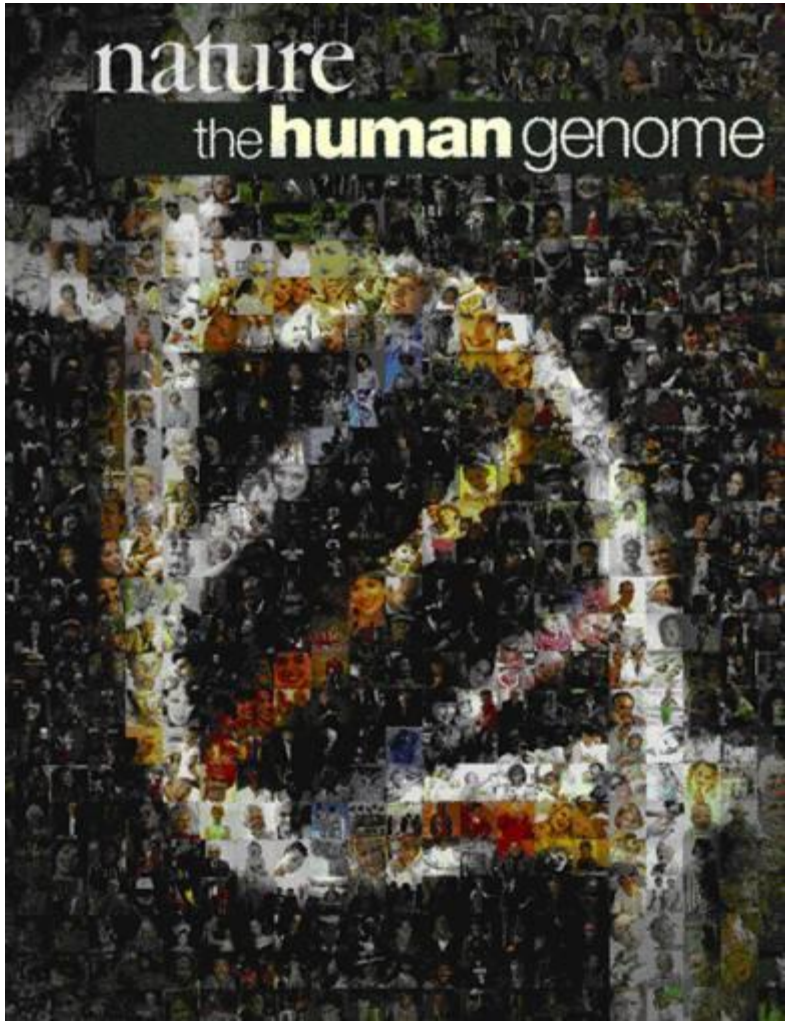
USING BIOLOGY TO IMPROVE AI (AND OTHER) APPLICATIONS

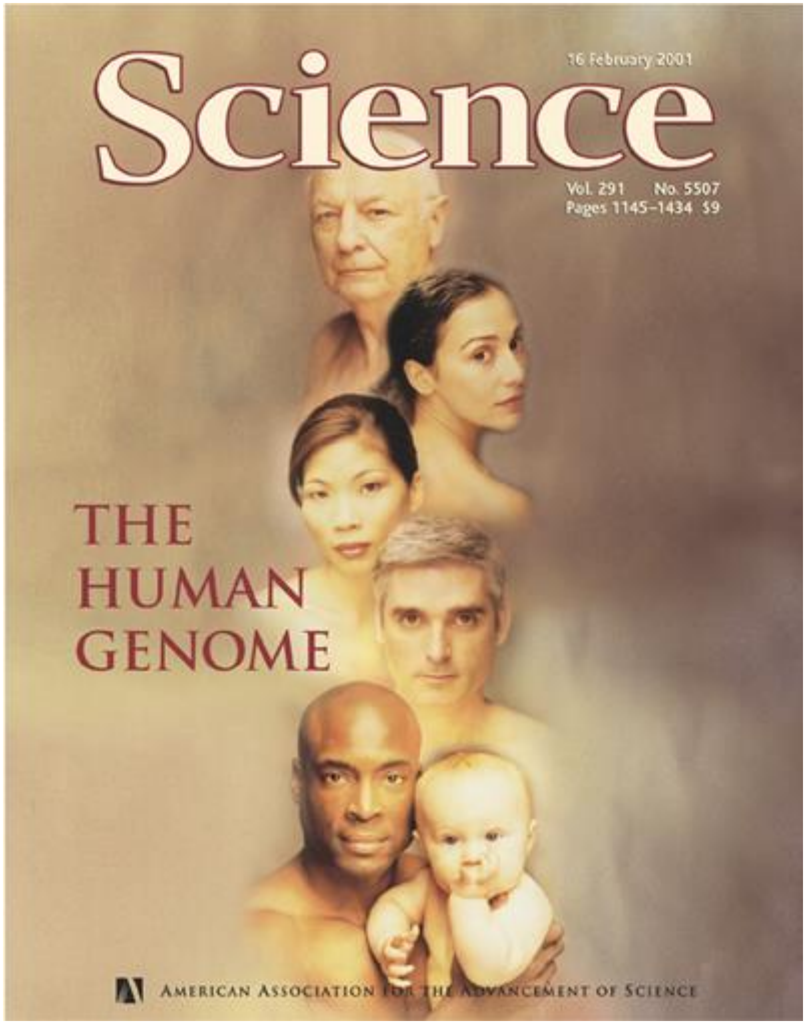
John Quackenbush
Harvard TH Chan School of Public Health
Channing Division of Network Medicine
Dana-Farber Cancer Institute

