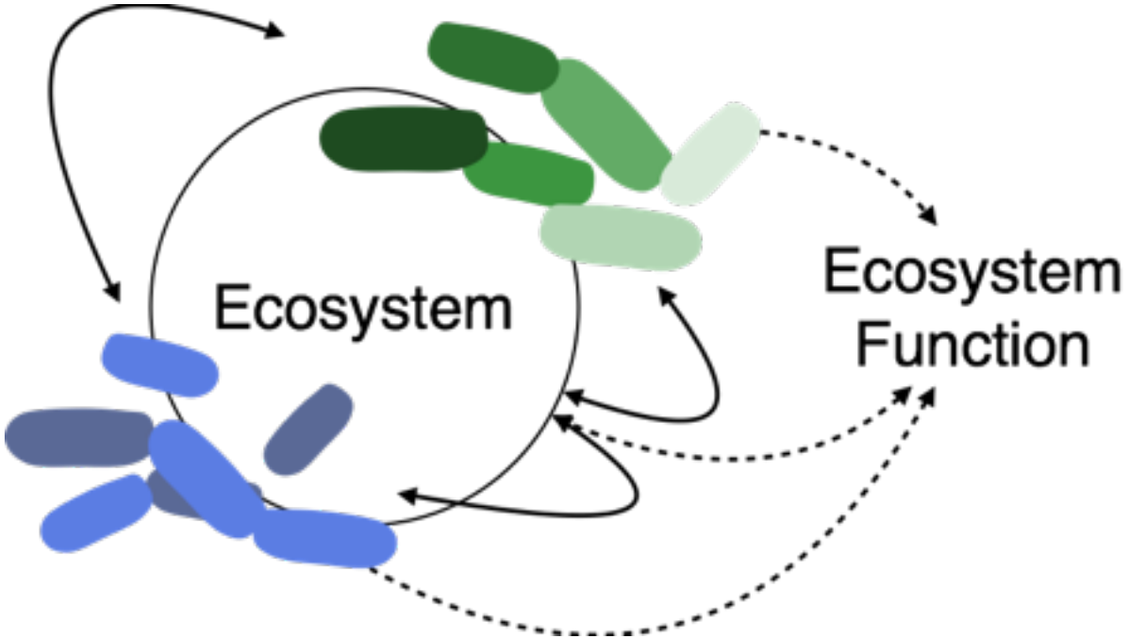

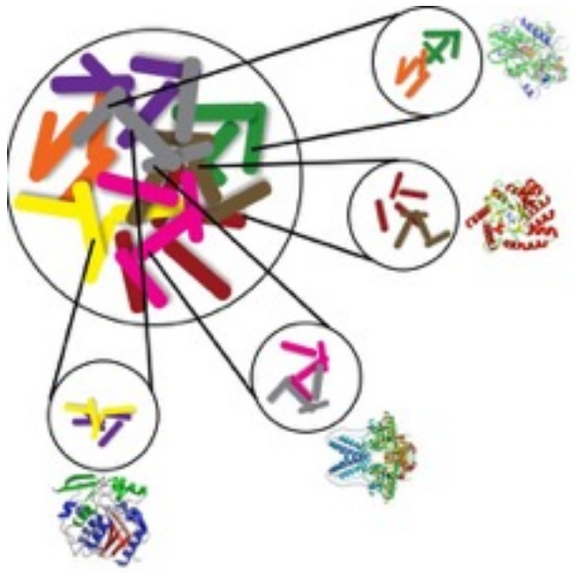

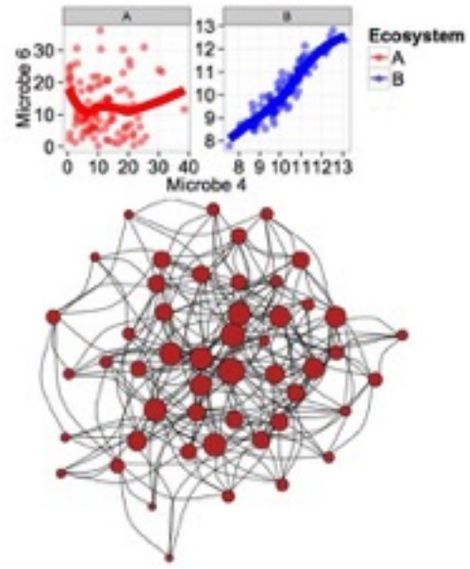

Ryan Williams
Post(Ghost)-doctoral Researcher
Agricultural and Biosystems Engineering
Iowa State University

Modeling and Simulating Data for a Better Understanding of Microbial Ecology

Ryan J. Williams

What is a model?

