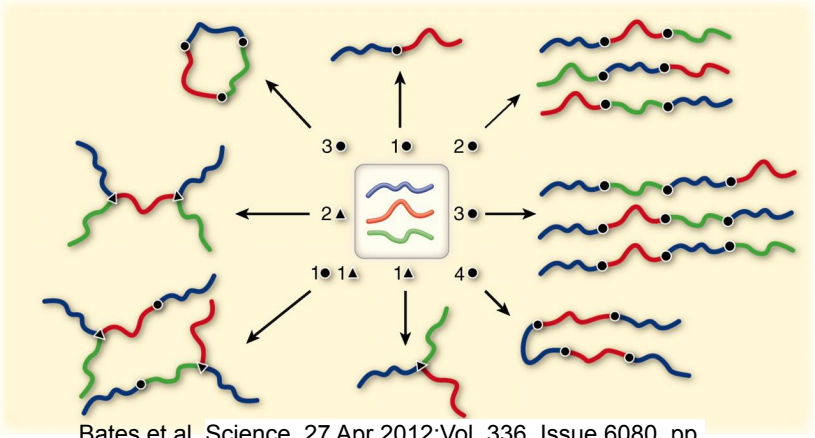
Classification Methods for Block Copolymer Phase Behavior

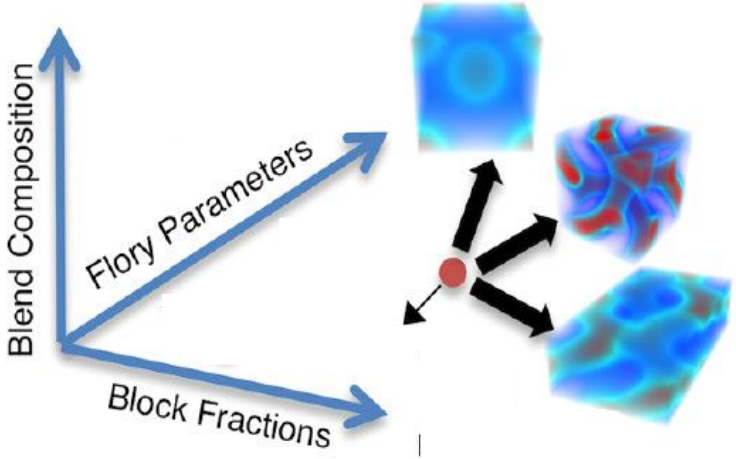
Timothy Quah

Motivation

- There are many parameters or dimensions that govern the phase behavior of block copolymers



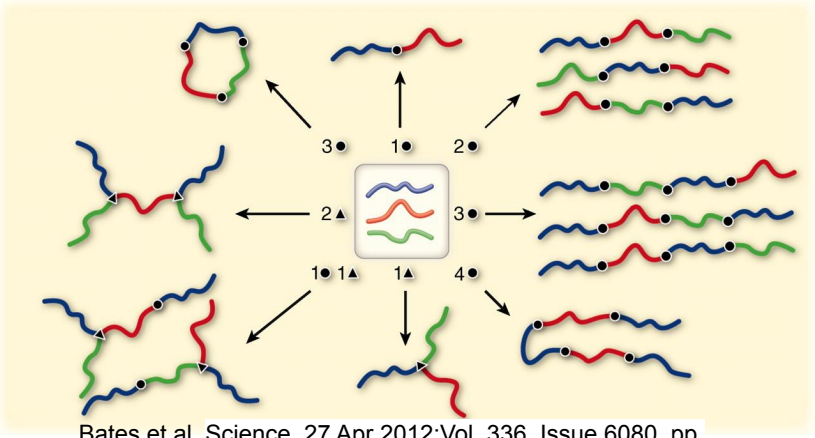
Bates et al. Science 27 Apr 2012:Vol. 336, Issue 6080, pp. 434-440 DOI: 10.1126/science.1215368



Khadilkar et al., Macromolecules 2017 *50* (17), 6702-6709 DOI:10.1021/acs.macromol.7b01204

Motivation

- There are many parameters or dimensions that govern the phase behavior of block copolymers
- Alternatives to grid searching?