We are awash in data…

February 2001: Completion of the Draft Human Genome



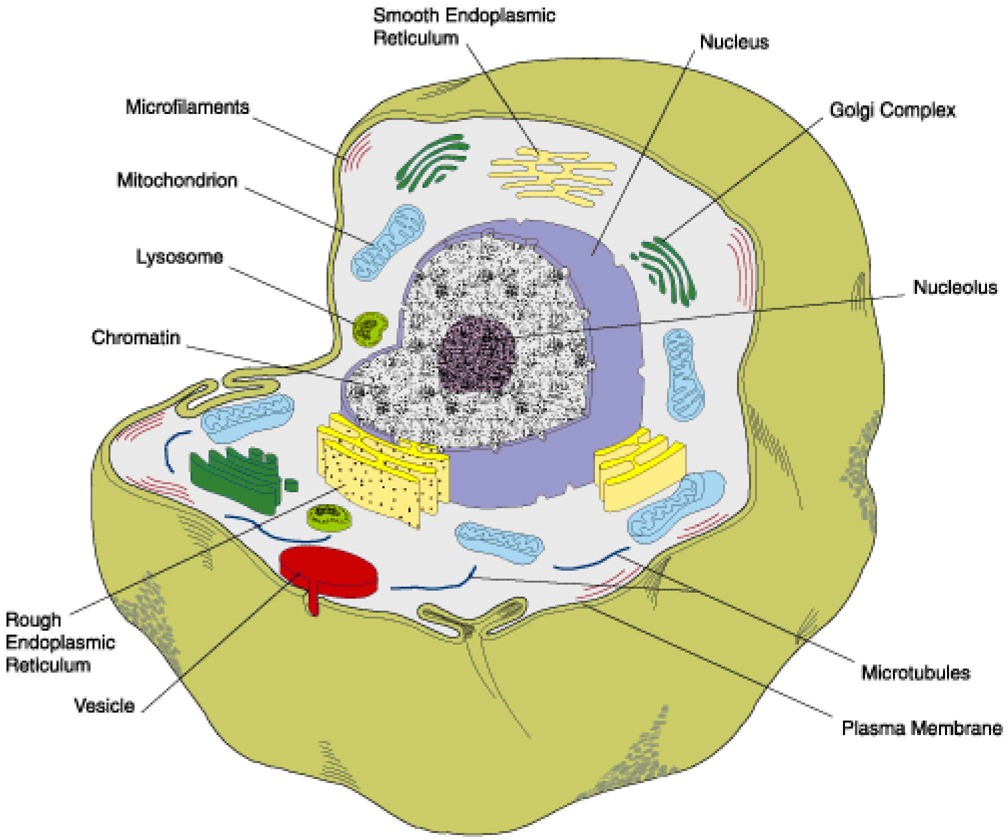
Public HGP



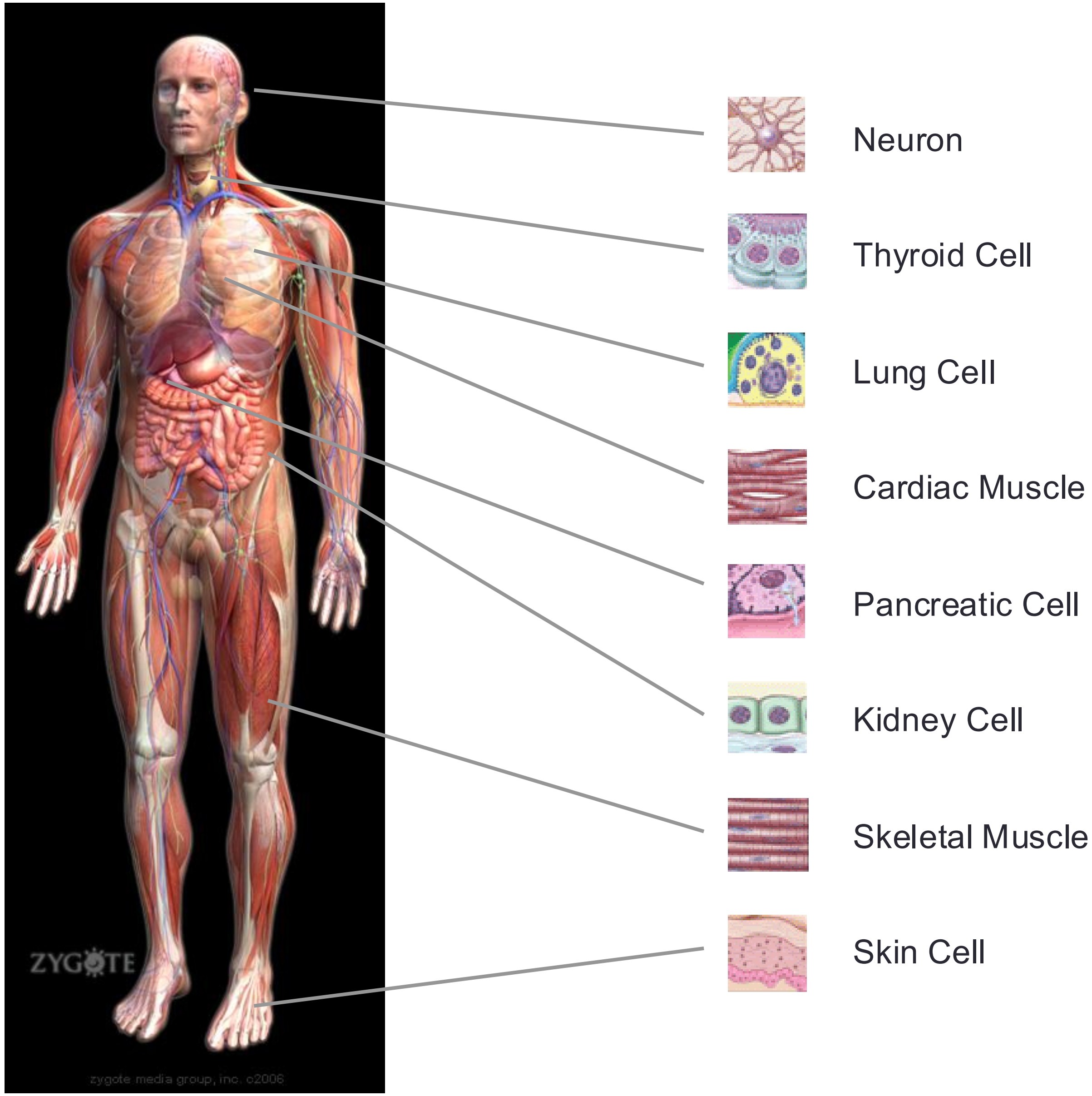
Celera Genomics

Happy 25th Birthday, Human Genome!

The Genome Project has provided a "parts list" for the components of a human cell