- Conceptualization of how we understand phenomena in nature.

- All models are wrong but are based on the best information we have.

- Can be a cartoon

- Can be mathematical

- Can be statistical

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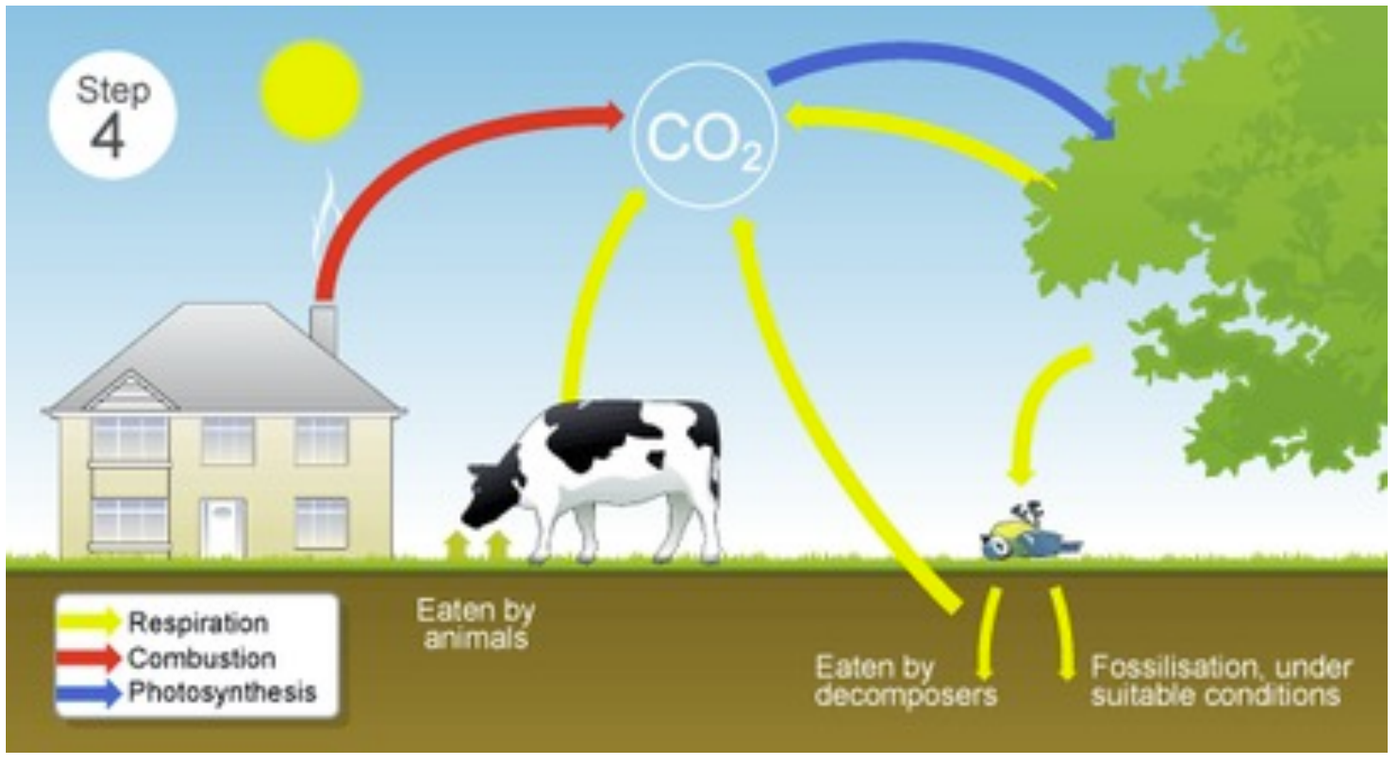

