Network Analysis

Alexander Bockmayr
Martin Vingron
Annika Röhl
SS 2017, FU Berlin

Organisational issues

- Slides and additional material will be made available through the course pages

    `http://www.mi.fu-berlin.de/w/AgMathLife/NetzWerkSS17`

- Note that these slides are not a script.

- Please take notes and read the recommended articles.

- Time slots: Monday 10-14, Friday, 9-10.30
  Precise schedule will be announced on course page

- Related Praxisseminar: Computational systems biology

Computational biology

- Biological macromolecules
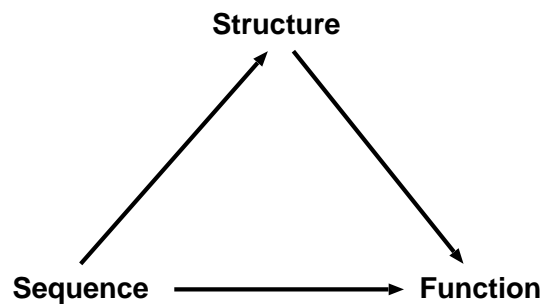
- Macromolecular interactions
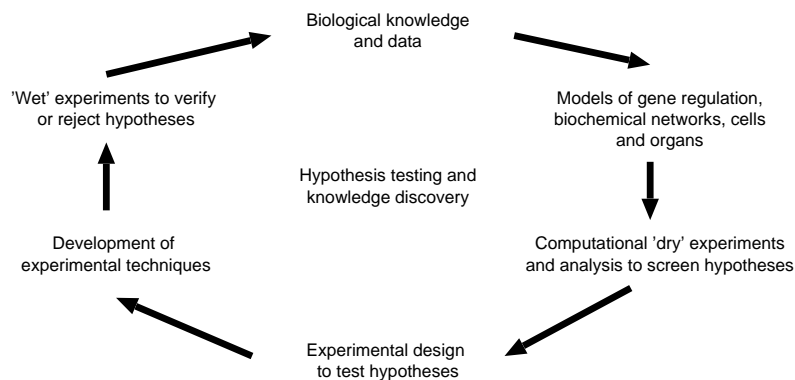
- Pathways, networks, systems

Computational systems biology

- **Systems biology:** Understand how *components* of a biological system *interact* to perform complex biological function

- Different levels of complexity

    - Many components, huge amount of data

    - Non-trivial interactions: non-linearity, feedback, ...

- Intuitive reasoning not sufficient

- Need for mathematical and computational models and tools

⤳ **predictive biology**

Systems biology research cycle

Kitano 2002

Biological knowledge
and data

'Wet' experiments to verify
or reject hypotheses

Models of gene regulation,
biochemical networks, cells
and organs

Hypothesis testing and
knowledge discovery

Development of
experimental techniques

Computational 'dry' experiments
and analysis to screen hypotheses

Experimental design
to test hypotheses

Biological networks

- Various network types

    - Metabolic networks

    - Gene regulatory networks

    - Signaling networks

    ⤳ syntax / semantics ?

- Structure/topology vs. dynamics:
  How does the dynamic behavior depend on the topology?

- Mathematical and computational study

    - Modeling

    - Simulation

    - Analysis ⤳ formal methods

    - Optimization

Mathematical modeling approaches

- Network topology

    – Graph-based modeling

    – Stoichiometric/constraint-based modeling

- Network dynamics

    – Continuous modeling

    – Discrete modeling

    – Stochastic modeling

    – Hybrid modeling

Important issues

- Abstraction vs. precision

- Quantitative vs. qualitative

- Deterministic vs. non-deterministic

Some activities

- Research Center MATHEON and Einstein Center for Mathematics ECMATH

- DFG Research and Training Group "Computational Systems Biology" (HU, FU, Charité, MDC, MPI)

- IMPRS "Computational Biology and Scientific Computing"

- Berlin Institute for Medical Systems Biology (BIMSB)

Outline

1. Continuous models $\rightsquigarrow$ simulation

2. Discrete models $\rightsquigarrow$ model checking

3. Constraint-based models $\rightsquigarrow$ optimization

4. Stochastic and hybrid models