Different cell types express different sets of genes


zygote media group, inc. c2006

Neuron

Thyroid Cell

Lung Cell

Cardiac Muscle

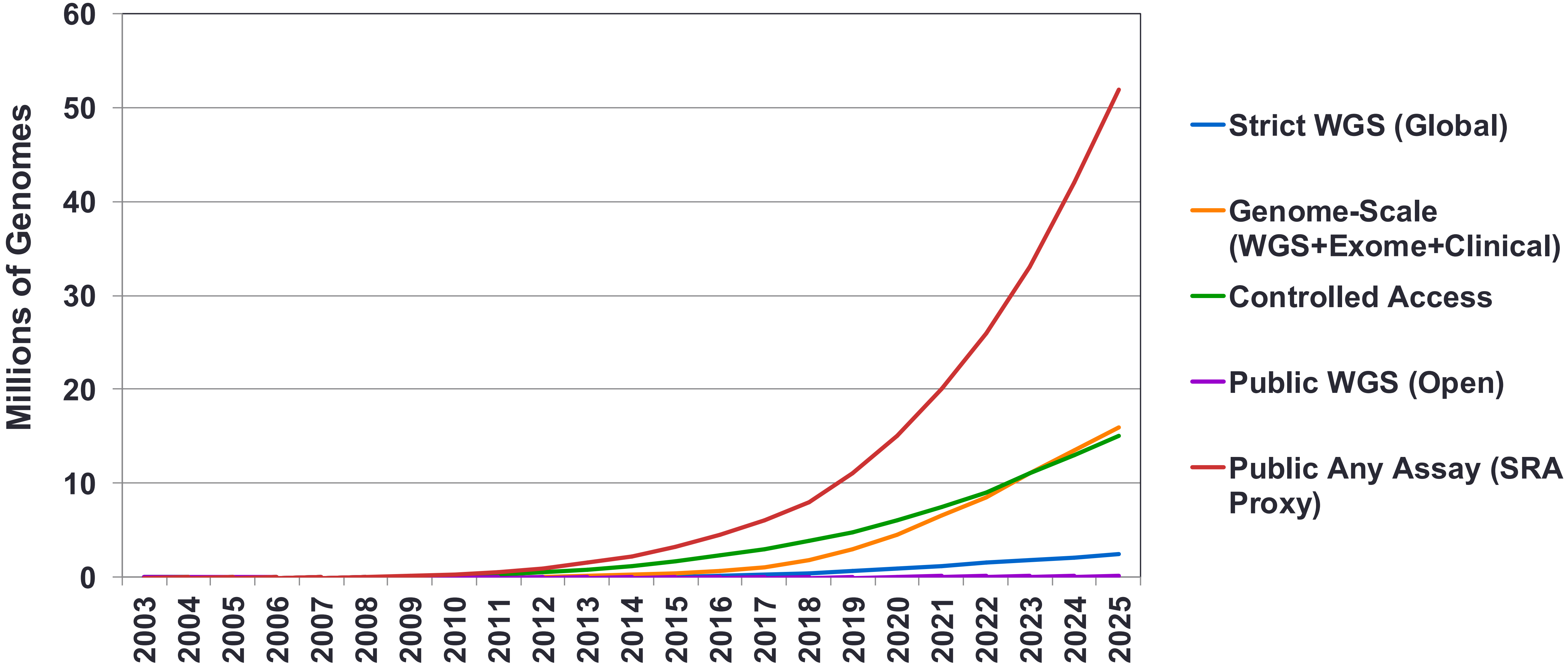
Pancreatic Cell

Kidney Cell

Skeletal Muscle

Skin Cell

Global Human Genome Sequencing Scale

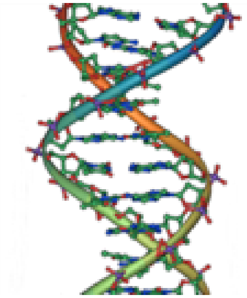


New Sources of Health and Medical Data

Drug Research

Social Media

Patient Records



Genomics

Test Results

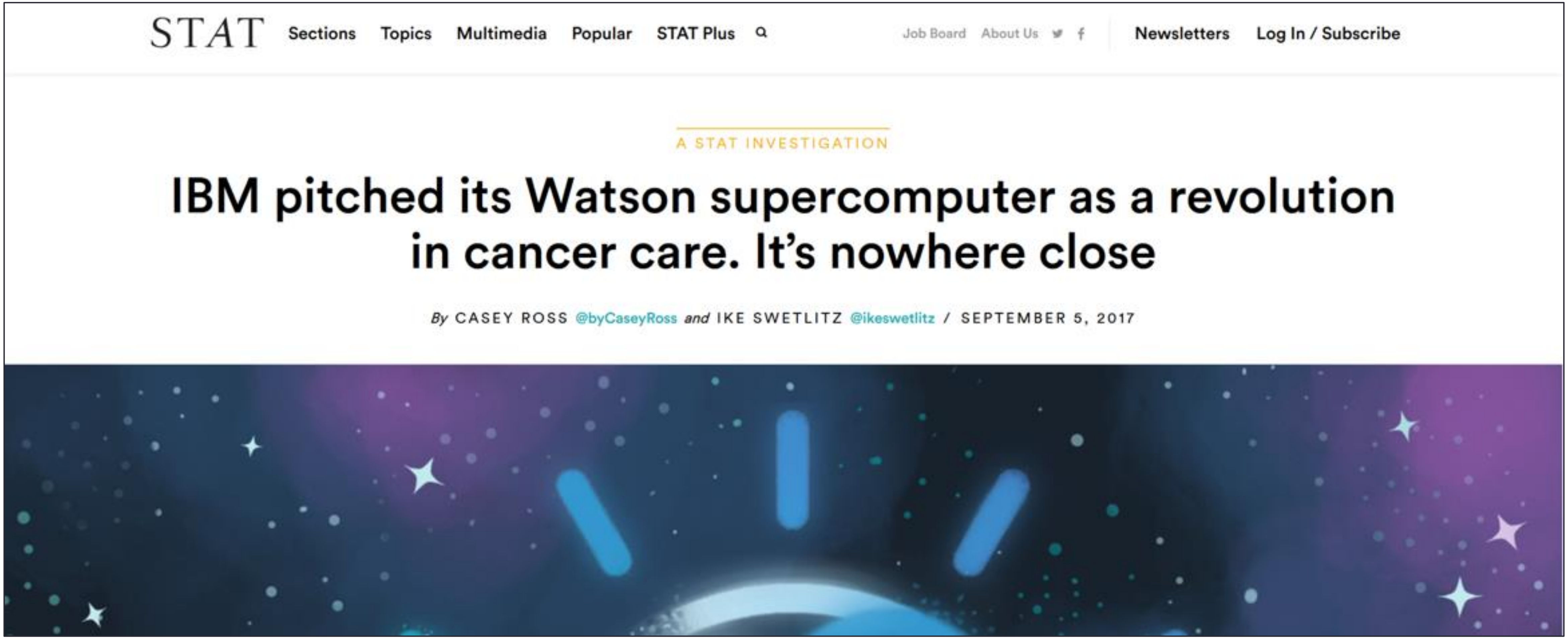
Claims Data

Home Monitoring

Mobile Apps

Is AI the solution for making full use of the genome?

Biology is Not Easy



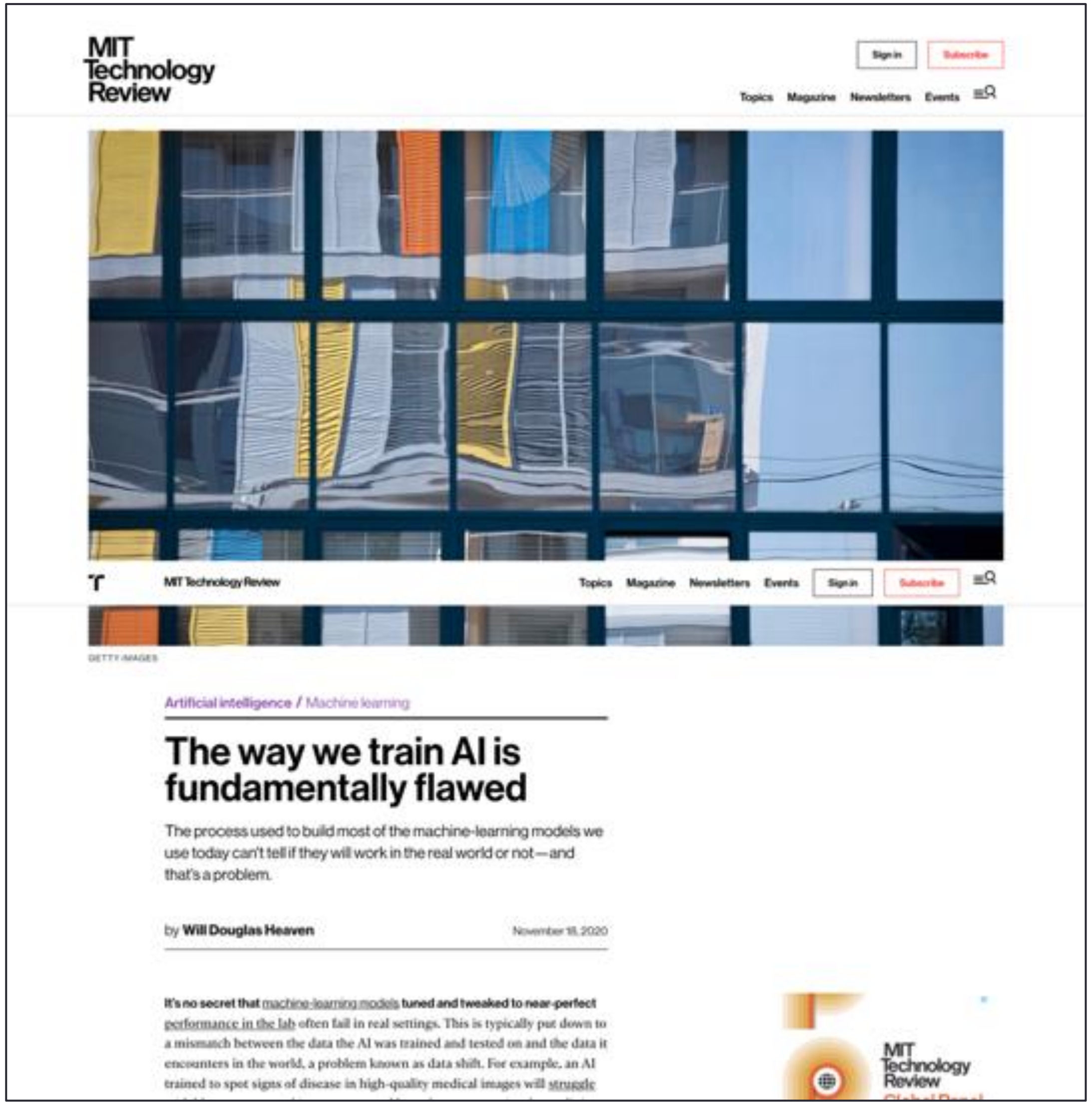
A STAT INVESTIGATION

IBM pitched its Watson supercomputer as a revolution in cancer care. It's nowhere close

By CASEY ROSS @byCaseyRoss *and* IKE SWETLITZ @ikeswetlitz / SEPTEMBER 5, 2017

https://www.statnews.com/2017/09/05/watson-ibm-cancer/

The way we train AI is fundamentally flawed



Artificial intelligence / Machine learning

The way we train AI is fundamentally flawed

The process used to build most of the machine-learning models we use today can't tell if they will work in the real world or not—and that's a problem.

by **Will Douglas Heaven** November 18, 2020

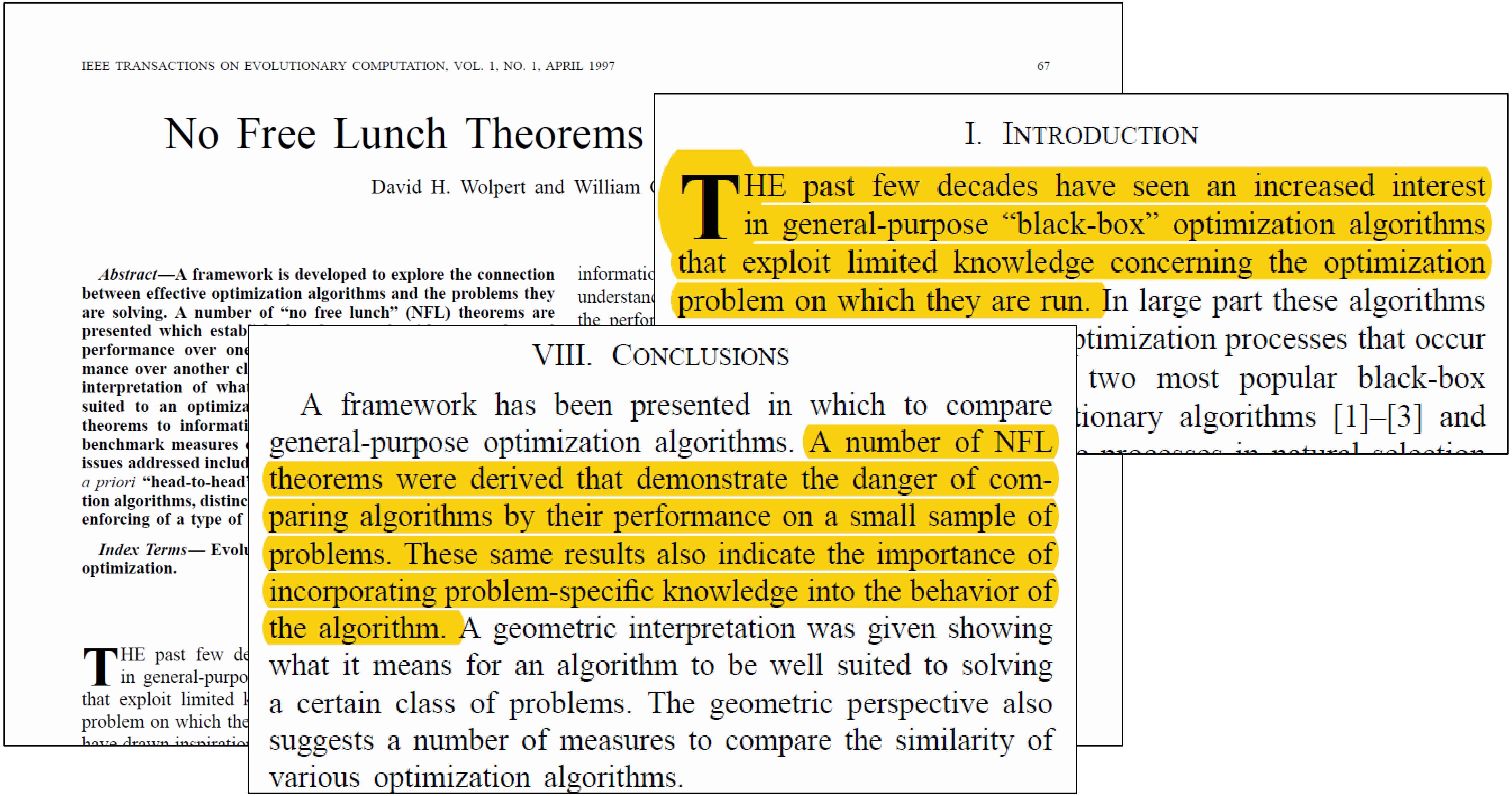
It's no secret that machine-learning models tuned and tweaked to near-perfect performance in the lab often fail in real settings. This is typically put down to a mismatch between the data the AI was trained and tested on and the data it encounters in the world, a problem known as data shift. For example, an AI trained to spot signs of disease in high-quality medical images will struggle