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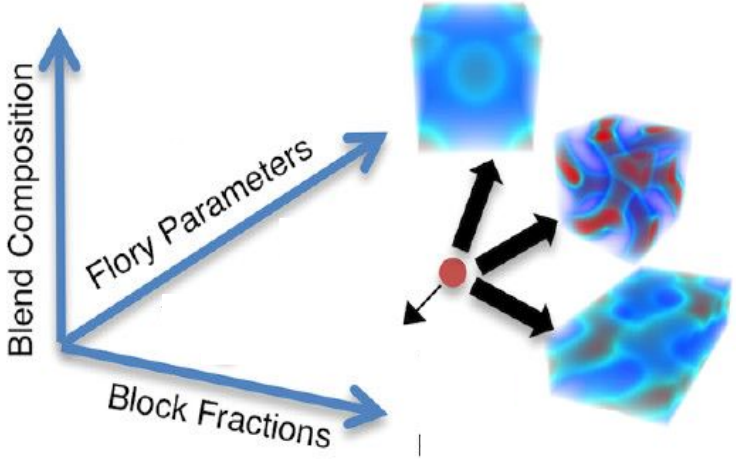

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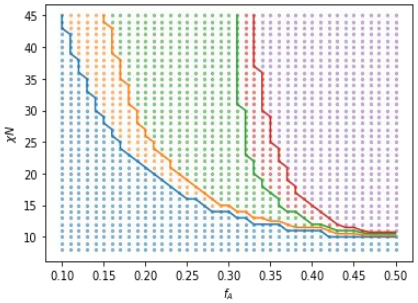
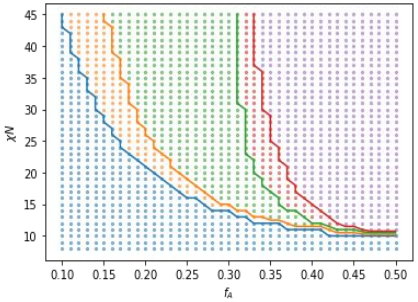
Methodology

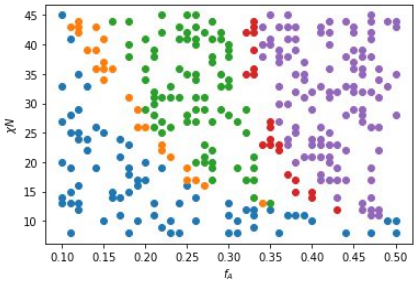


Data Preparation and Normalization

Methodology

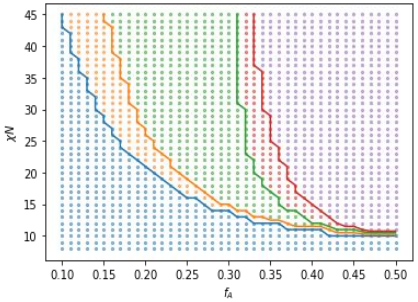


Data Preperation and Normalization



Data Splitting

Methodology



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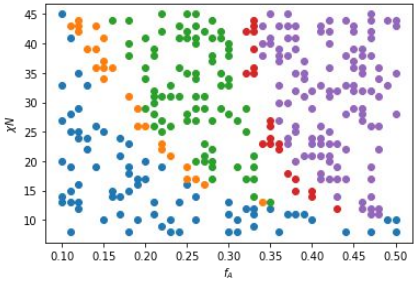

