Organization Theory applied to Chemical Reaction Networks

Gil Benkö

Graduiertenkolleg Wissensrepräsentation and
Lehrstuhl f. Bioinformatik, Institut f. Informatik,
Universität Leipzig

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Background

[Fontana & Buss '94]: Theory of Biological Organization
Classification of dynamical systems

- L0: cooperating replicators
- L1: *organizations*, features include : boundaries, self-maintenance
- L2: organizations of organizations

[Dittrich & Speroni d. F. '05]: Chemical organization theory

- Definition 1: Algebraic chemistry = set of molecules + reactions
- Definition 2: Closed set = all reactions produce only molecules of type already in the set
- Definition 3: Self-maintaining set = all molecules that are consumed by reactions are also produced by other reactions
- Definition 4: Semi-organization = closed and self-maintaining set

Application

Input a set of molecules and reactions (chemical reaction network)
Output all (sub)sets that are closed and self-maintaining = organizations
All those organizations form together a lattice of organizations

Connection to chemical dynamics

Loosely speaking, organizations are fixed points of the chemical reaction network, once all molecules in the reaction vessel belong to a organization, the system cannot escape as no new types of molecules are produced and the existing types of molecules are maintained.

Moving between organizations

If a type of molecule in an organization is consumed faster than it is produced, it will disappear, the system will move ("DOWN") to a smaller organization completely included in the original one.

Moving between organizations II

External influences like the addition from outside of a new type of molecule will result in moving ("UP") from the original organization to a bigger one.

Short explanation of the Toy Model

Given a list of starting molecules and allowed chemical reactions, we iteratively generate a chemical reaction network.
This might be interpreted in the framework of organizations as finding the closed set that includes the starting molecules.