November 2020

Two major problems:

- Data Shift
  (Insufficient Data)
  - A mismatch between the data the AI was trained and tested on and the data it encounters in the world.
- Underspecification
  (No Robust Underlying Model)
  - Underspecification is a known issue in statistics, where observed effects can have many possible causes.

This is not a new problem



IEEE TRANSACTIONS ON EVOLUTIONARY COMPUTATION, VOL. 1, NO. 1, APRIL 1997 67

No Free Lunch Theorems

David H. Wolpert and William

Abstract—A framework is developed to explore the connection between effective optimization algorithms and the problems they are solving. A number of "no free lunch" (NFL) theorems are presented which estab
performance over one
mance over another cl
interpretation of what
suited to an optimiza
theorems to informati
benchmark measures
issues addressed includ
a priori "head-to-head
tion algorithms, distinc
enforcing of a type of

Index Terms— Evolu
optimization.

informatic
understand
the perfor

THE past few de
in general-purpo
that exploit limited k
problem on which the
have drawn inspiratio

I. INTRODUCTION

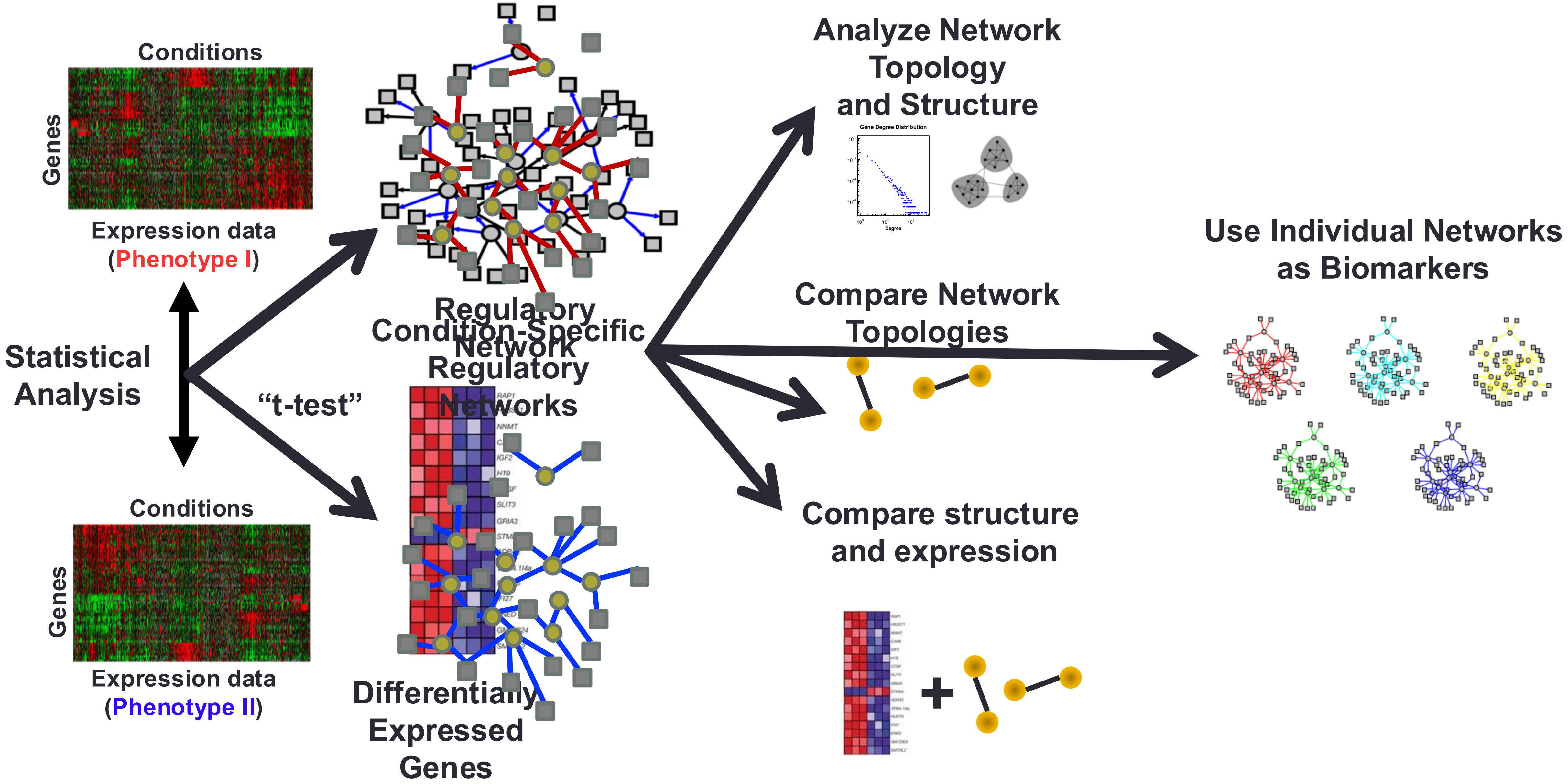
THE past few decades have seen an increased interest in general-purpose "black-box" optimization algorithms that exploit limited knowledge concerning the optimization problem on which they are run. In large part these algorithms
ptimization processes that occur
two most popular black-box
tionary algorithms [1]–[3] and

VIII. CONCLUSIONS

A framework has been presented in which to compare general-purpose optimization algorithms. A number of NFL theorems were derived that demonstrate the danger of comparing algorithms by their performance on a small sample of problems. These same results also indicate the importance of incorporating problem-specific knowledge into the behavior of the algorithm. A geometric interpretation was given showing what it means for an algorithm to be well suited to solving a certain class of problems. The geometric perspective also suggests a number of measures to compare the similarity of various optimization algorithms.

Networks: A biological constraint

Networks Beyond Simple Differences



Expression data (Phenotype I)

Statistical Analysis

"t-test"

Expression data (Phenotype II)

