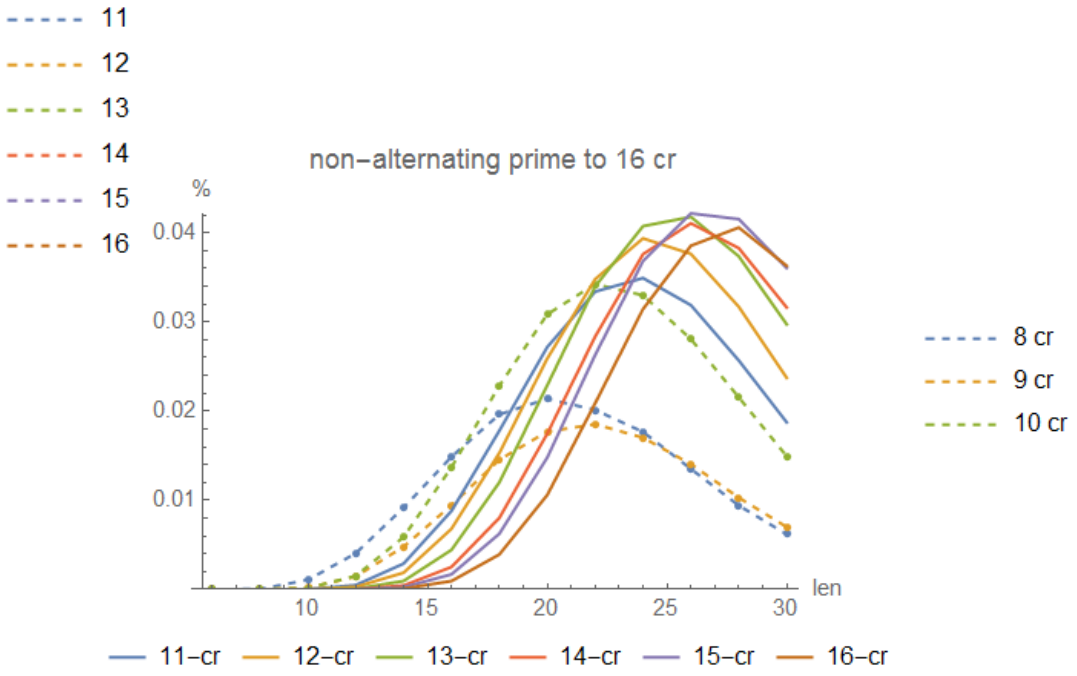
cr 17 to cr 26: solid



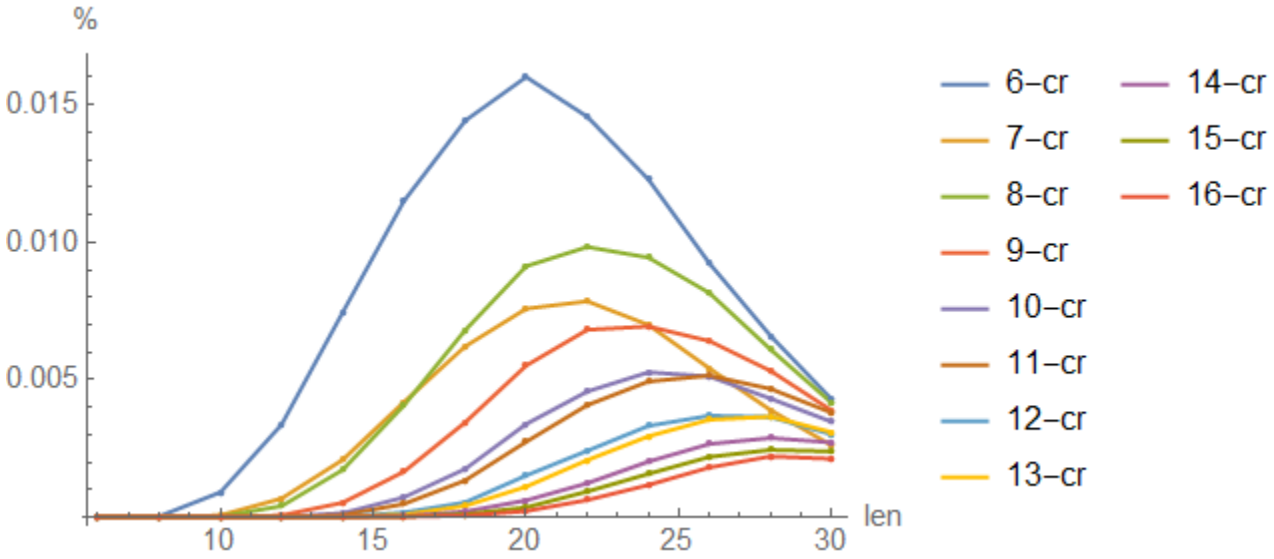
correct labels: cr 17 to cr 46

Alternating and non-alternating distribution

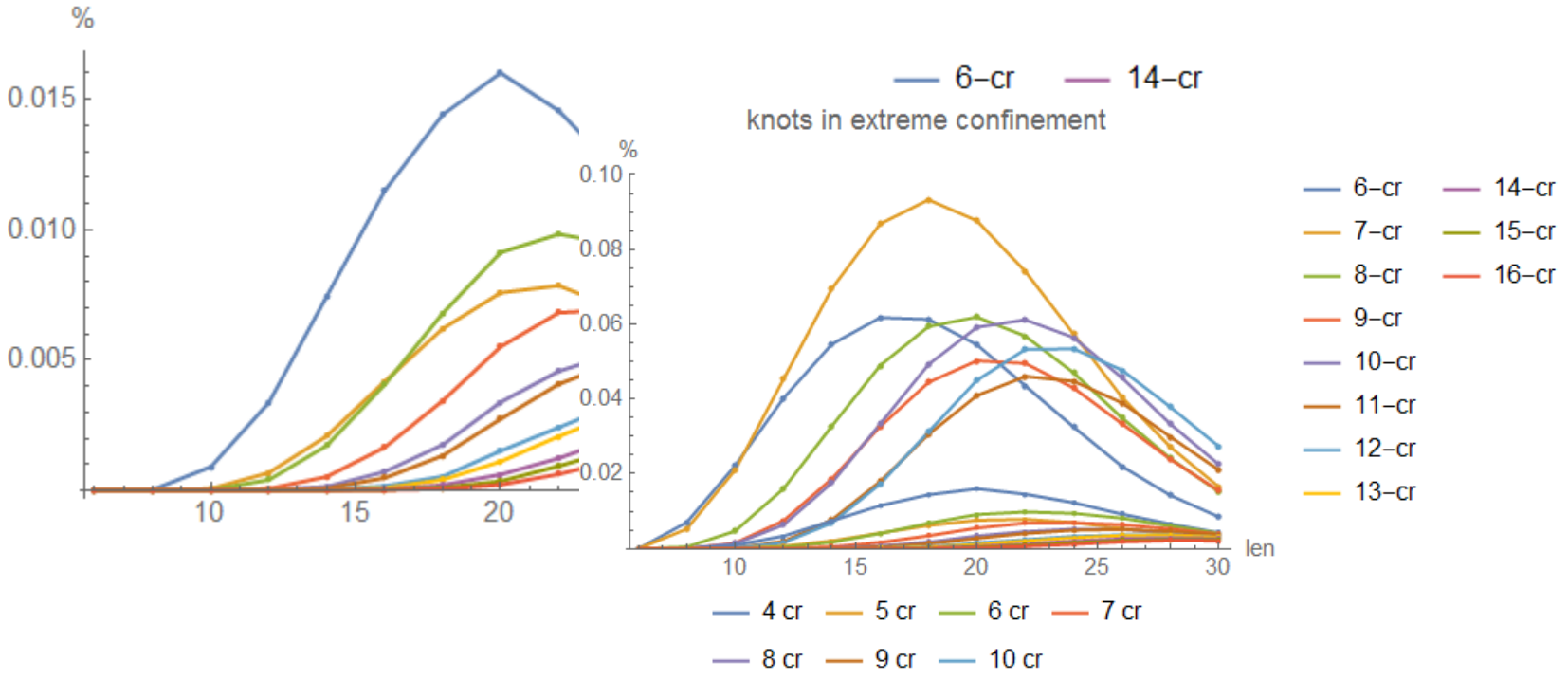




Knot type distributions – composite knots