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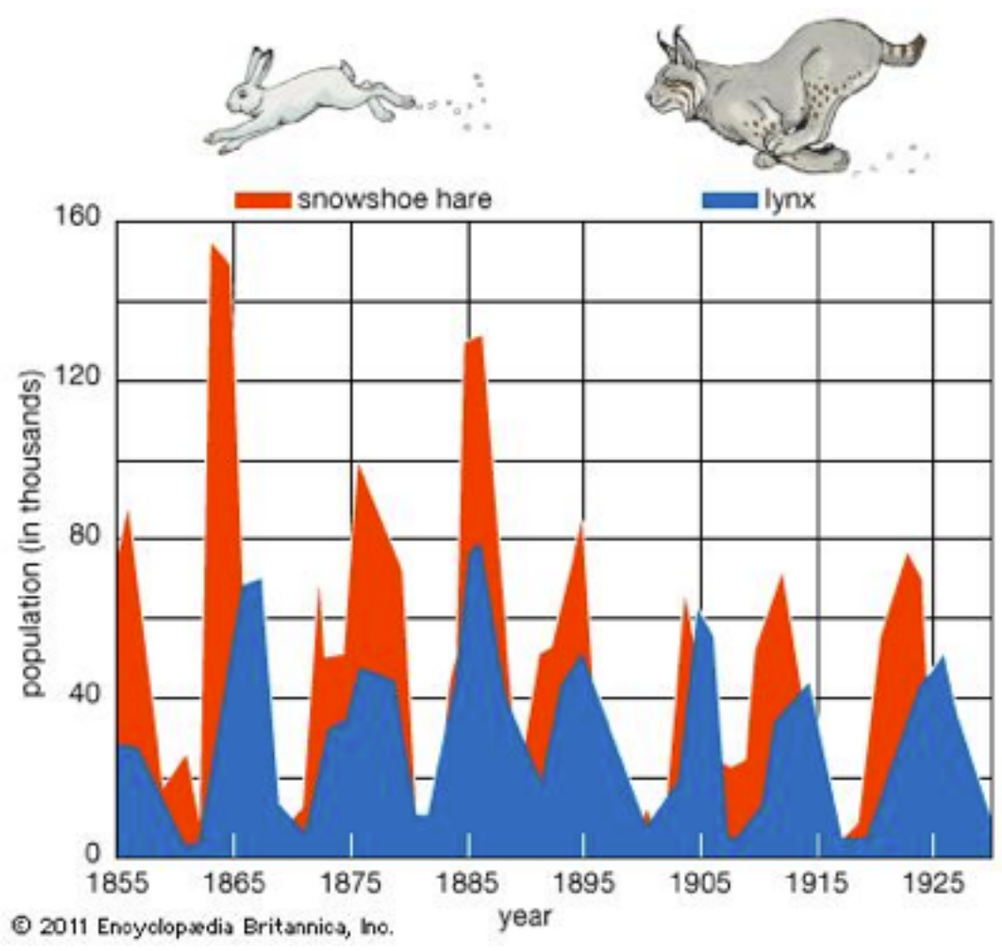