Regulatory Network

Condition-Specific Regulatory Networks

Differentially Expressed Genes

Analyze Network Topology and Structure

Compare Network Topologies

Compare structure and expression

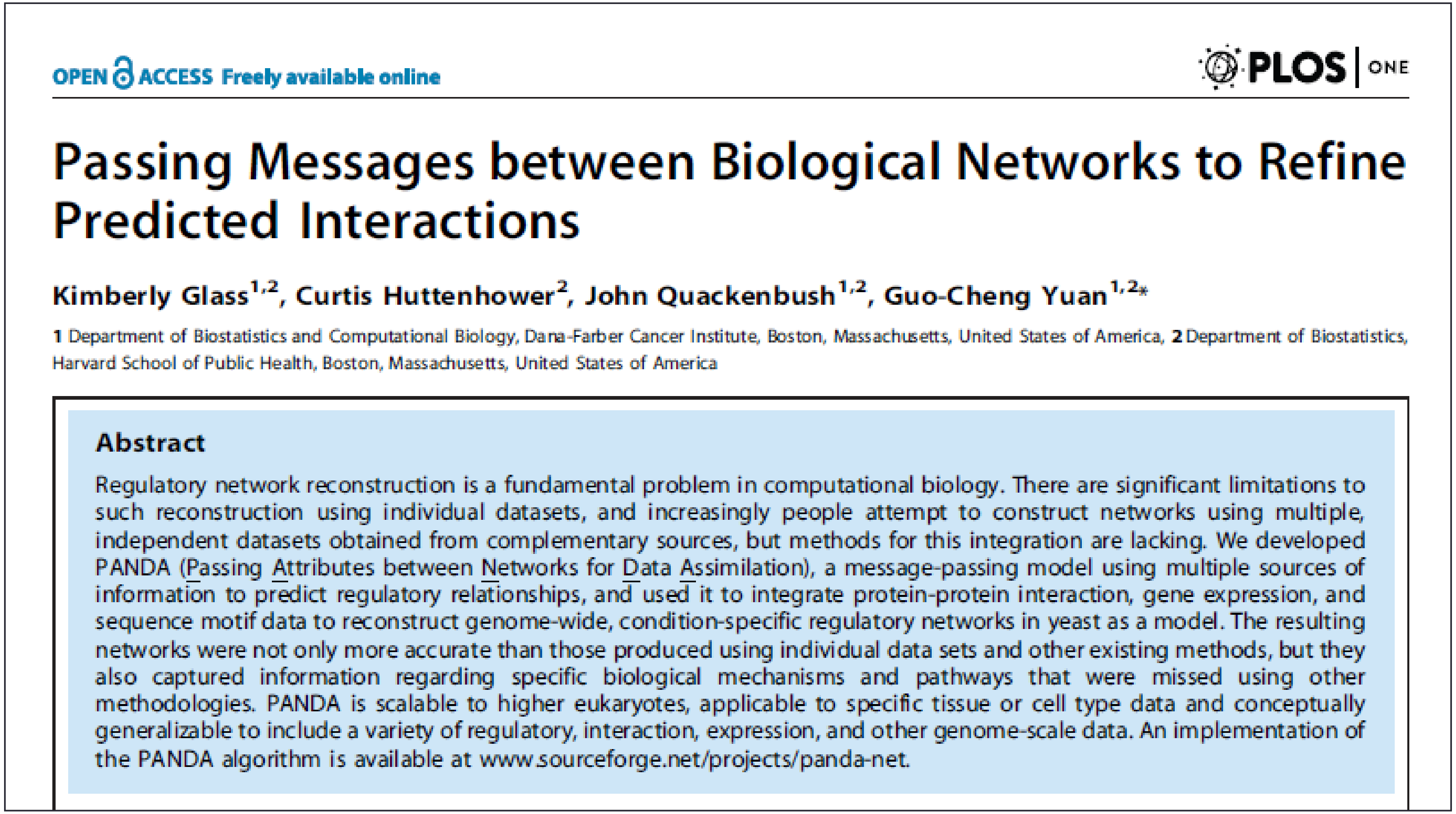
Use Individual Networks as Biomarkers

Core Ideas

- Biological systems are driven by complex networks
- The structure of the network is important and informs our understanding of the biology of the system we are studying
- There is no single right network—the network in each tissue, in each biological state, in each individual is unique
- The real question is “Does a network model inform our understanding of biology?”

Can we model
Gene Regulatory Processes?

Integrative Network Inference: PANDA



OPEN ACCESS Freely available online

PLOS | ONE

Passing Messages between Biological Networks to Refine Predicted Interactions

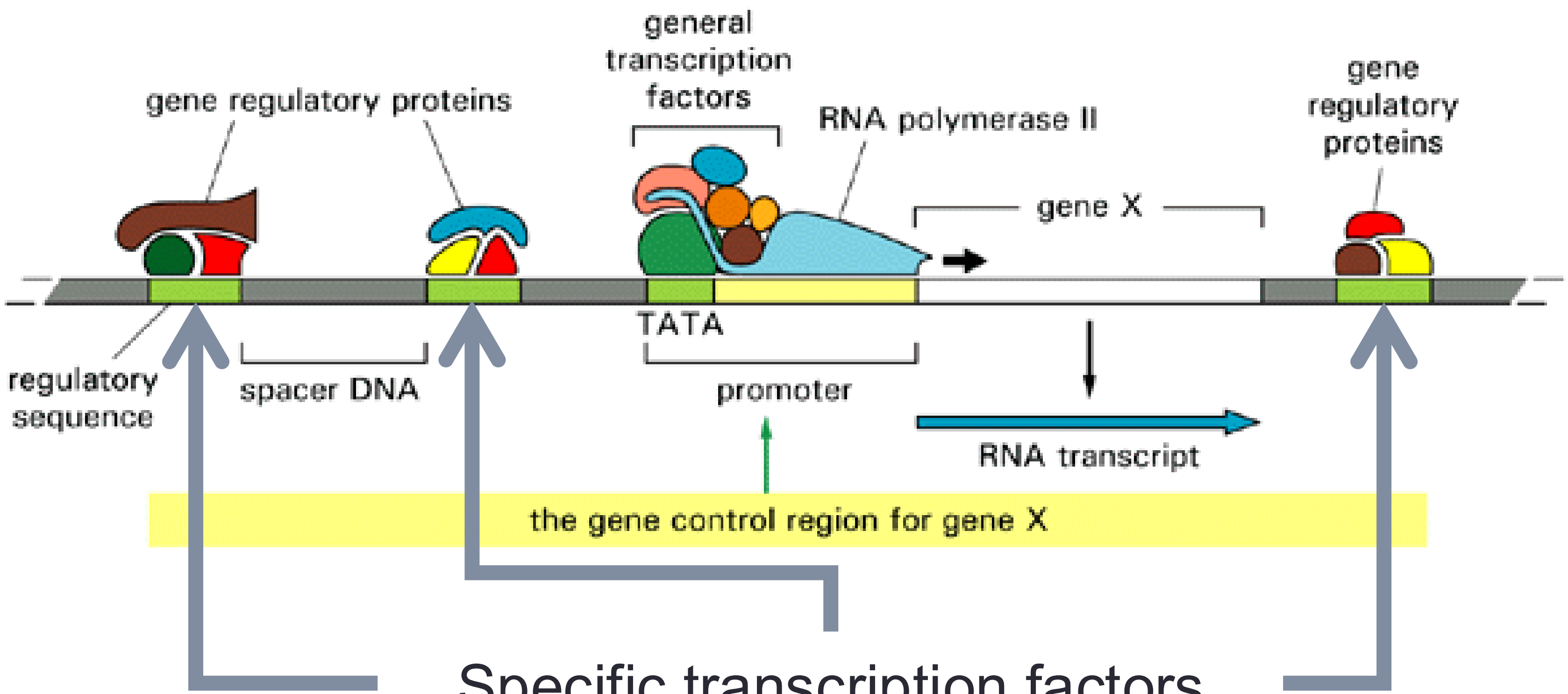
Kimberly Glass[1,2], Curtis Huttenhower[2], John Quackenbush[1,2], Guo-Cheng Yuan[1,2]*

1 Department of Biostatistics and Computational Biology, Dana-Farber Cancer Institute, Boston, Massachusetts, United States of America, **2** Department of Biostatistics, Harvard School of Public Health, Boston, Massachusetts, United States of America

Abstract

Regulatory network reconstruction is a fundamental problem in computational biology. There are significant limitations to such reconstruction using individual datasets, and increasingly people attempt to construct networks using multiple, independent datasets obtained from complementary sources, but methods for this integration are lacking. We developed PANDA (Passing Attributes between Networks for Data Assimilation), a message-passing model using multiple sources of information to predict regulatory relationships, and used it to integrate protein-protein interaction, gene expression, and sequence motif data to reconstruct genome-wide, condition-specific regulatory networks in yeast as a model. The resulting networks were not only more accurate than those produced using individual data sets and other existing methods, but they also captured information regarding specific biological mechanisms and pathways that were missed using other methodologies. PANDA is scalable to higher eukaryotes, applicable to specific tissue or cell type data and conceptually generalizable to include a variety of regulatory, interaction, expression, and other genome-scale data. An implementation of the PANDA algorithm is available at www.sourceforge.net/projects/panda-net.