Knot type distributions – composite knots

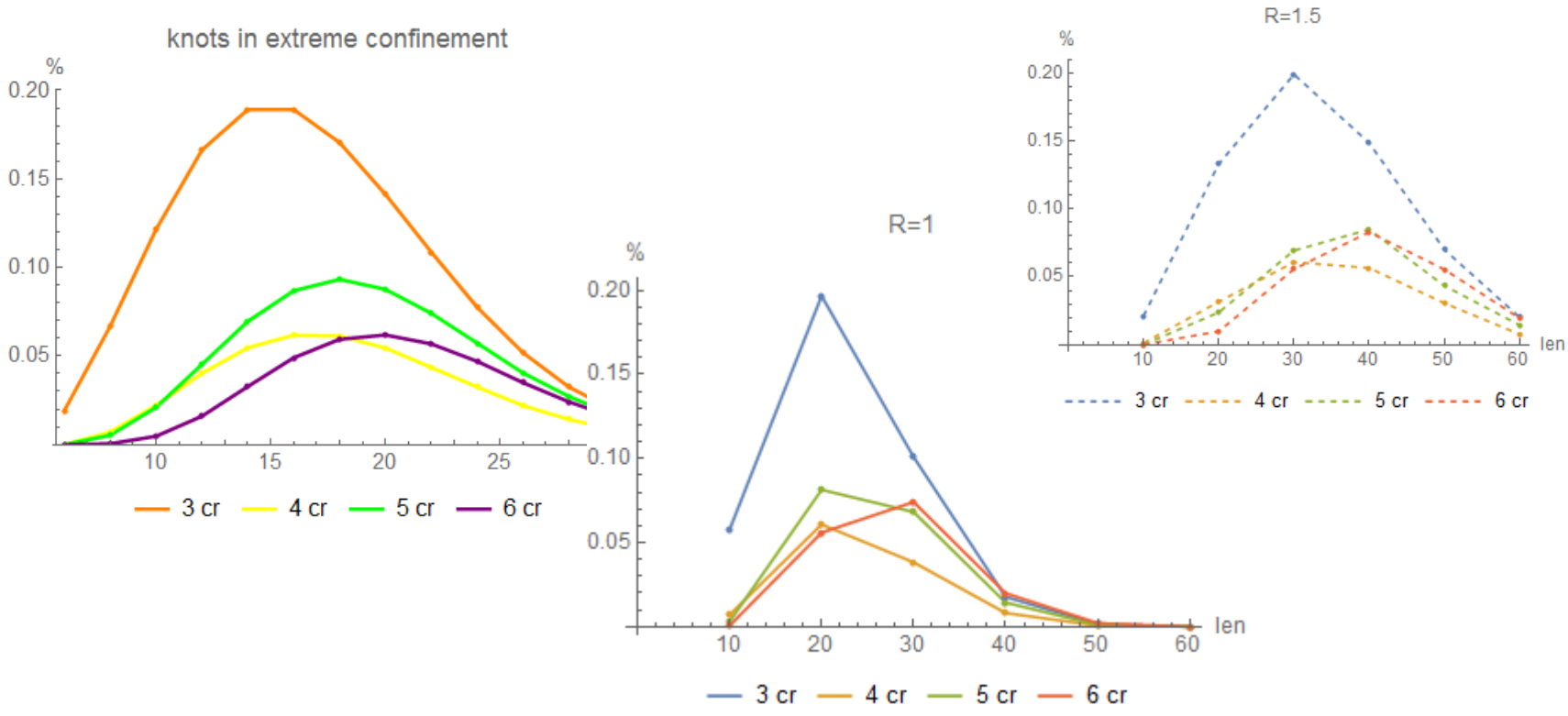


Extension of earlier results

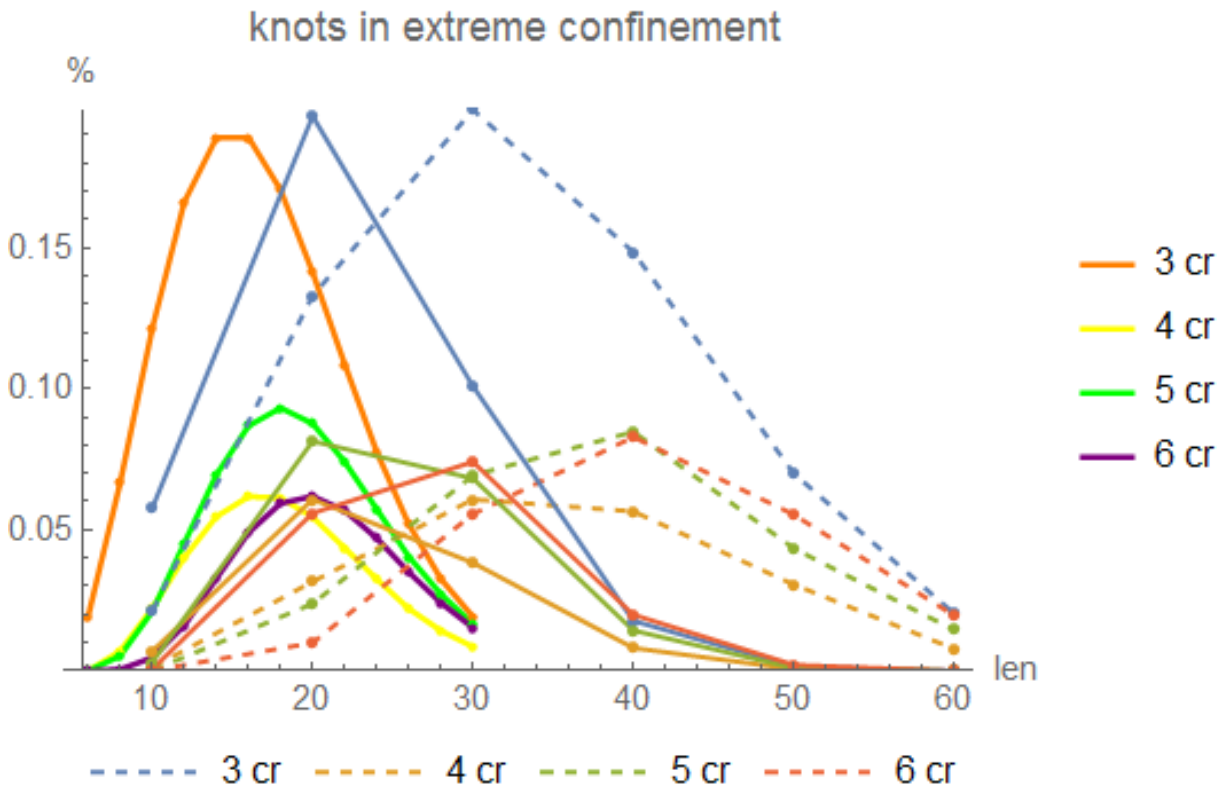
Confinement pressures is increased with increased length and decreased radius of confinement