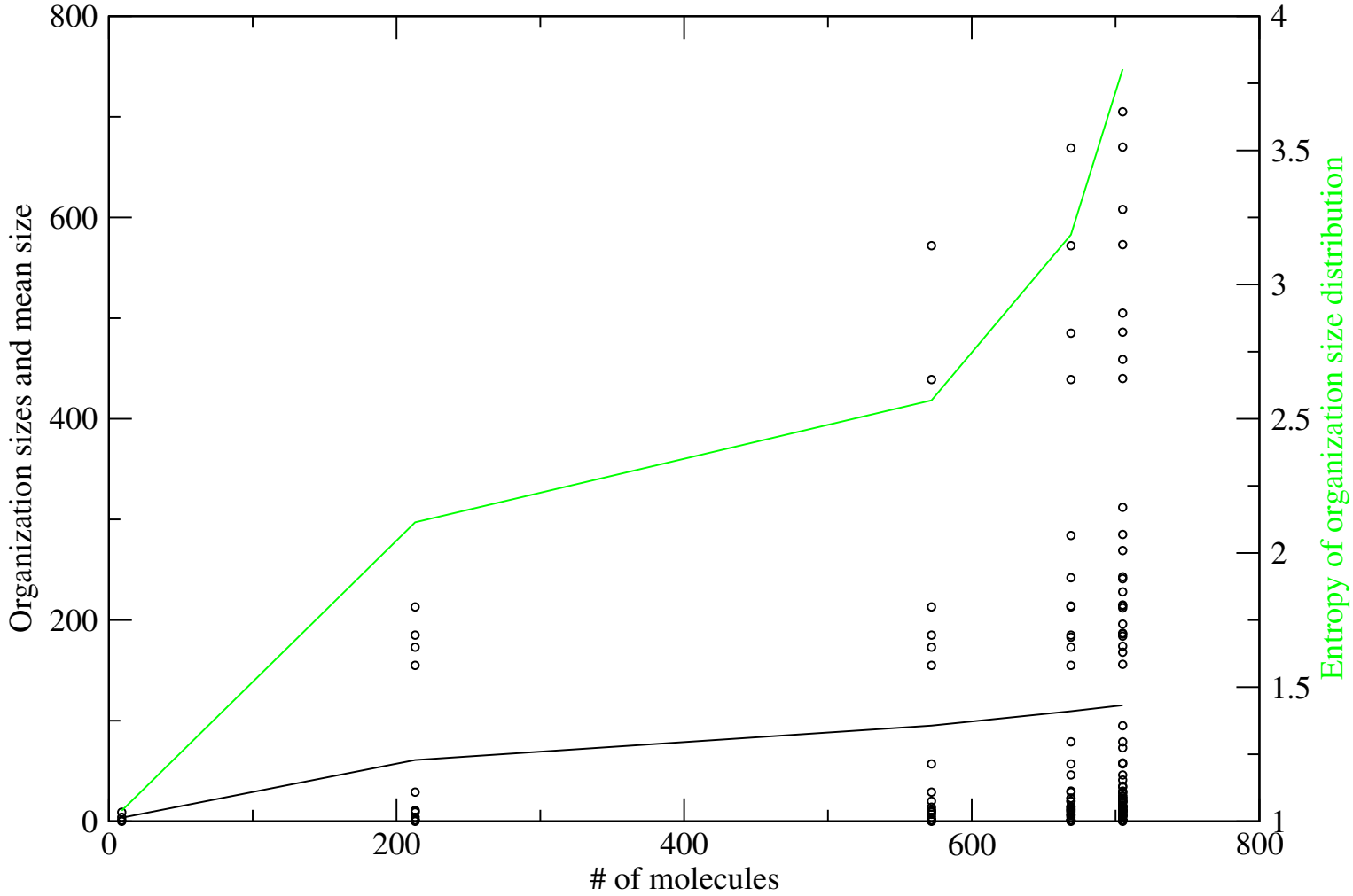
Example

Starting molecules $\longrightarrow$ Network

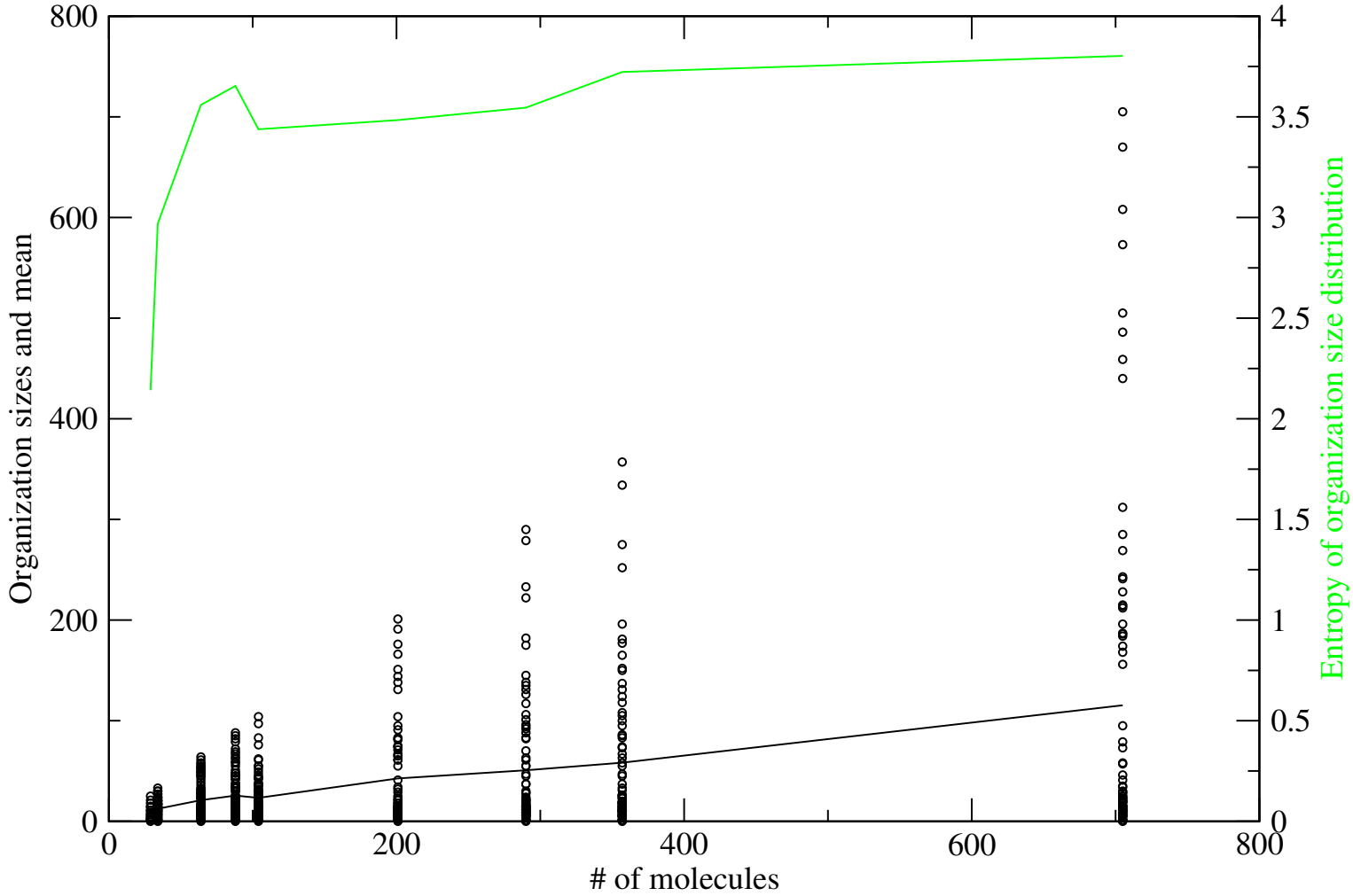
Objective

How does the lattice of organizations change with growing chemical reaction networks? We generated networks of