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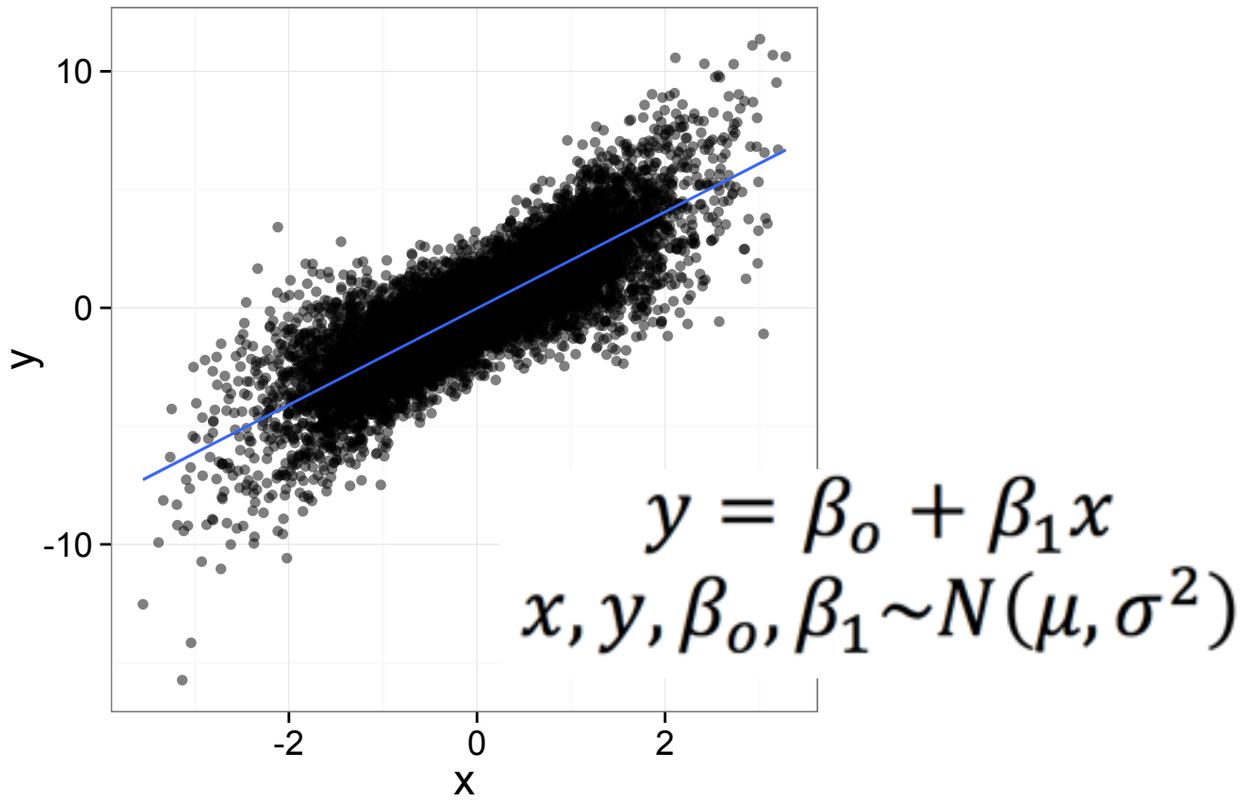

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  - Simulating sequences
  - Simulating numerical data

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MetaSim

Daniel H. Huson and Felix Ott

with contributions from:
R. Schmid, A.F. Auch and D.C. Richter

www-ab.informatik.uni-tuebingen.de/software/metasim

OPEN ACCESS Freely available online

PLOS | ONE

NeSSM: A Next-Generation Sequencing Simulator for Metagenomics

Ben Jia[1,3], Liming Xuan[3,4,5], Kaiye Cai[4,5], Zhiqiang Hu[2,4], Liangxiao Ma[4],

1 School of Biomedical Engineering, Shanghai Jiao Tong University, Shanghai, China, 2 Department of Bioinformat Biotechnology, Shanghai Jiao Tong University, Shanghai, China, 3 School of Bioengineering, East China University of Sci Center for Bioinformation Technology, Shanghai, China

Johnson et al. BMC Bioinformatics 2014, 15(Suppl 9):S14
http://www.biomedcentral.com/1471-2105/15/S9/S14

BMC Bioinformatics

PROCEEDINGS Open Access

Grinder: a versatile amplicon and shotg sequence simulator

Florent E. Angly[1,*], Dana Willner[1,2], Forest Rohwer[3], Philip Hugenh Gene W. Tyson[1,5]

A better sequence-read simulator program for metagenomics

Stephen Johnson[1*], Brett Trost[1], Jeffrey R Long[1], Vanessa Pittet[2], Anthony Kusalik[1]

From RECOMB-Seq: Fourth Annual RECOMB Satellite Workshop on Massively Parallel Sequencing Pittsburgh, PA, USA. 31 March - 05 April 2014