- Frequency of certain knots
- Relative frequencies – of knot types with same crossing number
- Relative percentage of alt, non-alt, and composite knots with same crossing number
- Mean total curvature and Mean ACN

Extension of prior results – Frequency of knots



Extension of prior results – Frequency of knots



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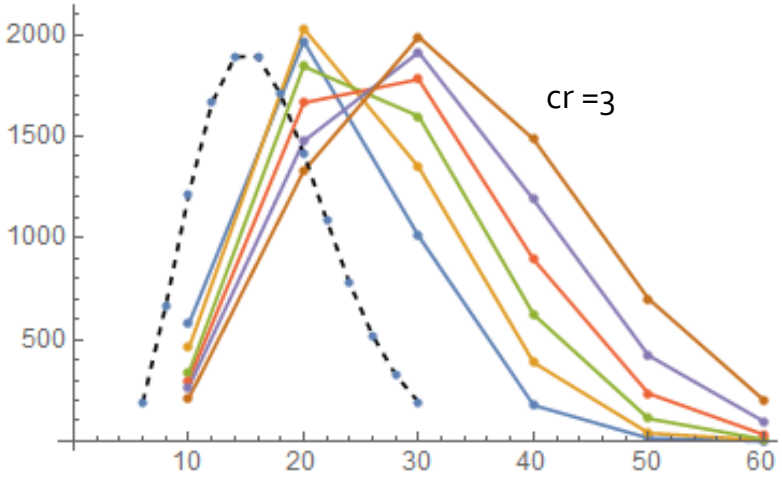

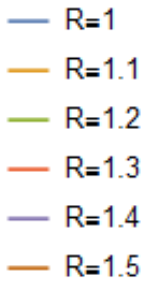

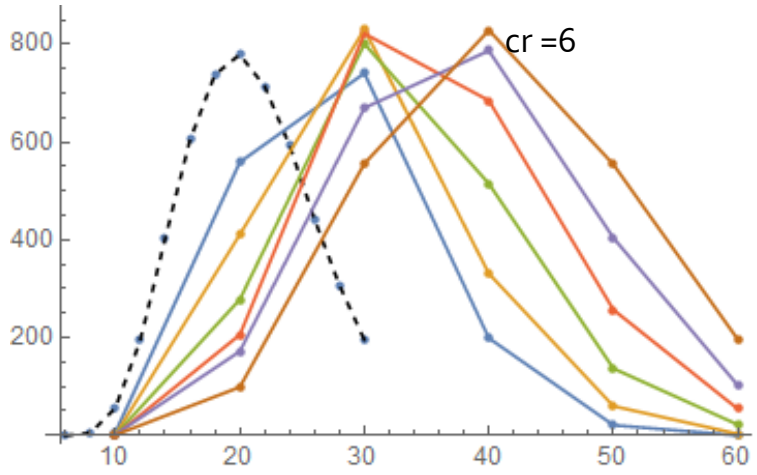

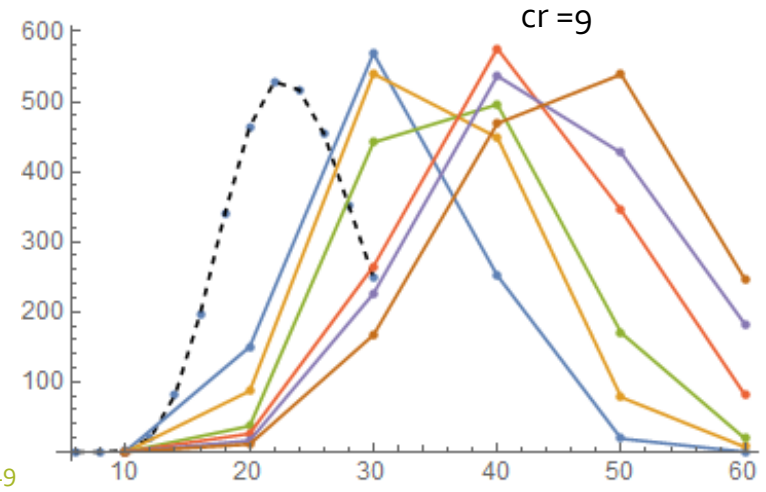

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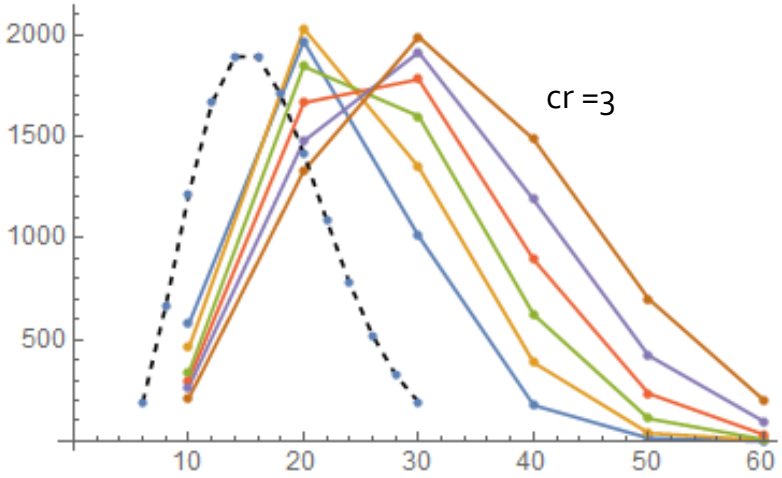
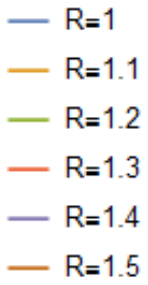
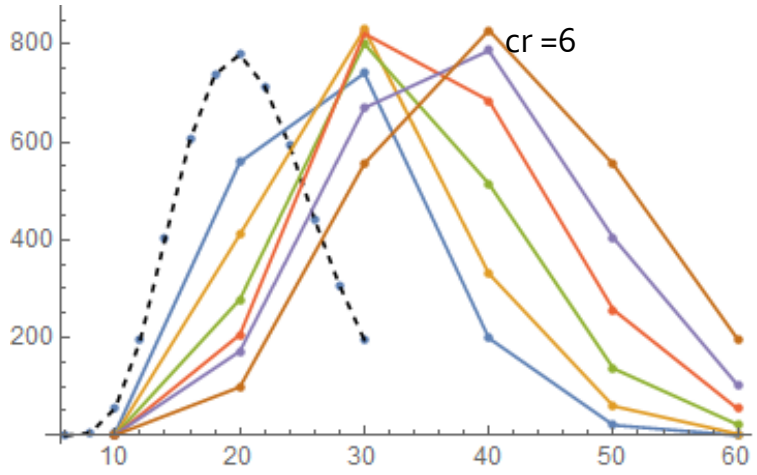
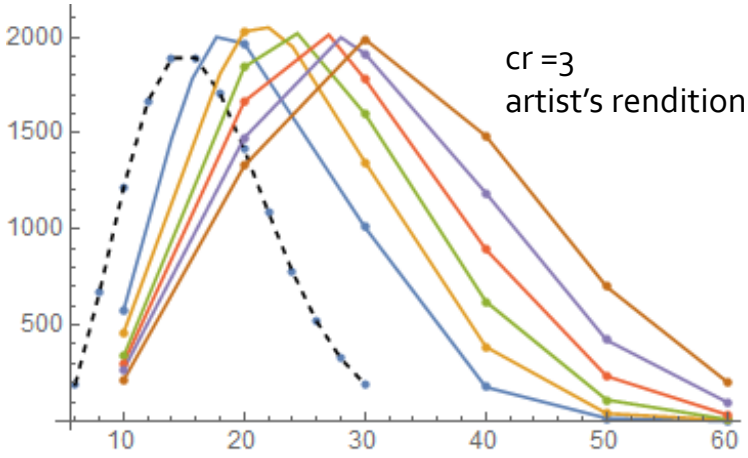
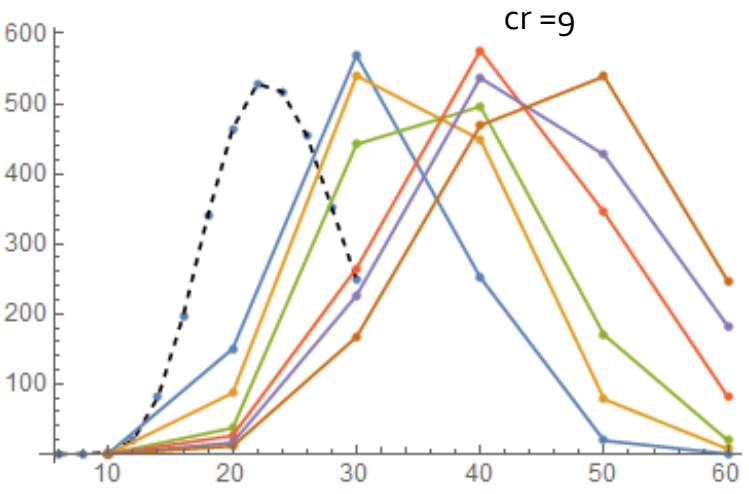