increasing size by using increasingly complex chemistries, i.e. by increasing the number of starting molecules or by increasing the size of molecules allowed.

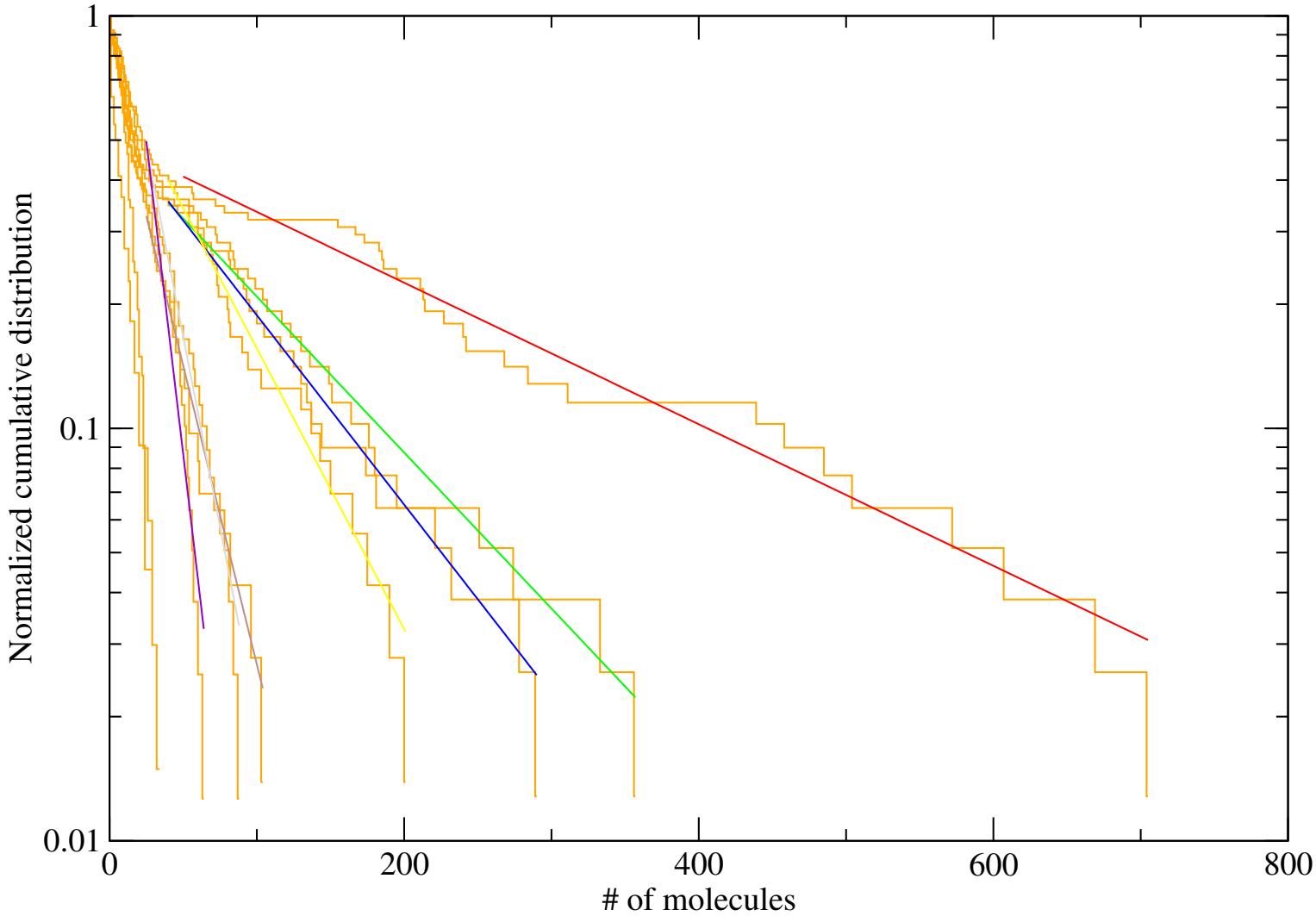
Results:
Increasing the number of starting molecules