Regulation of Transcription

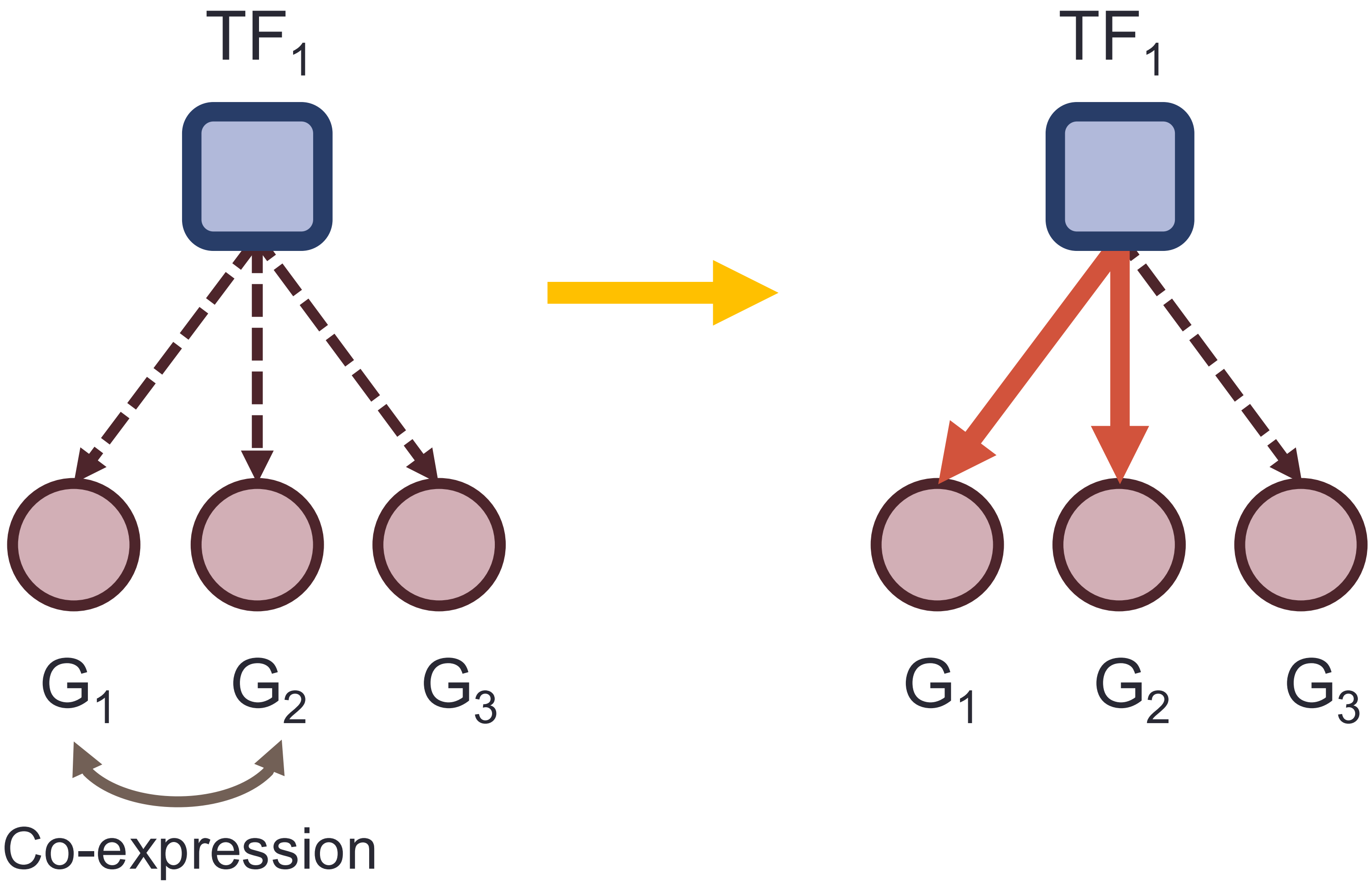


regulatory
sequences

promoter

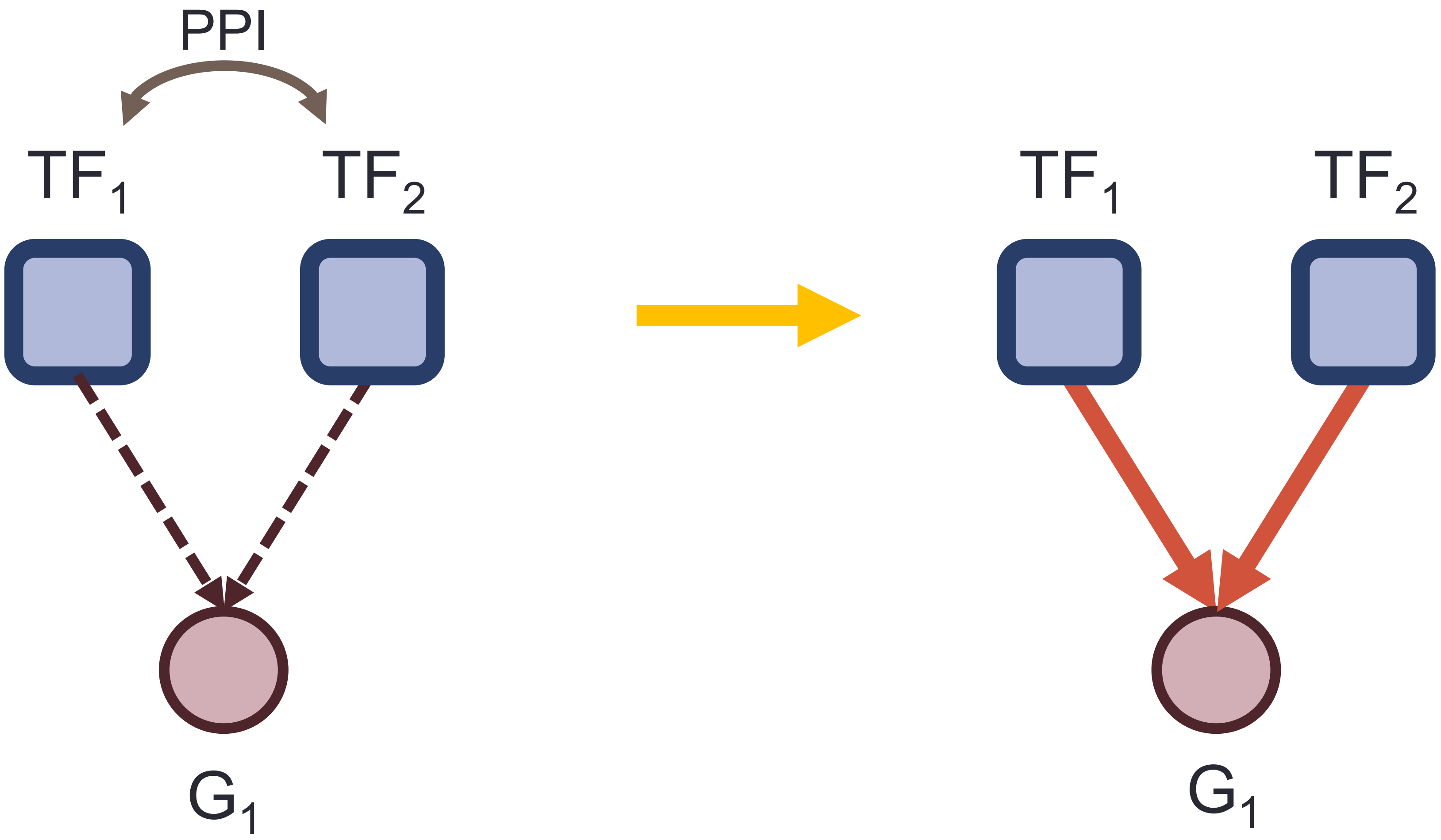
Specific transcription factors

Co-expression is evidence for regulation



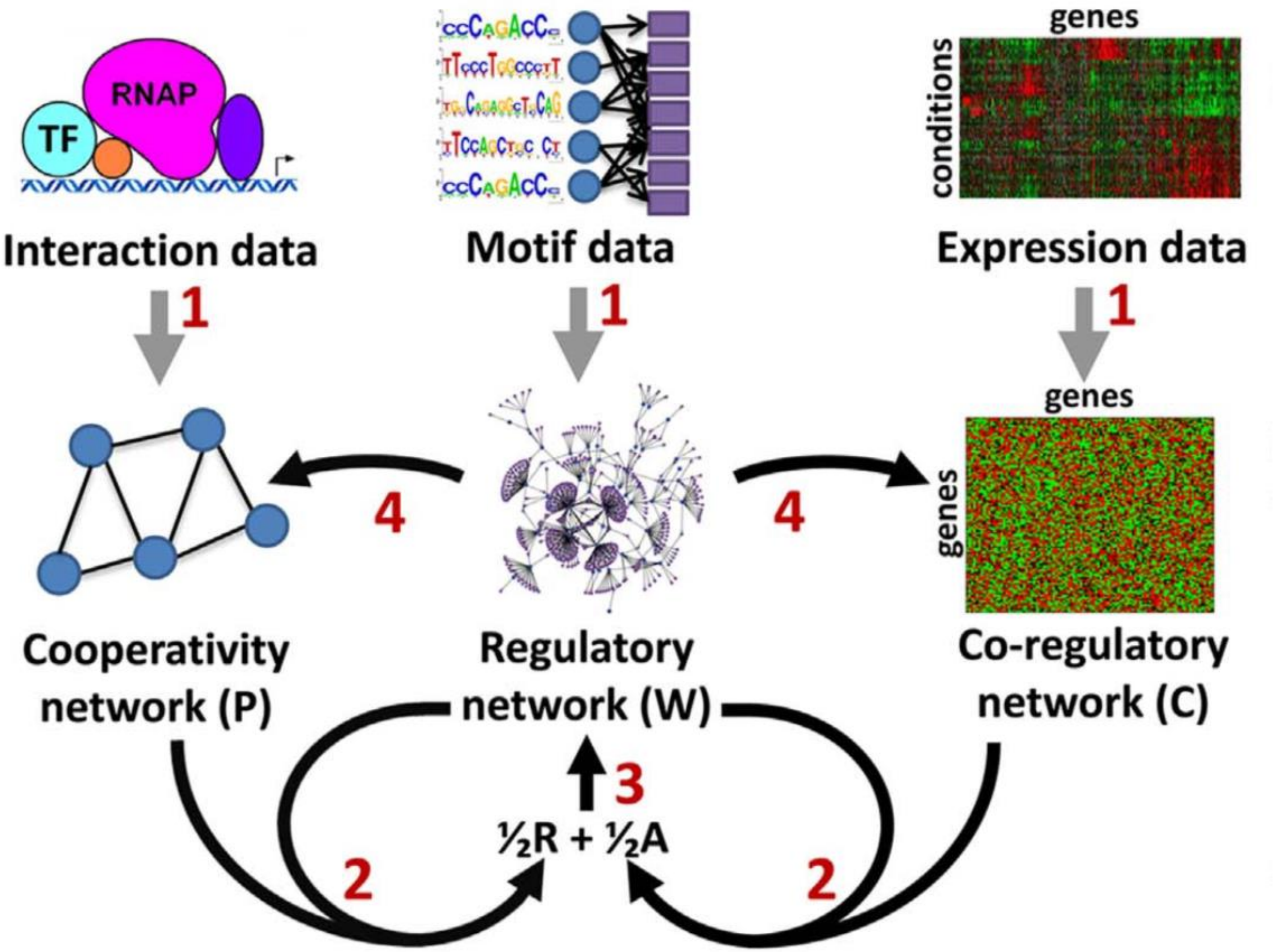
Des Weighill

PPI is evidence for regulation

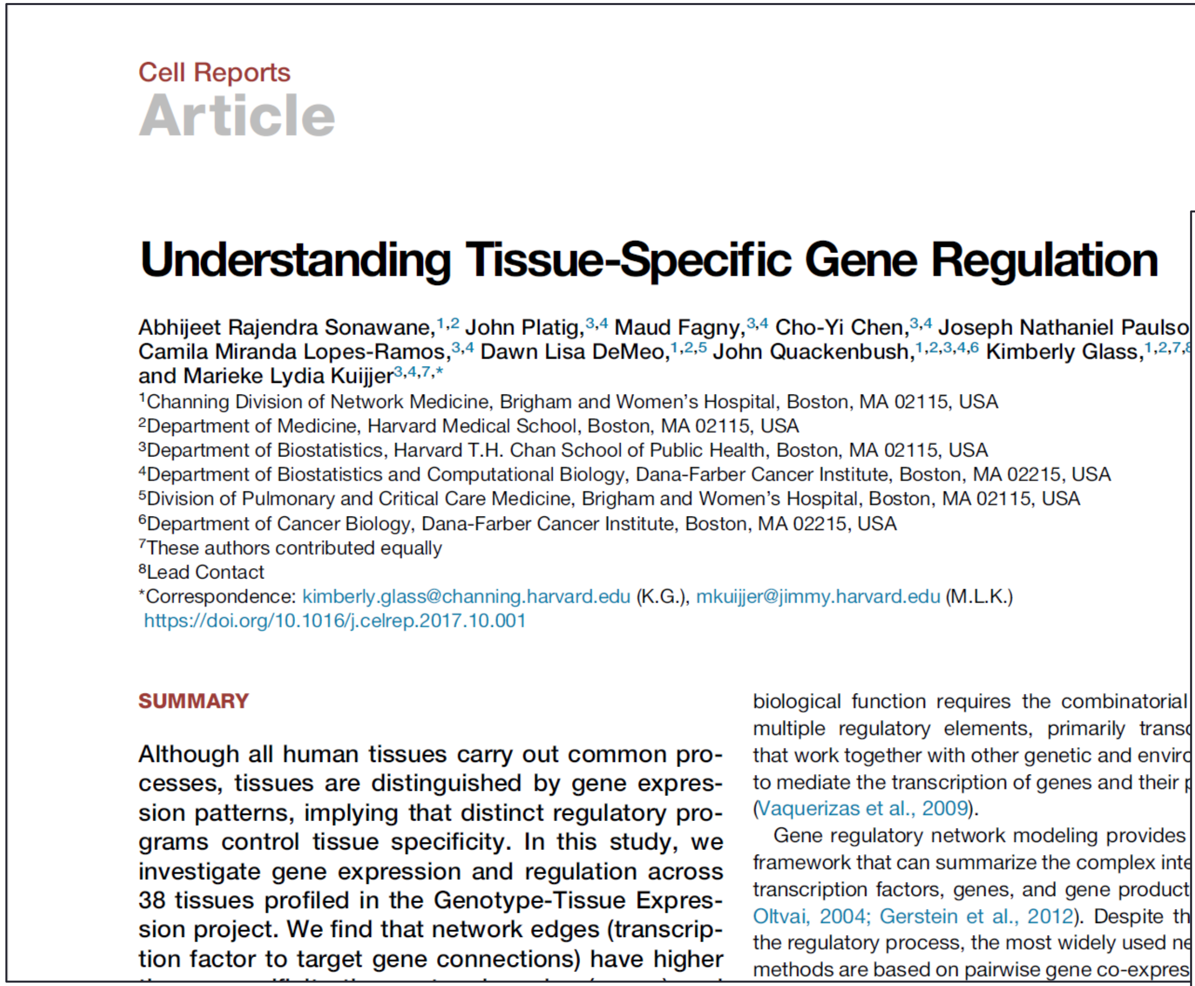


Des Weighill

PANDA: Integrating Data to Infer Networks



PANDA (Passing Attributes between Networks for Data Assimilation) Glass et. al. PLOS one (2013)



Cell Reports

Article

OPEN ACCESS CellPress

Understanding Tissue-Specific Gene Regulation

Abhijeet Rajendra Sonawane,[1,2] John Platig,[3,4] Maud Fagny,[3,4] Cho-Yi Chen,[3,4] Joseph Nathaniel Paulso
Camila Miranda Lopes-Ramos,[3,4] Dawn Lisa DeMeo,[1,2,5] John Quackenbush,[1,2,3,4,6] Kimberly Glass,[1,2,7,
and Marieke Lydia Kuijjer[3,4,7,*]