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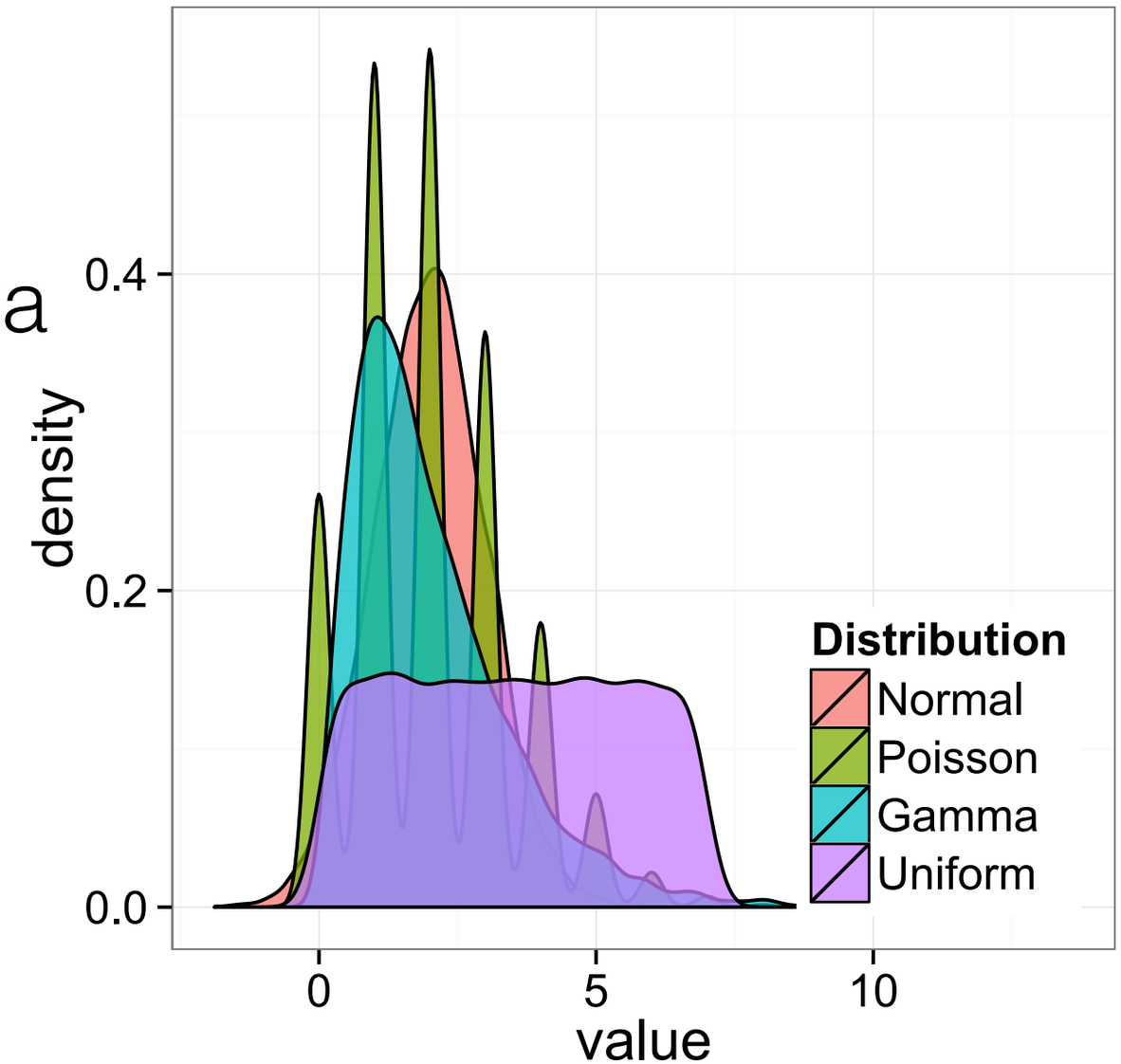


What's the use?

- Microbes are hard to observe in nature, and data describing them can be expensive