Results:
Increasing the size of molecules allowed



The distributions are exponential:



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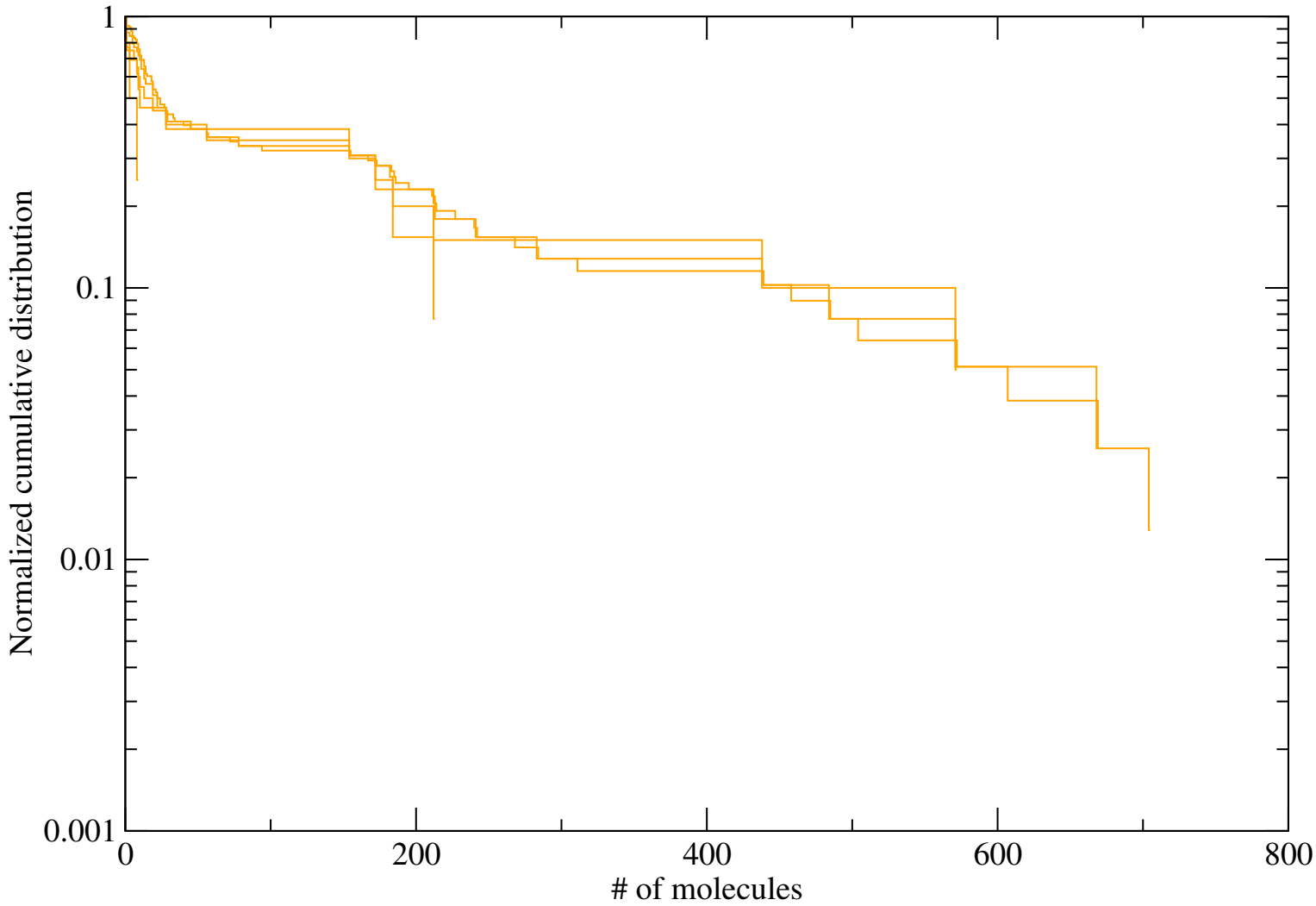
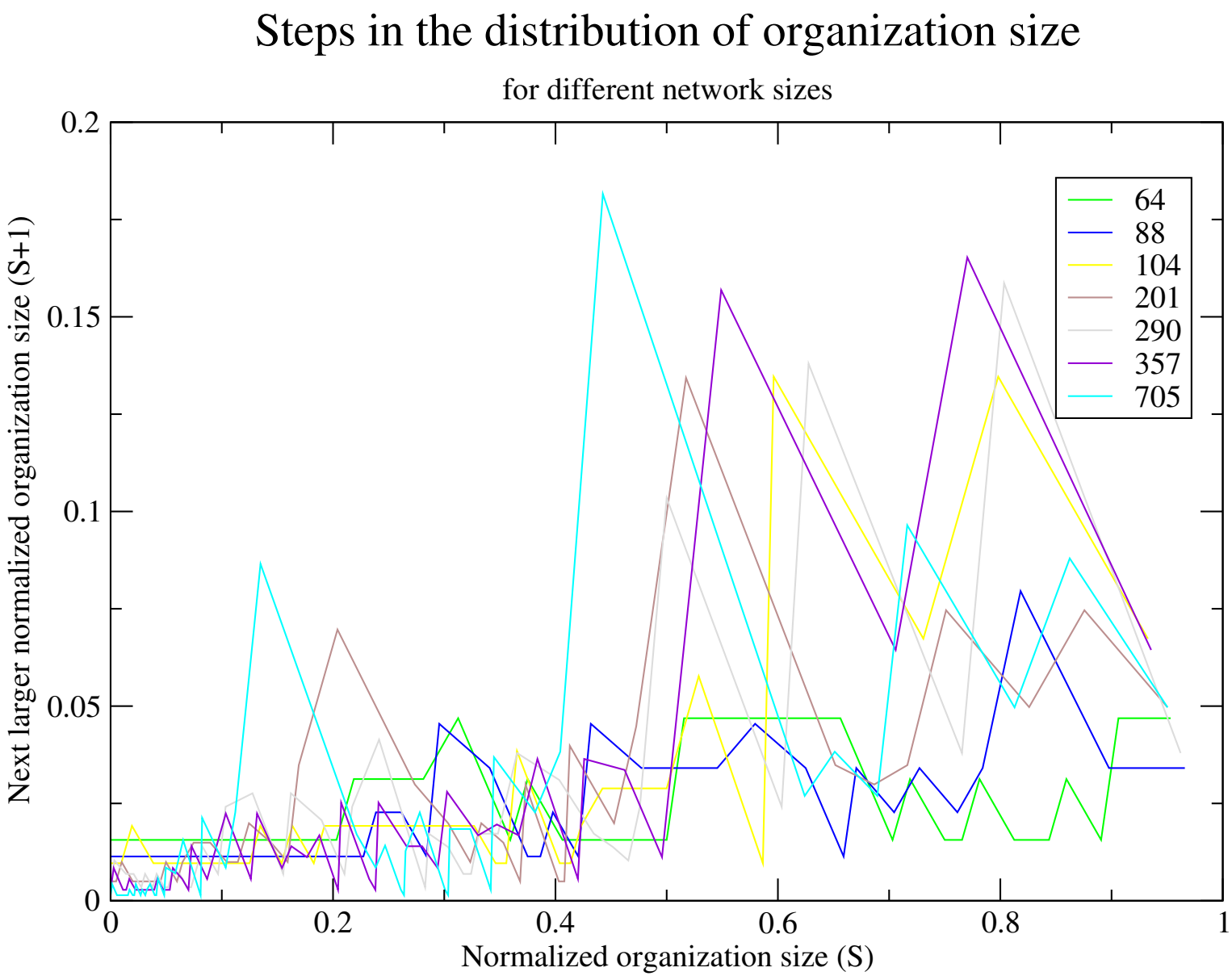