[1]Channing Division of Network Medicine, Brigham and Women's Hospital, Boston, MA 02115, USA
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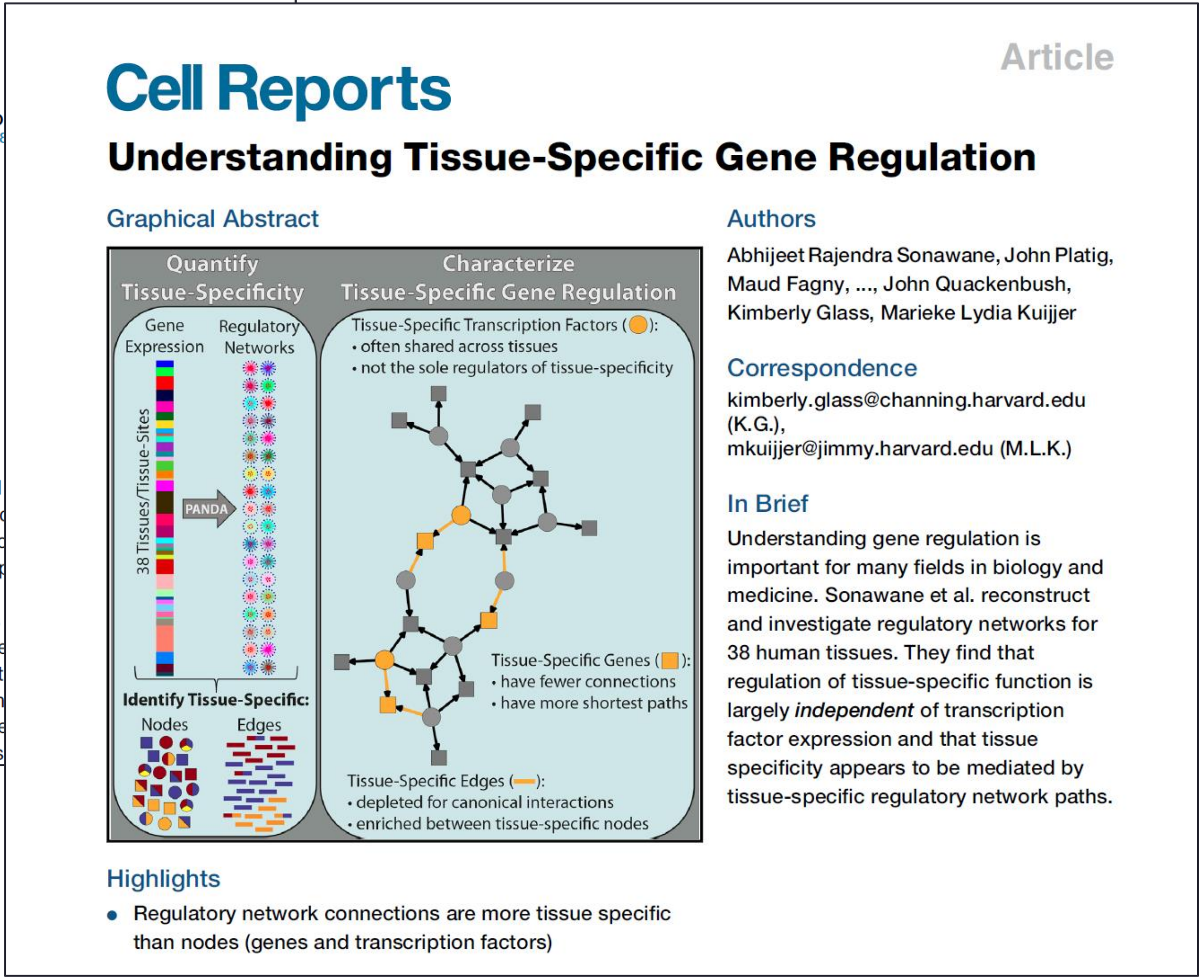
https://doi.org/10.1016/j.celrep.2017.10.001

SUMMARY

Although all human tissues carry out common processes, tissues are distinguished by gene expression patterns, implying that distinct regulatory programs control tissue specificity. In this study, we investigate gene expression and regulation across 38 tissues profiled in the Genotype-Tissue Expression project. We find that network edges (transcription factor to target gene connections) have higher

biological function requires the combinatorial
multiple regulatory elements, primarily trans
that work together with other genetic and enviro
to mediate the transcription of genes and their
(Vaquerizas et al., 2009).