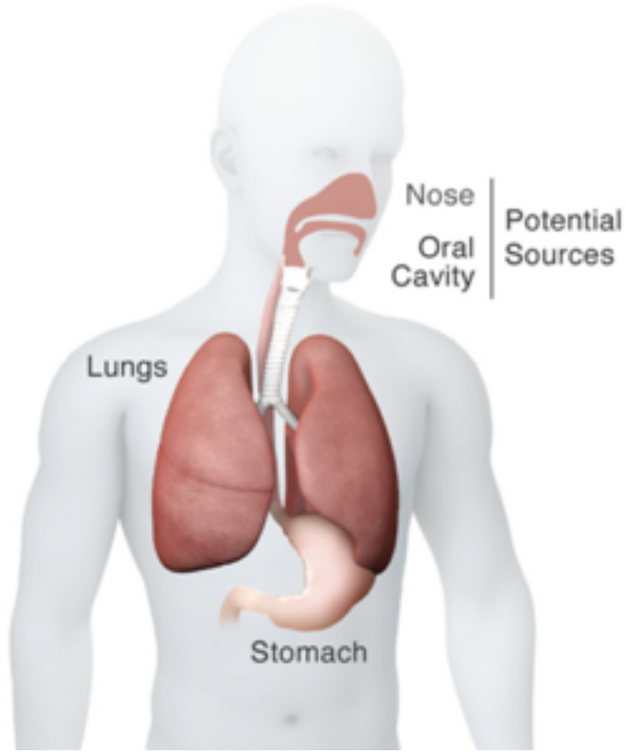
- Microbial data is highly multivariate

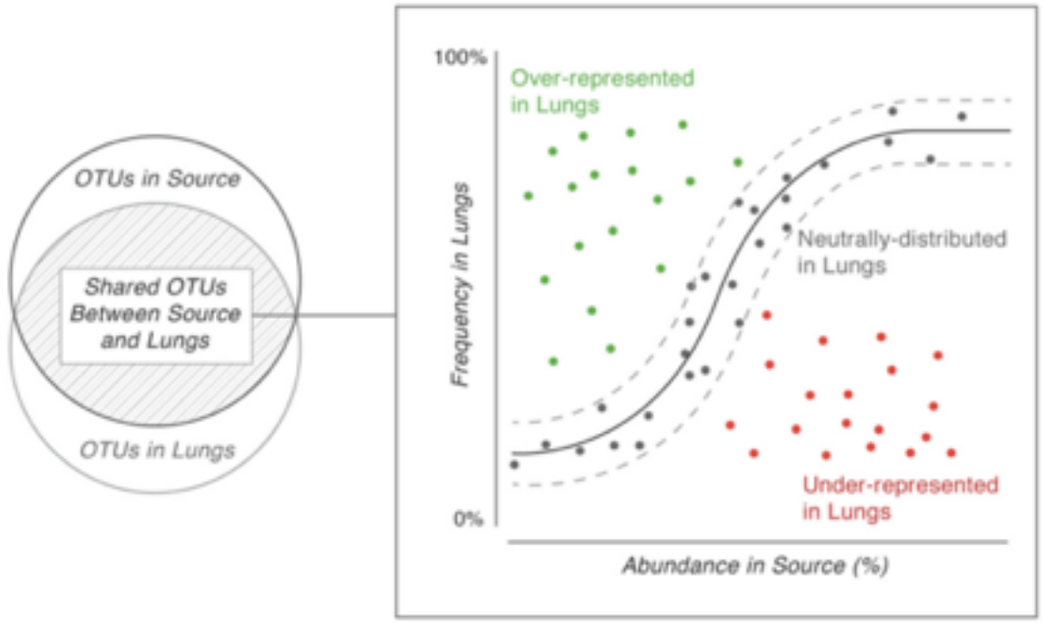
- Microbial ecologists love to use a variety of methods and pre-packaged tools that are not necessarily easy to understand

- Numerical simulation is universal; simulating sequences is applied (both can be very slick but simple tools!)

- Simulation modeling can be used to explain complex natural phenomena

Application of a neutral community model to assess structuring of the human lung microbiome