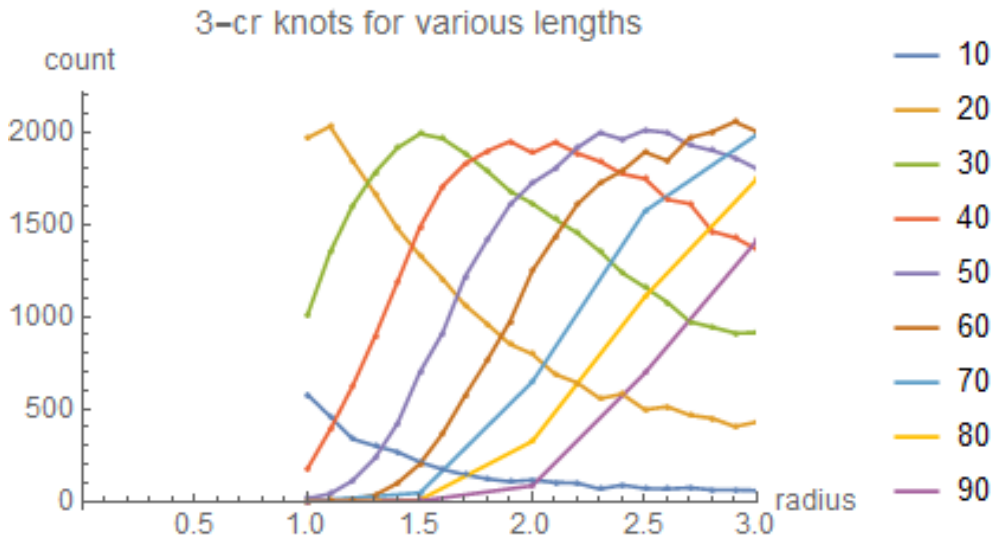








Extension of prior results – Frequency of knots



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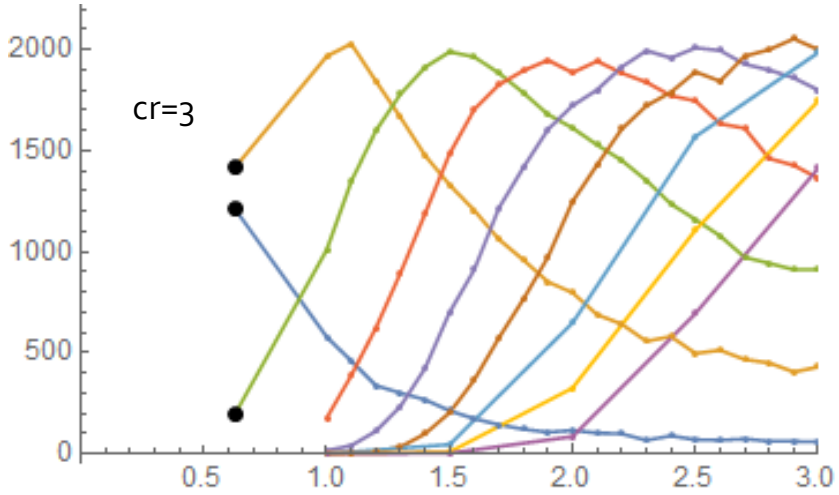
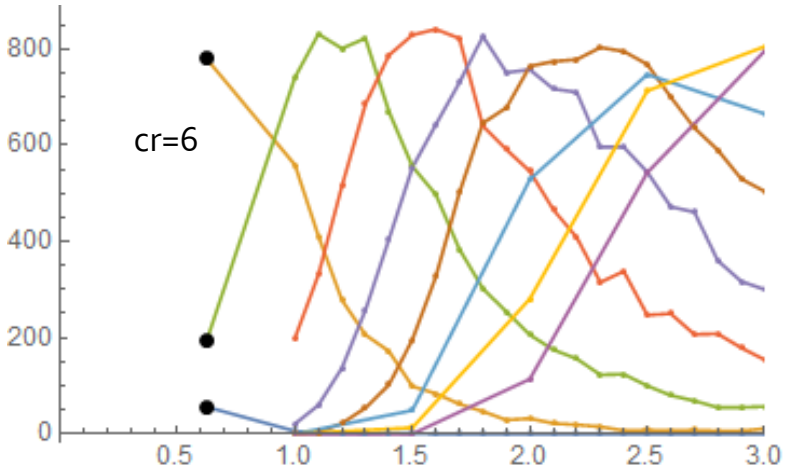
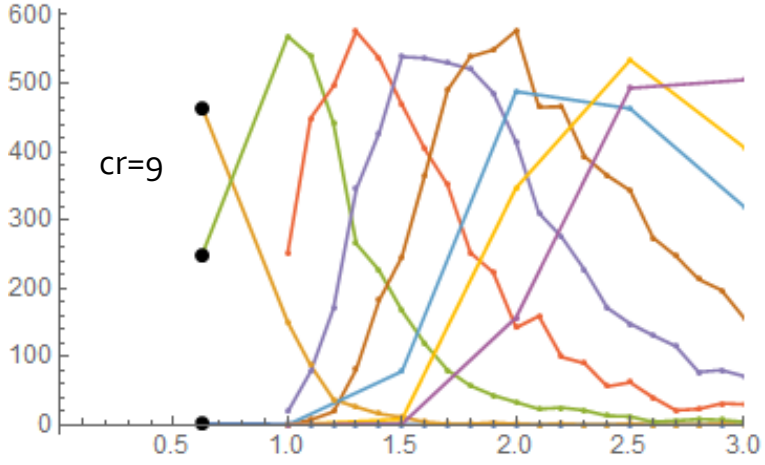