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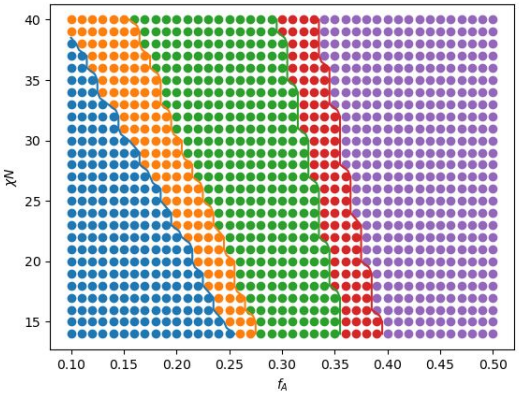
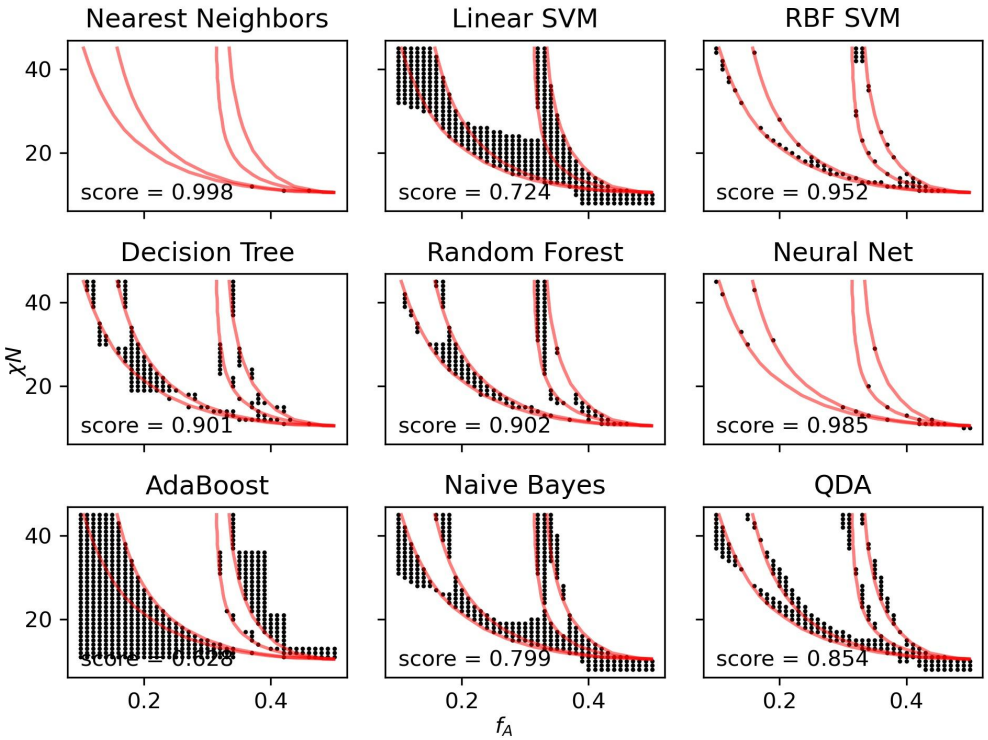
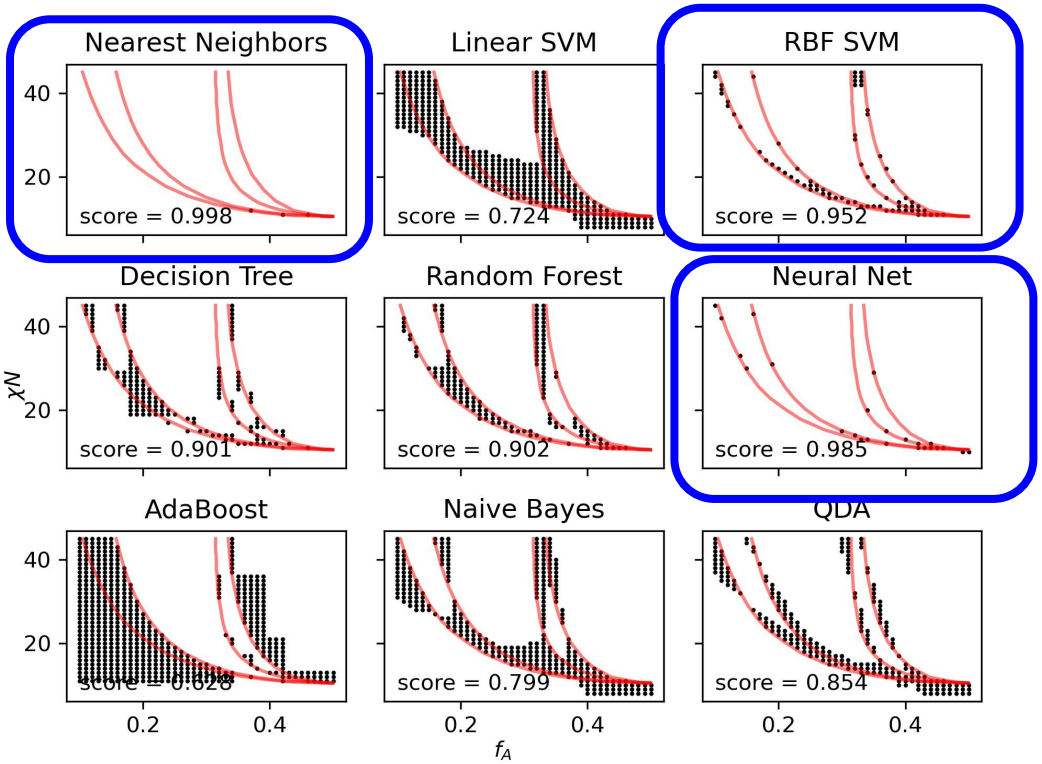