1
0.1
0.01
0.001
Normalized cumulative distribution
0
200
400
600
800
# of molecules

The distributions have gaps that partition it:



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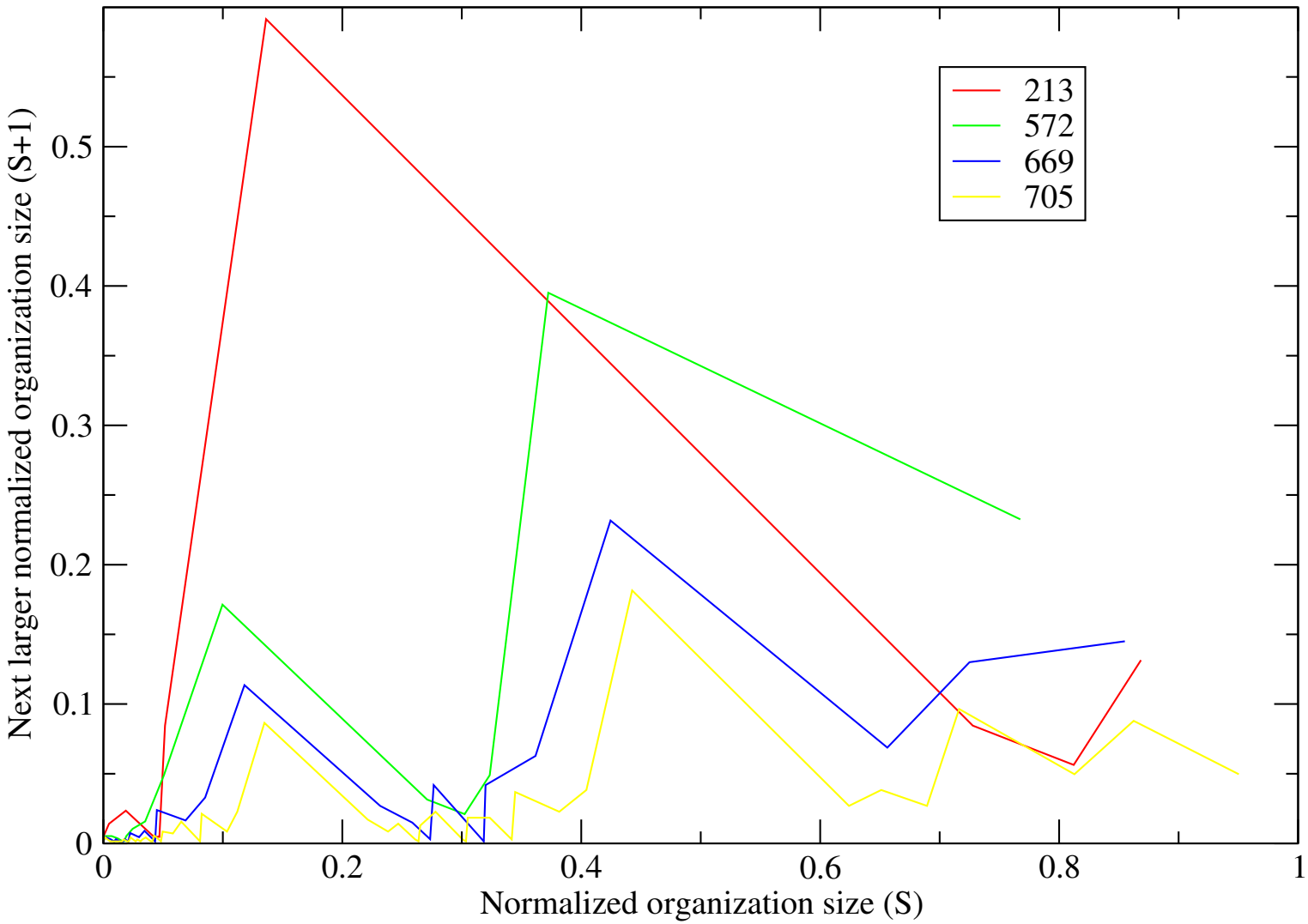
213
572
669
705
Next larger normalized organization size (S+1)
Normalized organization size (S)
0
0.1
0.2
0.3
0.4
0.5
0
0.2
0.4
0.6
0.8
1

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