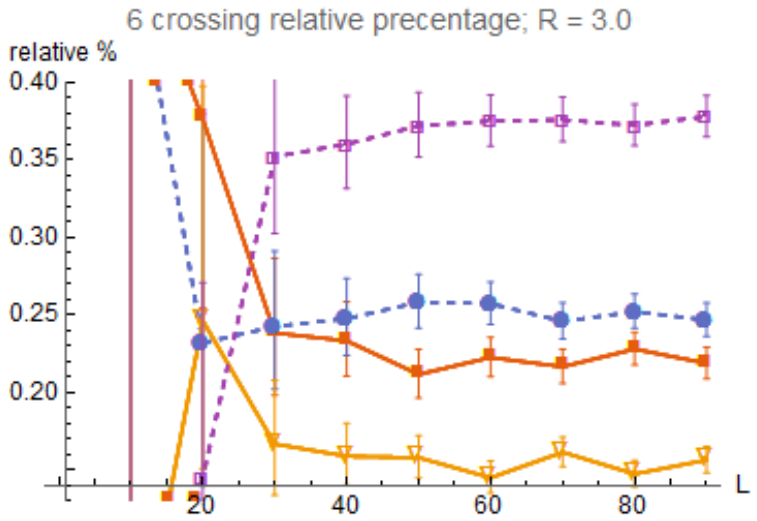


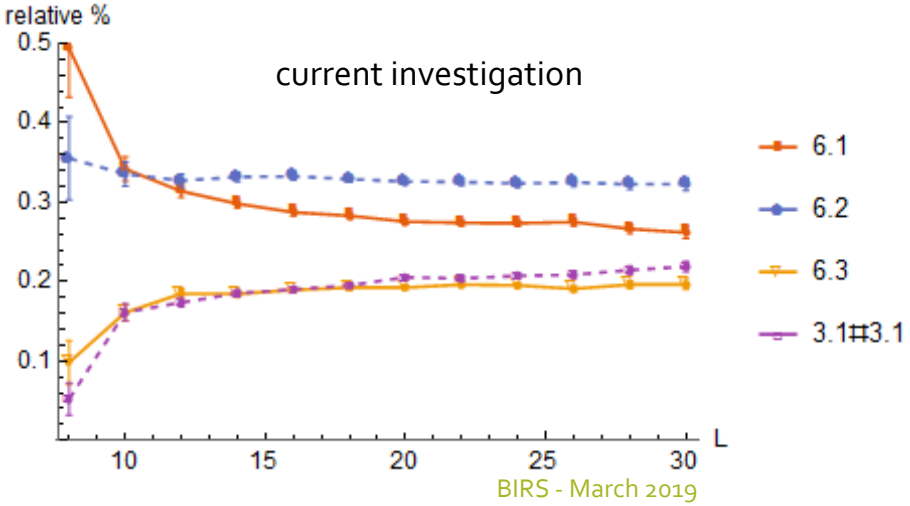


Relative frequencies of knot types with same crossing number

The frequencies for a fixed length add up to 1

Error bars are shows for all data points





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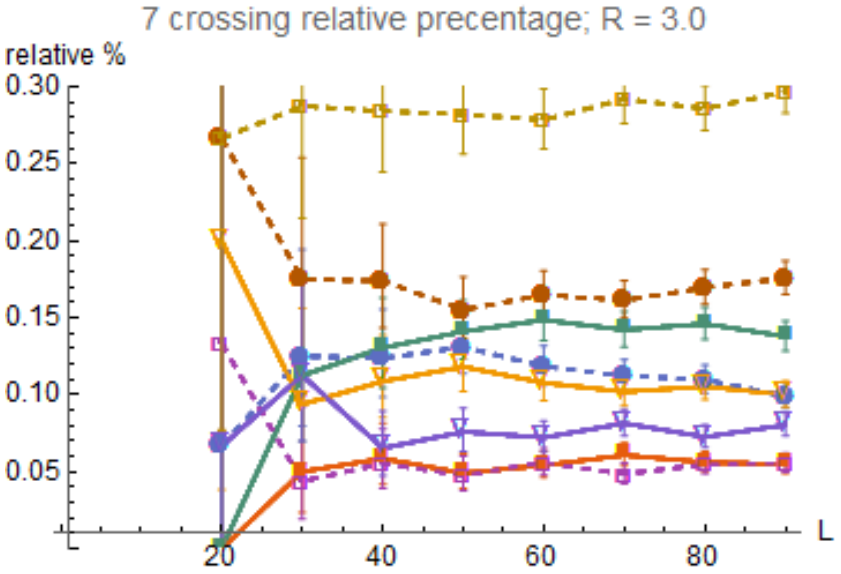

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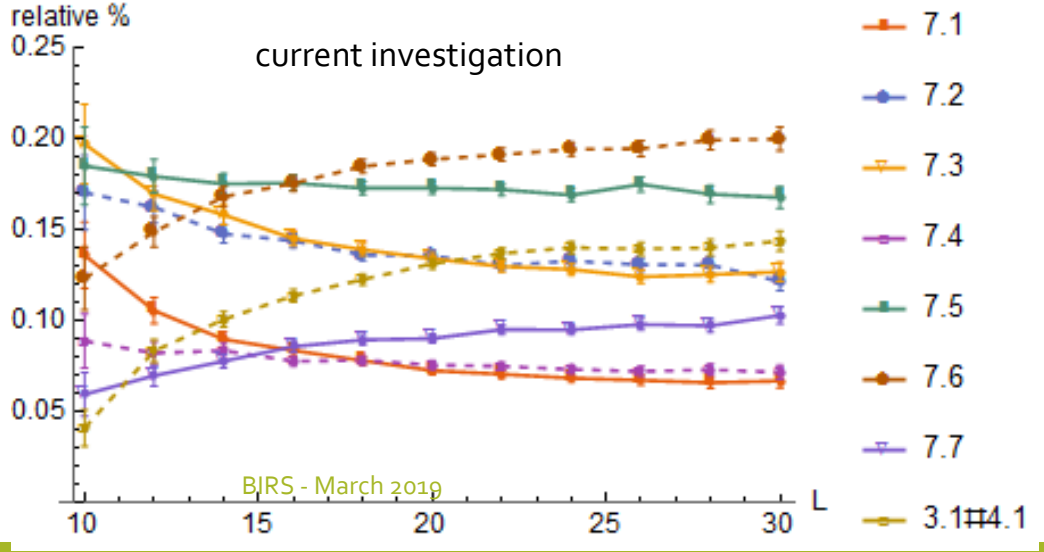

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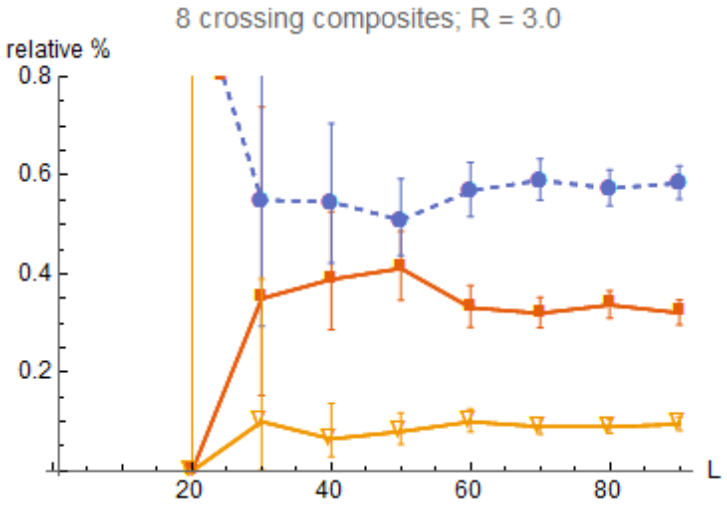