Classification and Decision Boundary

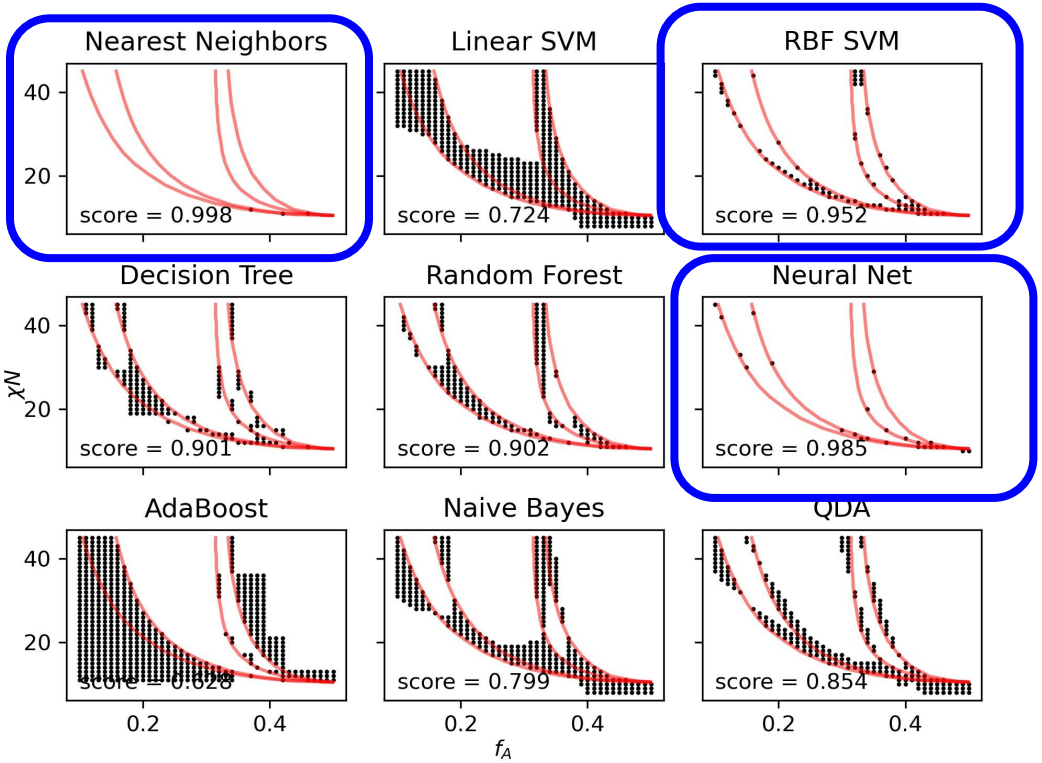
Results: Classification

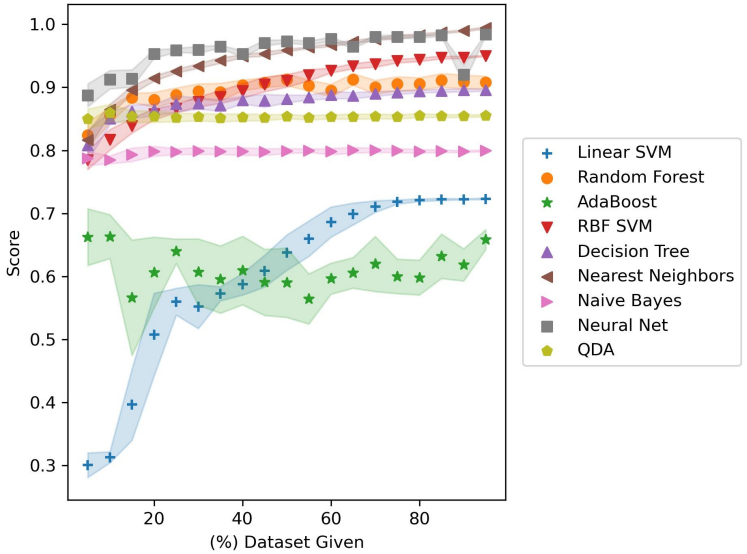


Results: Classification