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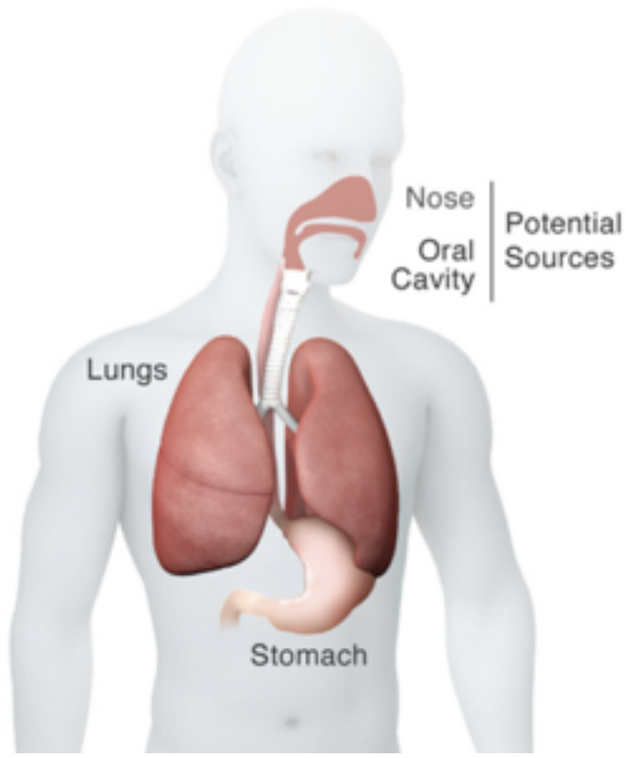
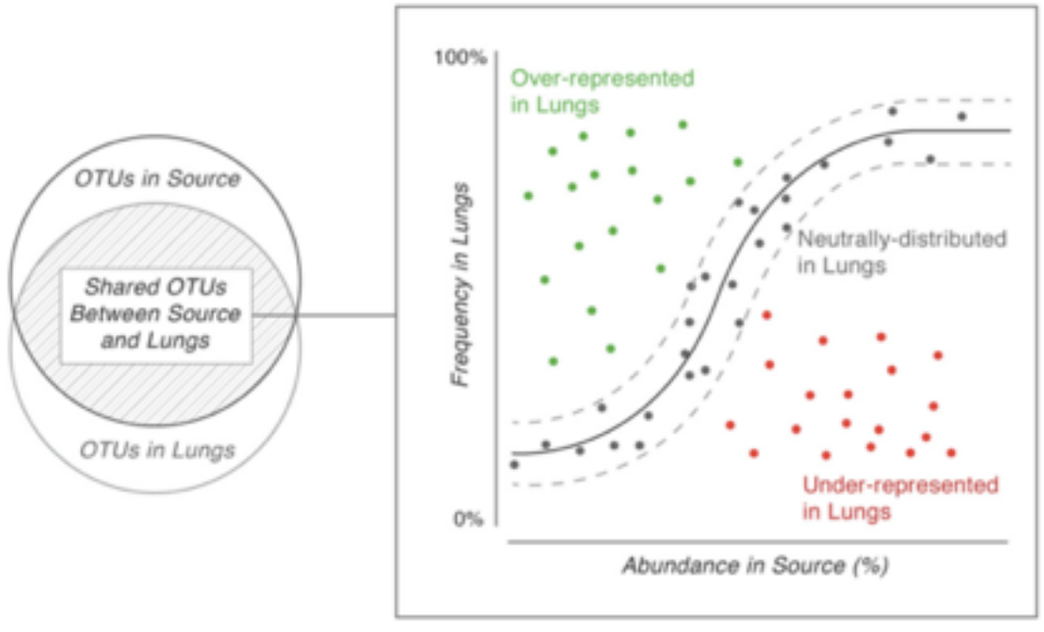
Application of a neutral community model to assess structuring of the human lung microbiome

- Modeled OTU abundances as probabilities of detection in either one environment or another. Similar probabilities across environments suggests neutral community assembly