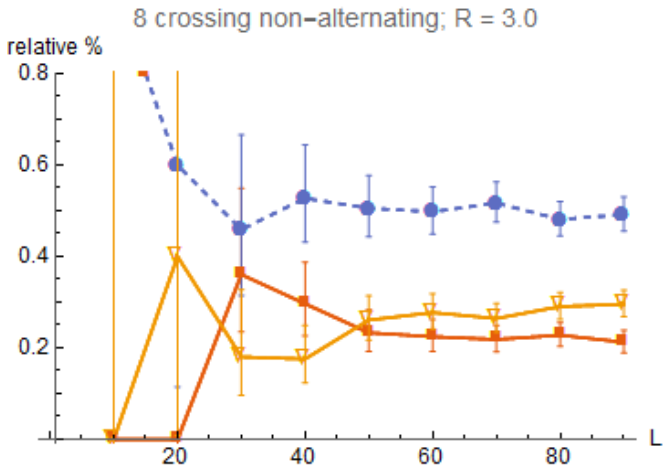

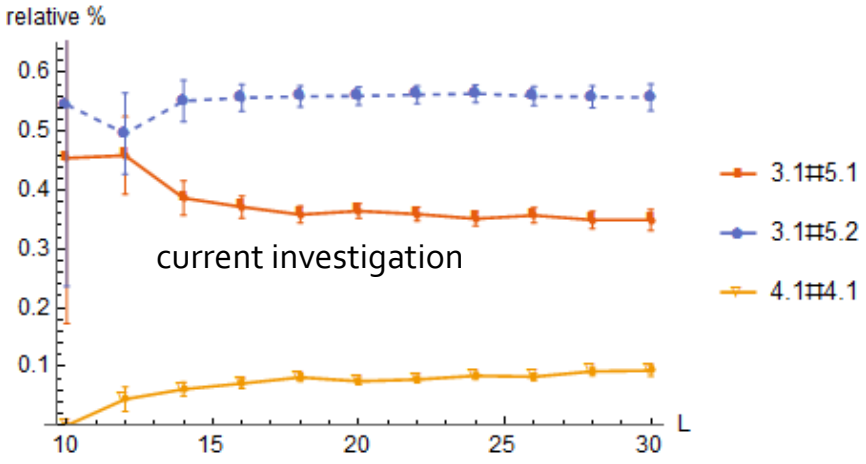

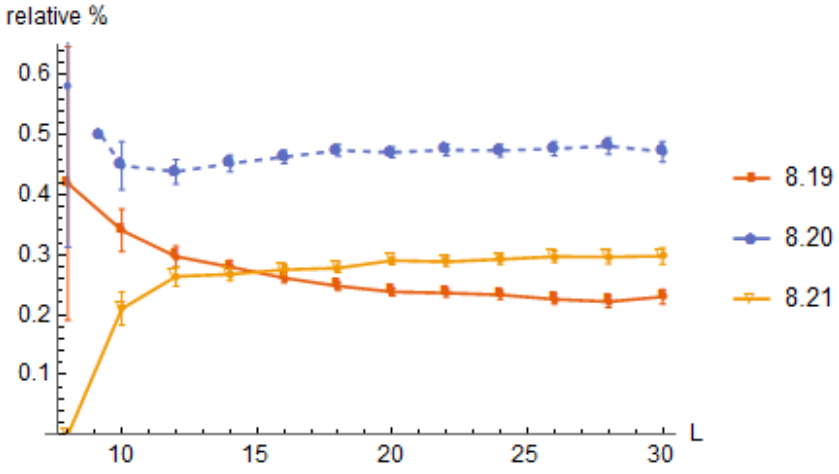

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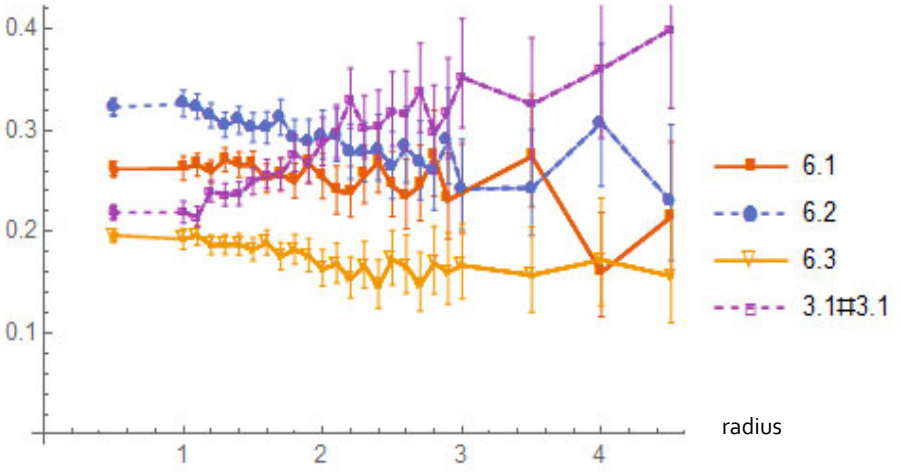
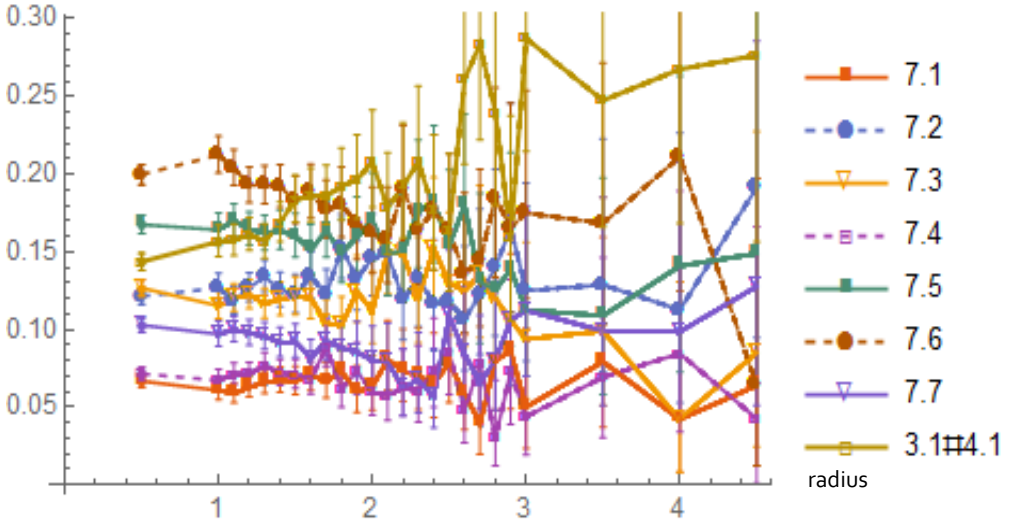
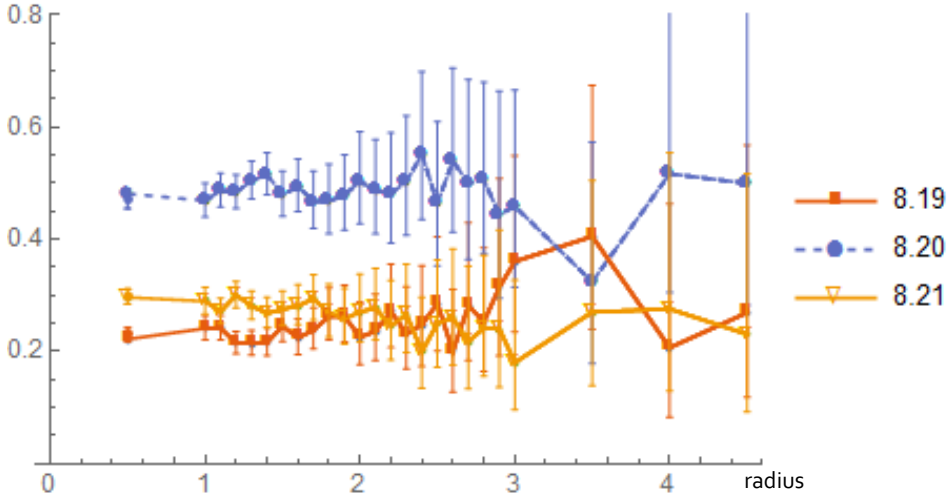