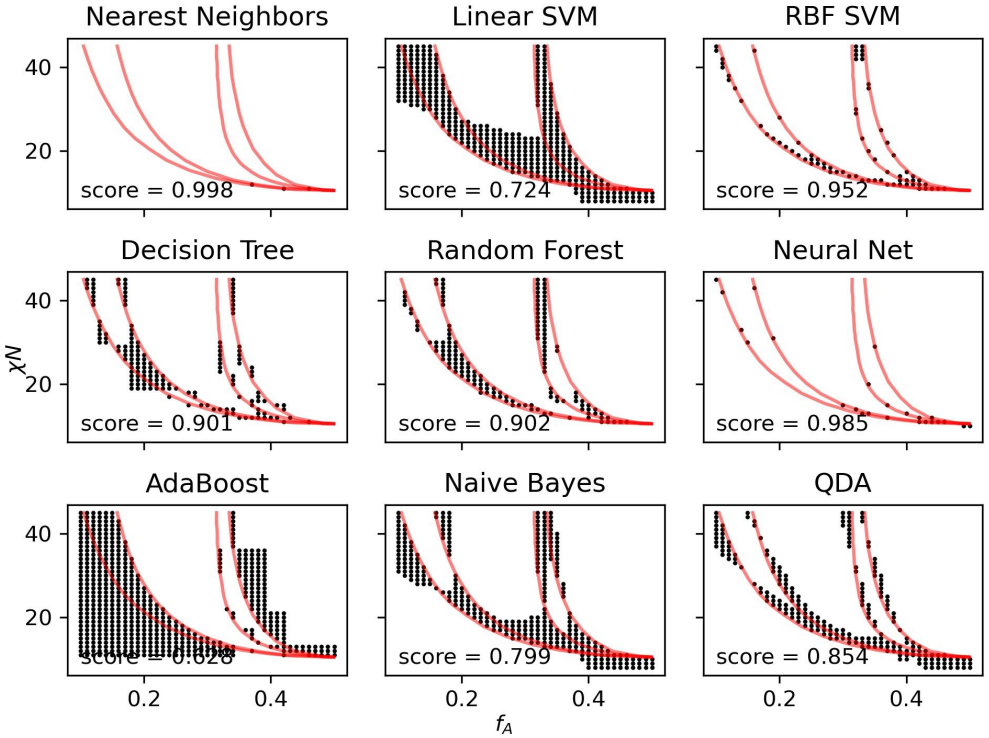


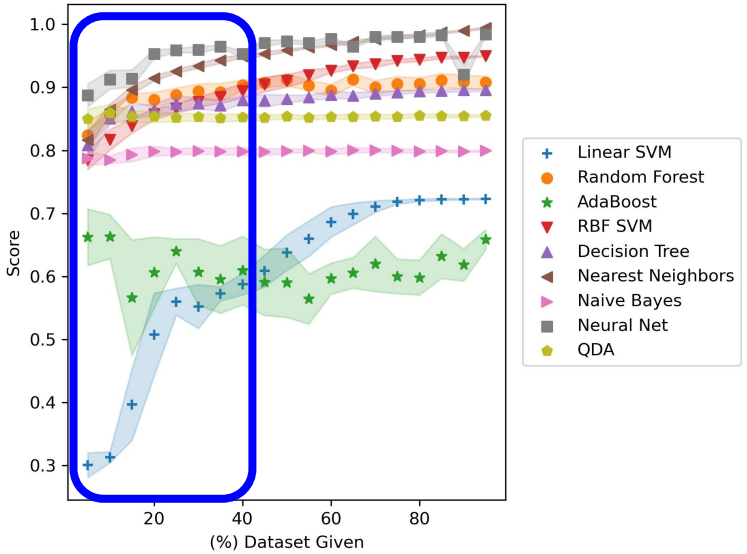
Results: Classification





Results: Classification