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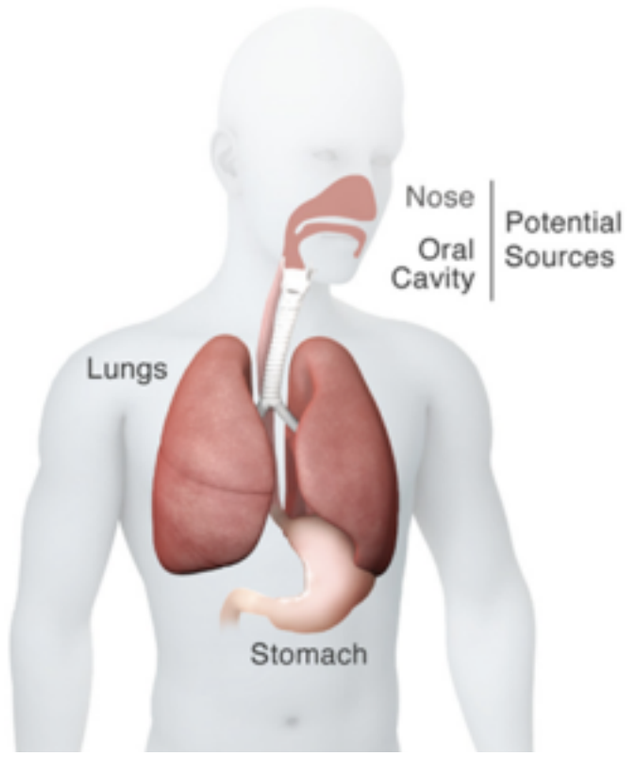
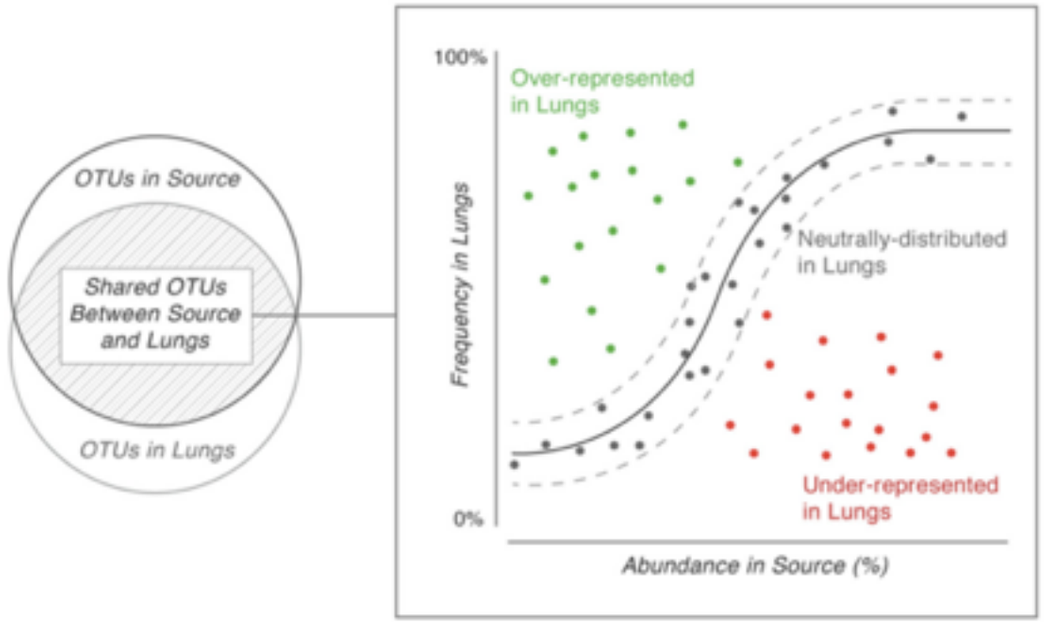
Application of a neutral community model to assess structuring of the human lung microbiome

- Though the model is simple, it represents a statistical expectation for OTU frequencies based on theory that can be simulated from various distributions

- What are pros and cons of this approach? Did you find this approach useful?





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Important things to consider when modeling/simulating…

- Processes generate patterns and not the other way around
- How do we determine randomness driven by nature vs. natural variation in a distribution? Am I observing complex natural phenomenon that create a random pattern (neutral theory) or am I observing natural variation? (Google Brian McGill, U of Maine if interested)

Say you are reviewing literature, and you stumble across an interesting analysis…

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Conditionally Rare Taxa Disproportionately Contribute to Temporal Changes in Microbial Diversity

Ashley Shade,[a] Stuart E. Jones,[b] J. Gregory Caporaso,[c,d] Jo Handelsman,[e] Rob Knight,[f,g] Noah Fierer,[h,i] Jack A. Gilbert[c,j]

Department of Microbiology and Molecular Genetics, Michigan State University, East Lansing, Michigan, USA[a]; Department of Biological Sciences, University of Notre Dame, Notre Dame, Indiana, USA[b]; Institute for Genomic and Systems Biology, Argonne National Laboratory, Argonne, Illinois, USA[c]; Department of Biological Sciences, Northern Arizona University, Flagstaff, Arizona, USA[d]; Department of Molecular, Cellular, and Developmental Biology, Yale University, New Haven, Connecticut, USA[e]; Howard Hughes Medical Institute, Boulder, Colorado, USA[f]; Department of Chemistry and Biochemistry and BioFrontiers Institute, University of Colorado, Boulder, Colorado, USA[g]; Department of Ecology and Evolutionary Biology, University of Colorado, Boulder, Colorado, USA[h]; Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, Colorado, USA[i]; Department of Ecology and Evolution, University of Chicago, Chicago, Illinois, USA[j]

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- Now I can start identifying cool OTUs that are changing over time.

- What are some potential pitfalls to this analysis? Can I use simulation/modeling to address these concerns?

Walk through R script