The frequencies for a fixed R add up to 1

Error bars are shows for all data points

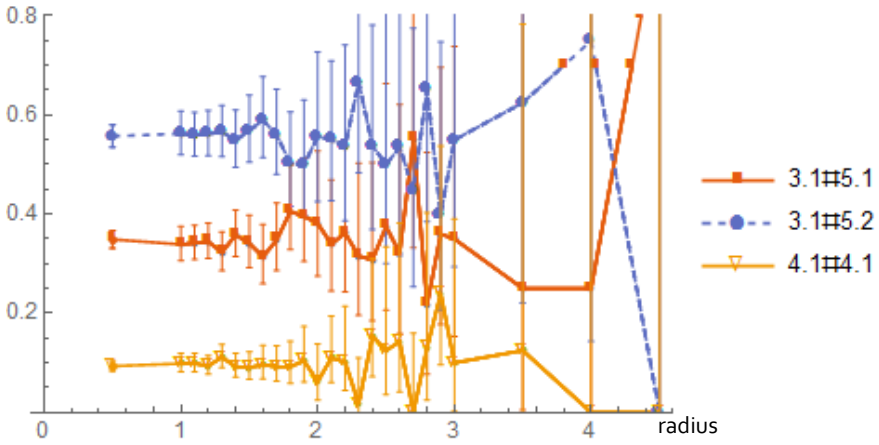


Relative frequencies of knot types with same crossing number



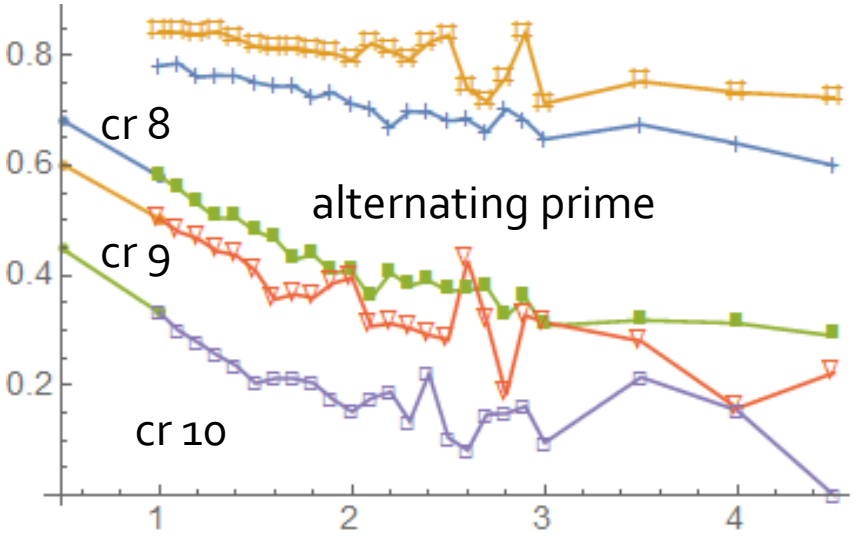
The frequencies for a fixed R add up to 1

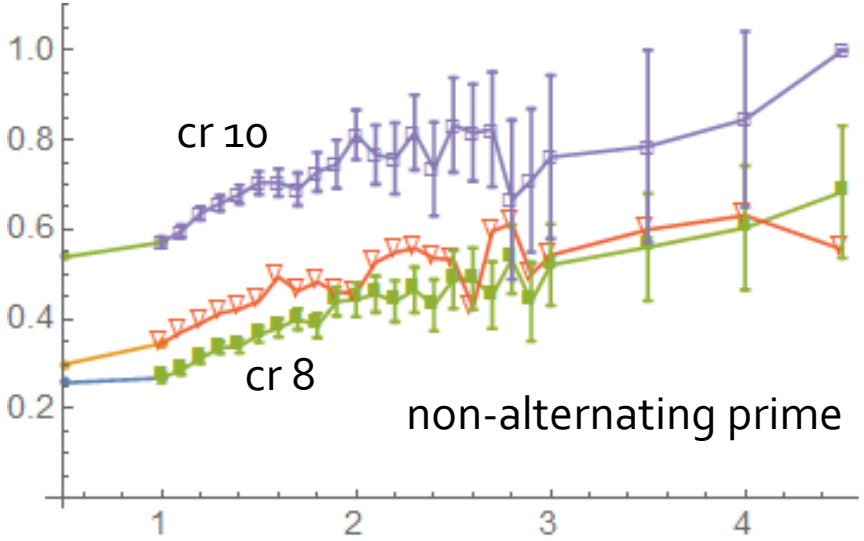
Error bars are shows for all data points



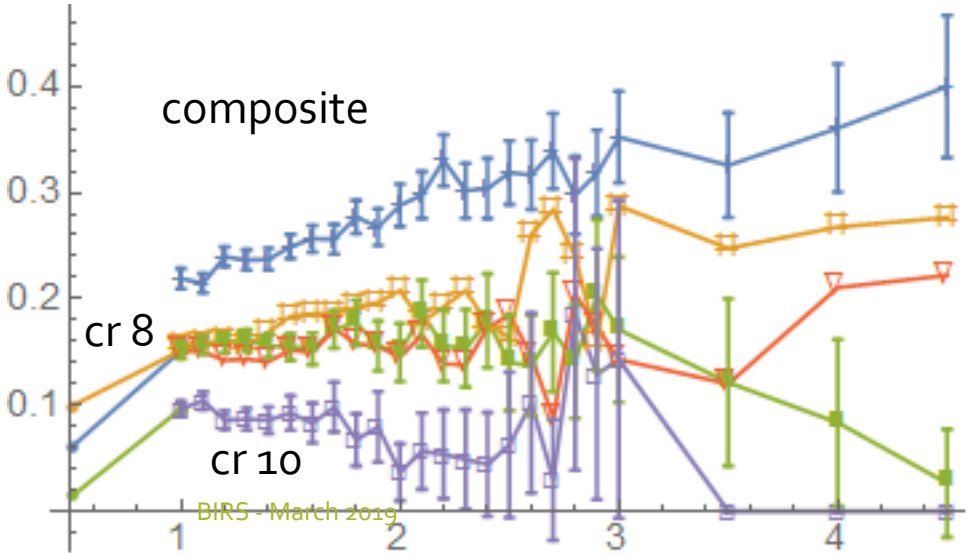
Relative percentage of alternating, non-alternating and composite knots with same crossing number