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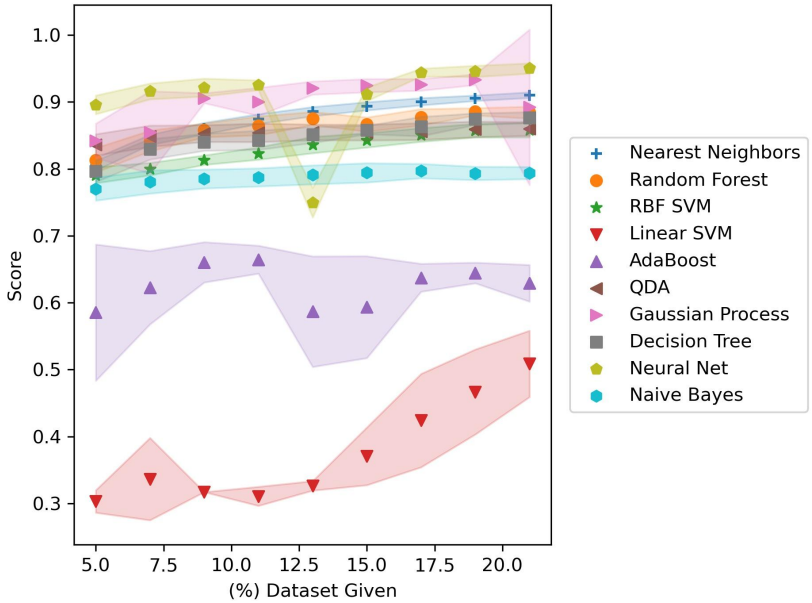
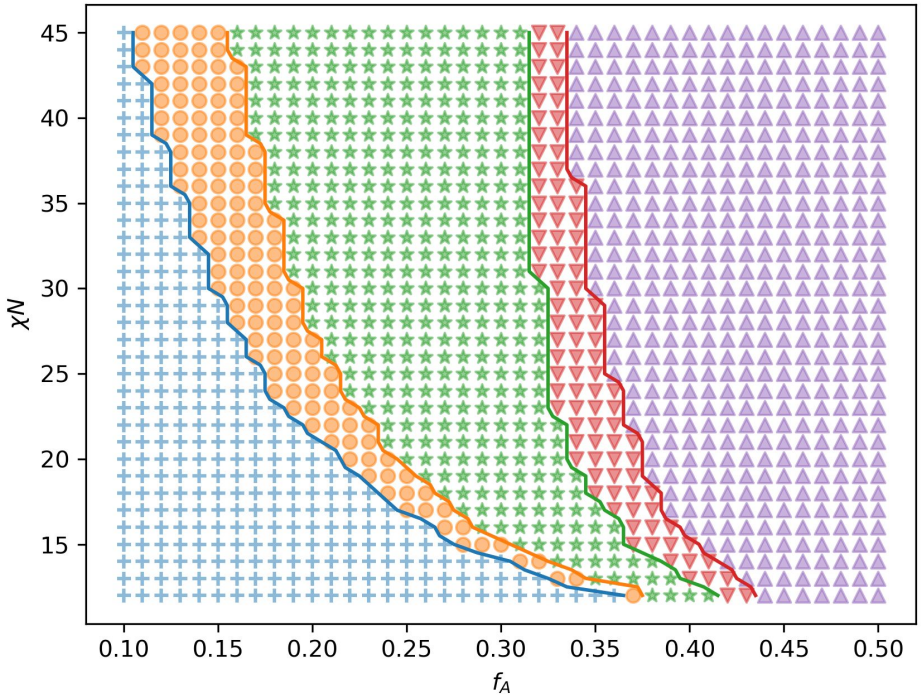
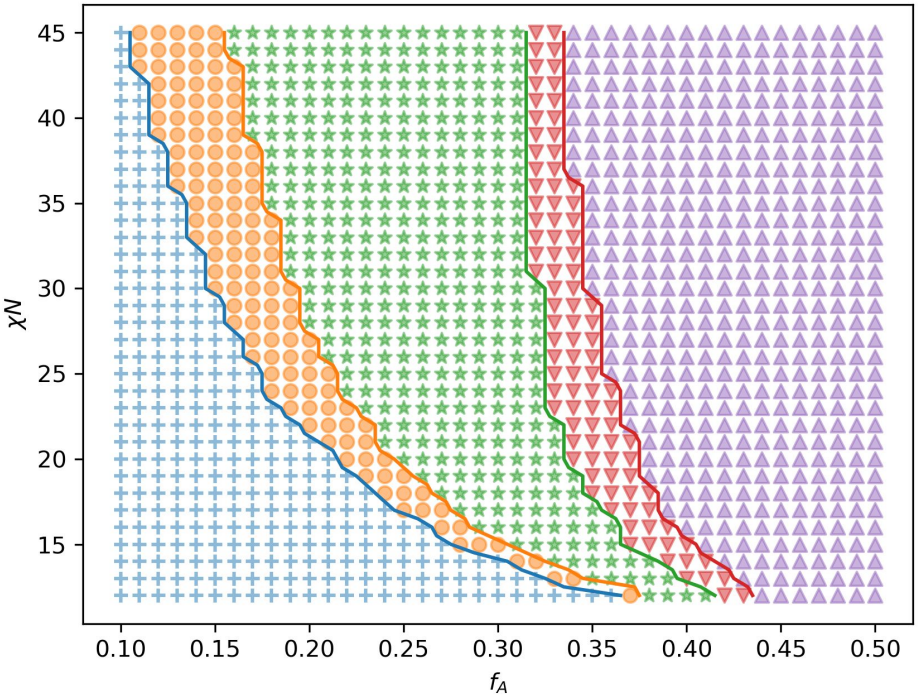