All polygons are of length 30

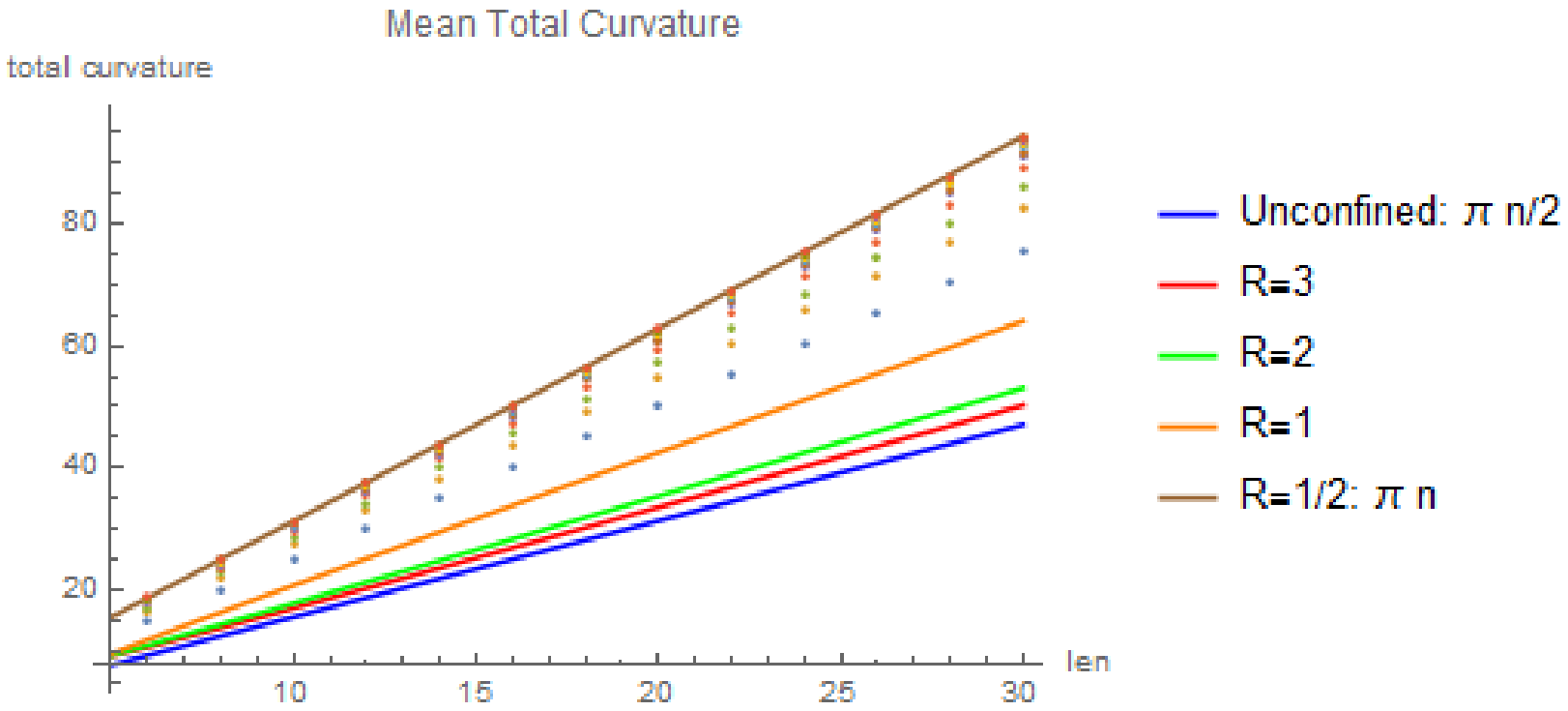




The frequencies for a given crossing number and given radius add up to 1 (over the three graphs).

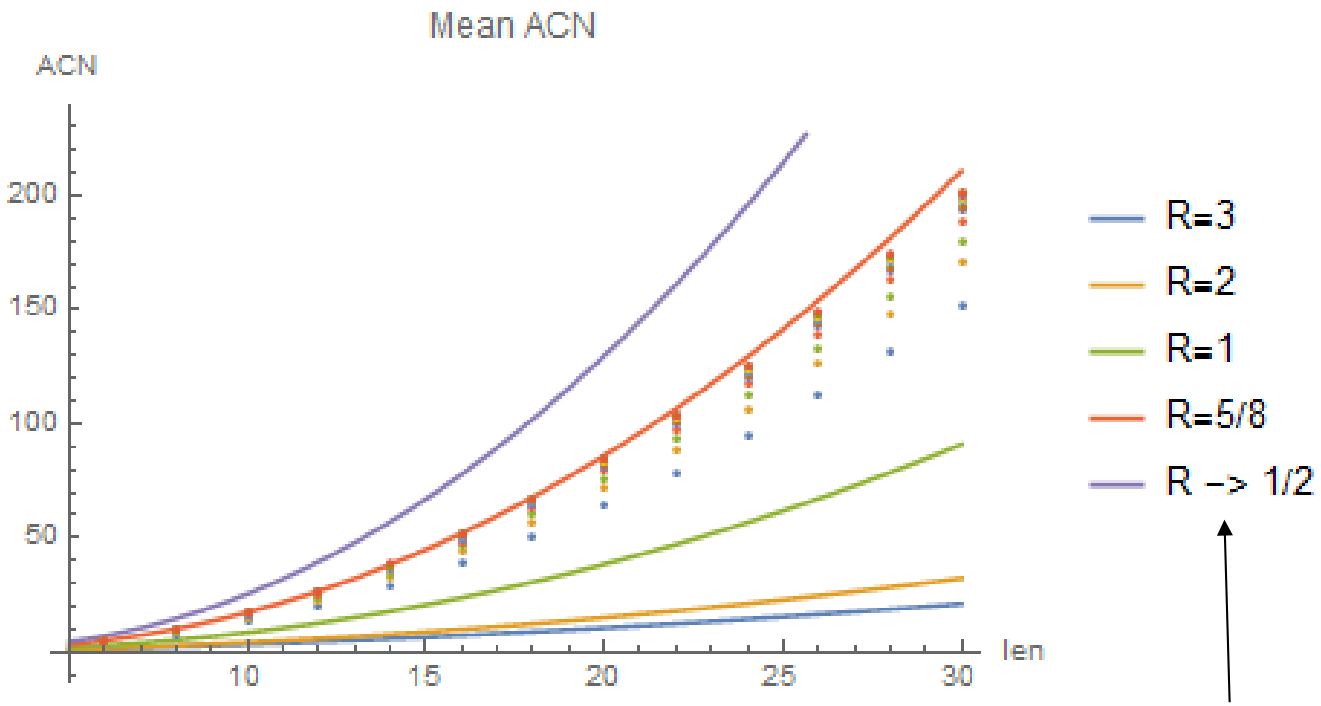


Geometric measure – curvature



(Diao-Ernst-Rawdon-Z 2018 a)

Geometric measure – ACN



(Diao-Ernst-Rawdon-Z 2018 b)

Take home…

- The described approach to ‘extreme’ confinement seems to be a valid extension of our previous investigation for decreasing the radius of confinement below 1

- < 1 and $> 1/2$, but unclear where exactly or whether it is equivalent to one fixed radius for the spherical confinement.

References

- Diao, Y., Ernst, C., Rawdon, E. Ziegler, U., (2018 b) Average crossing number and writhe of knotted random polygons in confinement, *Reactive and Functional Polymers*, **131,** pp 430-444, doi:10.1016/j.reactfunctpolym.2018.07.028
- Diao, Y., Ernst, C., Rawdon, E. Ziegler, U., (2018 a) Total curvature and total torsion of knotted random polygons in confinement, *J. Phys. A: Math. Theor*. **51** 154002 (33pp)
- Diao, Y., Ernst, C., Rawdon, E. Ziegler, U. (2017) *Relative Frequencies of Alternating and Non-alternating Prime Knots and Composite Knots in Random Knot Spaces*, Experimental Mathematics, doi:10.1080/10586458.2017.1320239
- Diao, Y., Ernst, C., Rawdon, E. Ziegler, U., (Dec 2018 c) The Knot Spectrum of Random Knot Spaces, in *New Directions in Geometric and Applied Knot Theory,* Eds P. Reiter, S. Blatt, A. Schikorra; accepted 2017 to be published by De Gruyter in the series OA Measure Theory (p. 205-237)
- Diao, Y., Ernst, C., Montemayor, A., Rawdon, E., Ziegler, U. (2014). *The Knot Spectrum of Confined Random Equilateral Polygons*. Molecular Based Mathematical Biology, *2*(1), pp. 19-33; doi: 10.2478/mlbmb-2014-0002