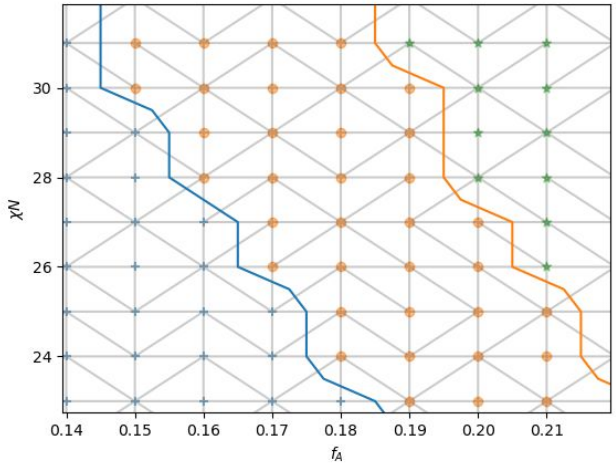
- Gaussian process classification (GPC) based on Laplace approximation works well on small datasets
- GPC is extremely computationally expensive on larger datasets
- As datasets become larger Neural Networks and Nearest Neighbors are better

Results: Phase Boundaries

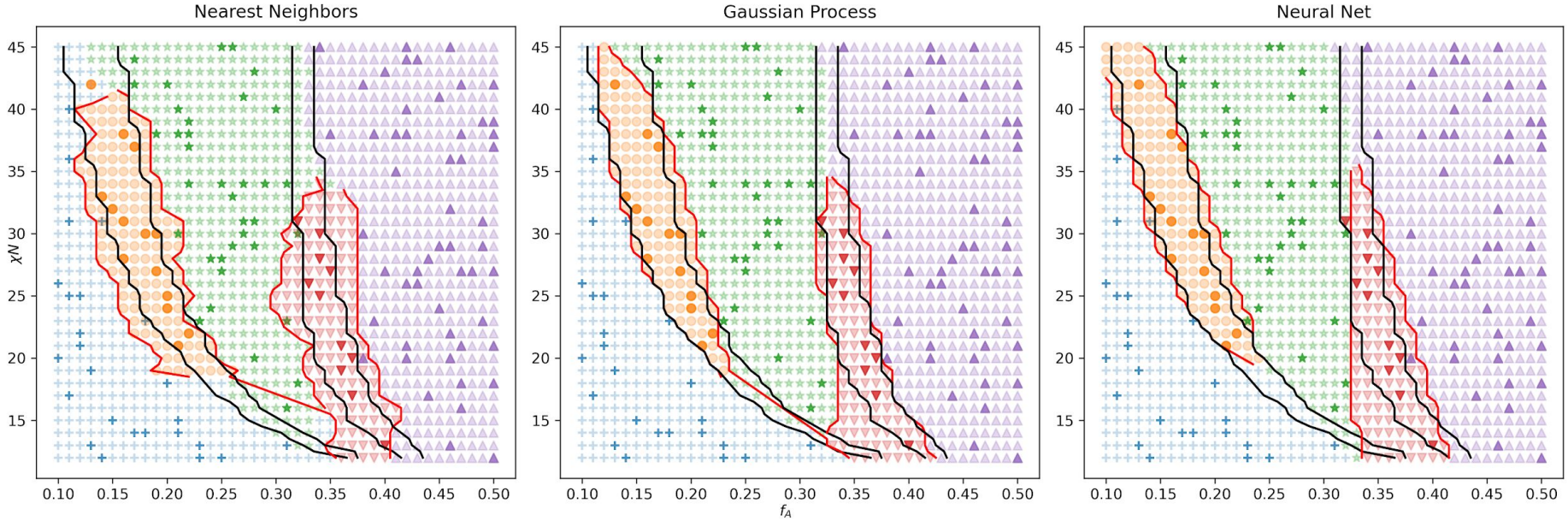


Results: Phase Boundaries

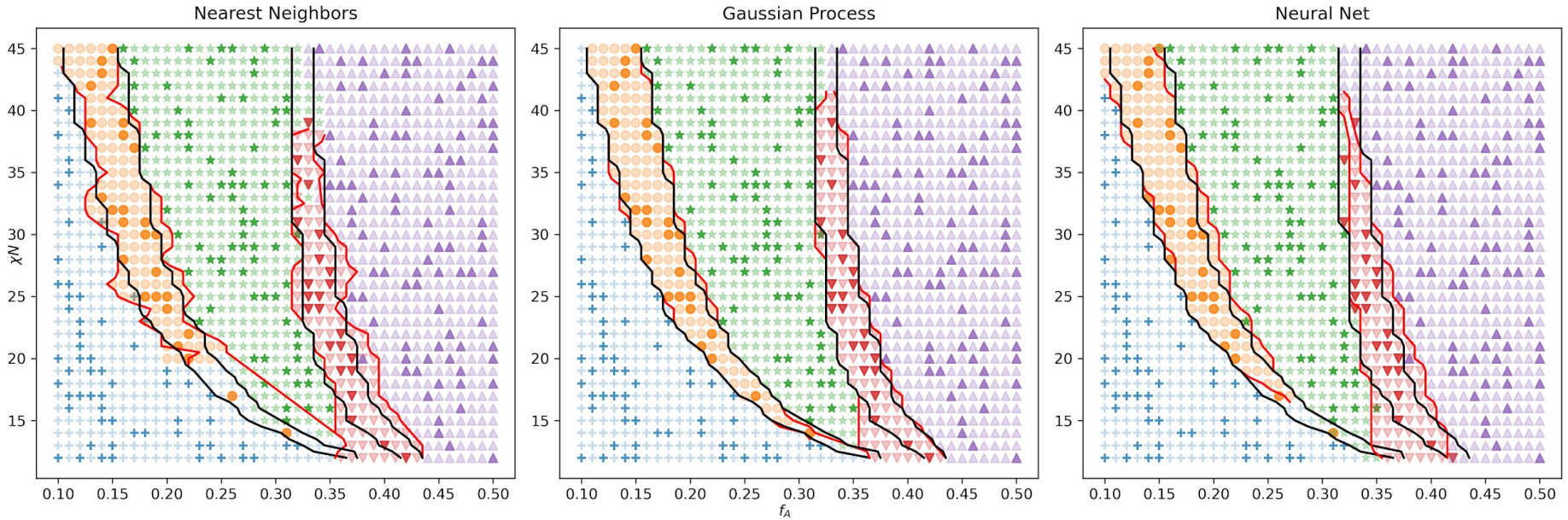




Results: Phase Boundaries-10% Percent of Data



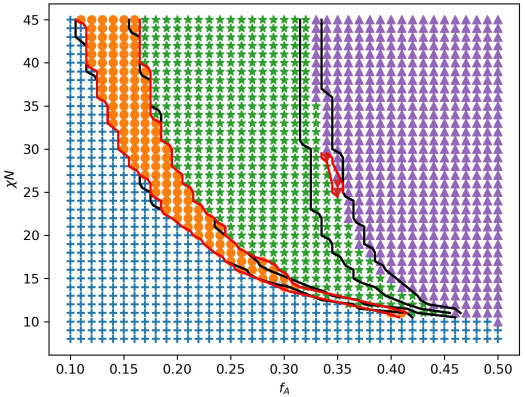
Results: Phase Boundaries-15% Percent of Data

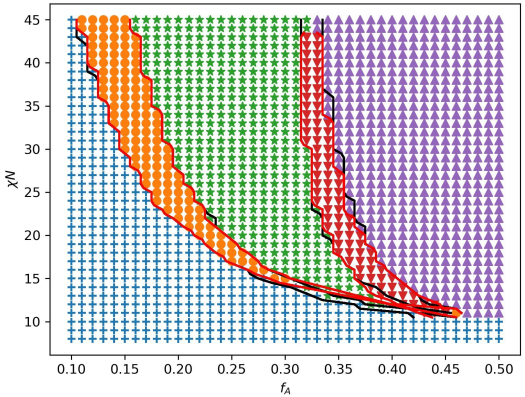


Active Learning

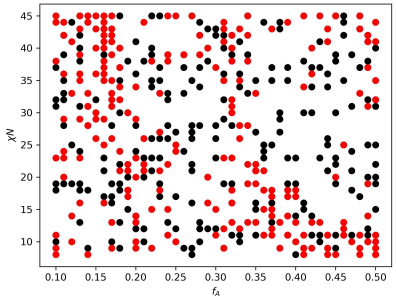
- Integrating GPC and Polymer Self-Consistent Theory
  - Get phases at random points using Self-Consistent Field Theory (SCFT)
  - Use a classification method to classify system
  - Compute points that will minimize uncertainty
  - Run those some of these points using SCFT
  - Rinse and Repeat

Active Learning





Both used similar amounts of points, but shows **which** points are chosen is important!



Future Directions

- Exploring if GPC can indeed explore higher dimensional spaces of block copolymer phase behavior
    - Architectural details
    - Chemistries/Interactions
    - Composition
- Revisit other similar bayesian methods using the iterative approach
    - If we run into large datasets GPC is slow will we need to use a quicker method?