Gene regulatory network modeling provides
framework that can summarize the complex inte
transcription factors, genes, and gene product
Oltvai, 2004; Gerstein et al., 2012). Despite th
the regulatory process, the most widely used ne
methods are based on pairwise gene co-expres



Cell Reports

Article

Understanding Tissue-Specific Gene Regulation

Graphical Abstract

Authors

Abhijeet Rajendra Sonawane, John Platig, Maud Fagny, ..., John Quackenbush, Kimberly Glass, Marieke Lydia Kuijjer

Correspondence

kimberly.glass@channing.harvard.edu (K.G.),
mkuijjer@jimmy.harvard.edu (M.L.K.)

In Brief

Understanding gene regulation is important for many fields in biology and medicine. Sonawane et al. reconstruct and investigate regulatory networks for 38 human tissues. They find that regulation of tissue-specific function is largely *independent* of transcription factor expression and that tissue specificity appears to be mediated by tissue-specific regulatory network paths.

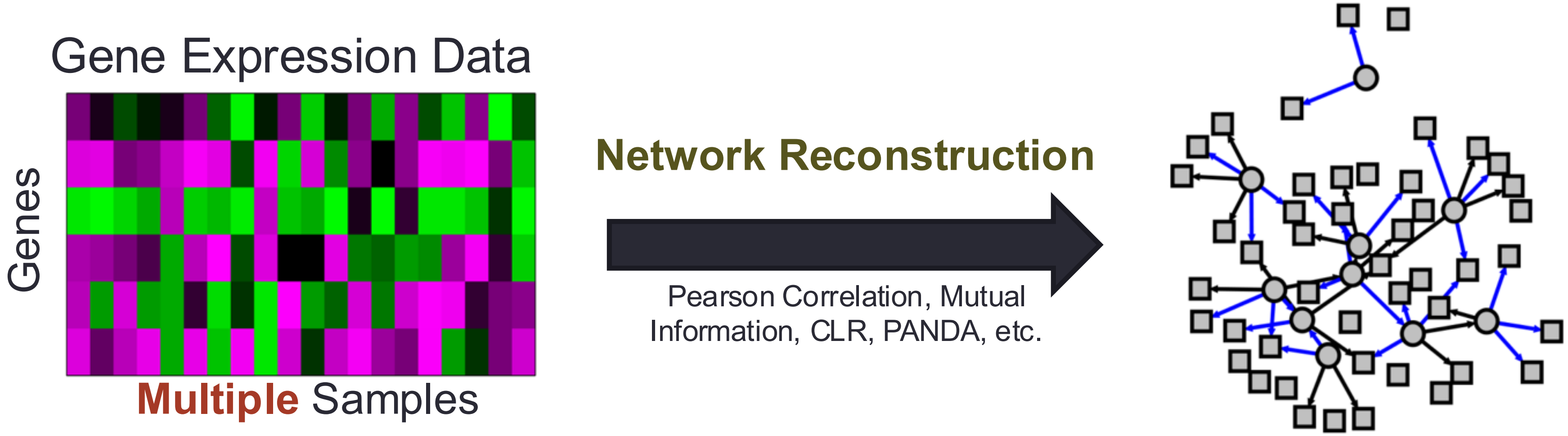
Highlights

- Regulatory network connections are more tissue specific than nodes (genes and transcription factors)

More application papers coming….

Can we move beyond THE Network?

Reconstructing Gene Regulatory Networks



Gene Expression Data

Genes

Multiple Samples

Network Reconstruction

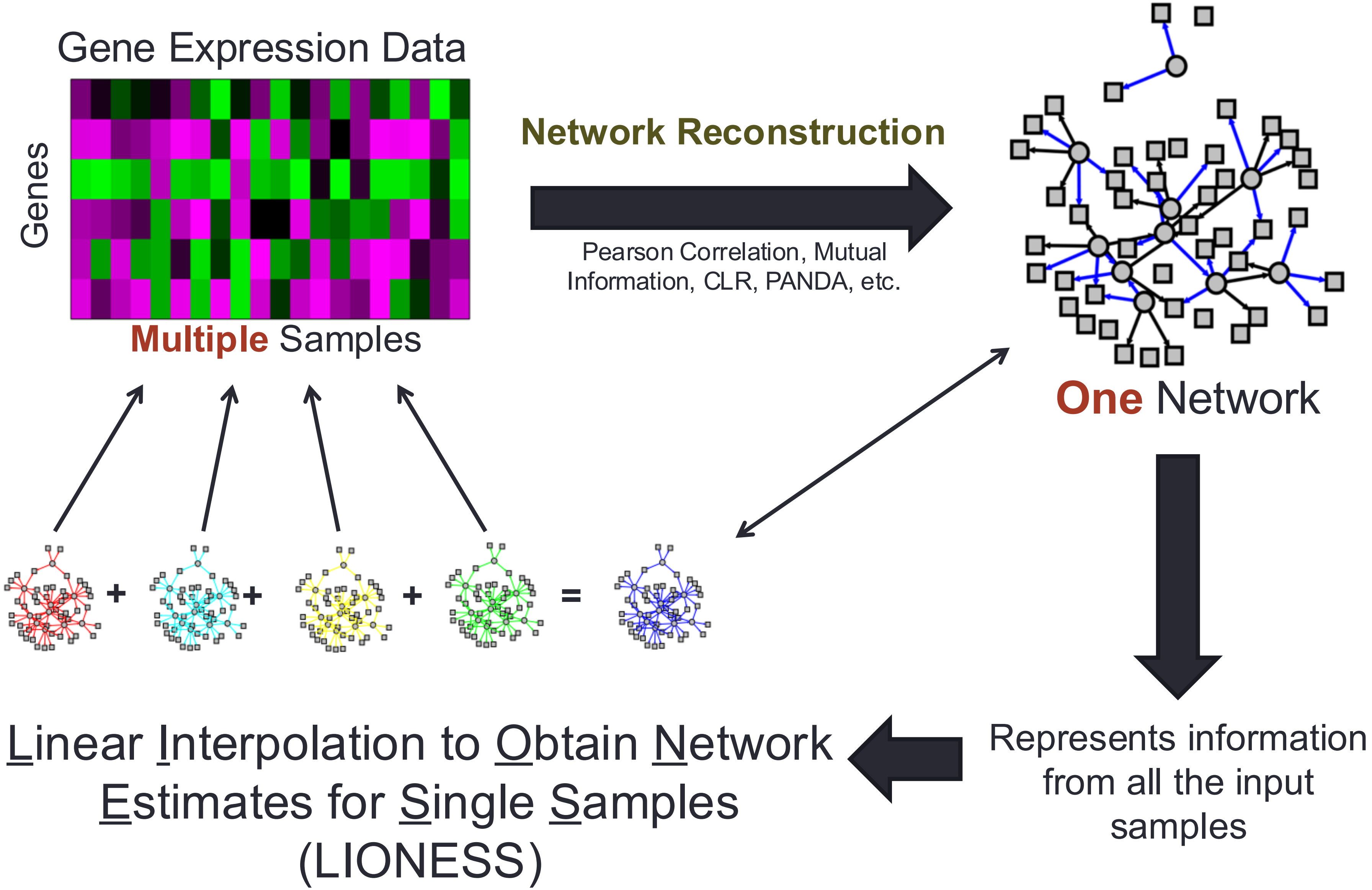
Pearson Correlation, Mutual Information, CLR, PANDA, etc.

One Network

We generally estimate “Aggregate” Networks.

Marieke Kuijjer, Matt Tung, Kimbie Glass

Reconstructing Gene Regulatory Networks



Gene Expression Data

Genes

Multiple Samples

Network Reconstruction

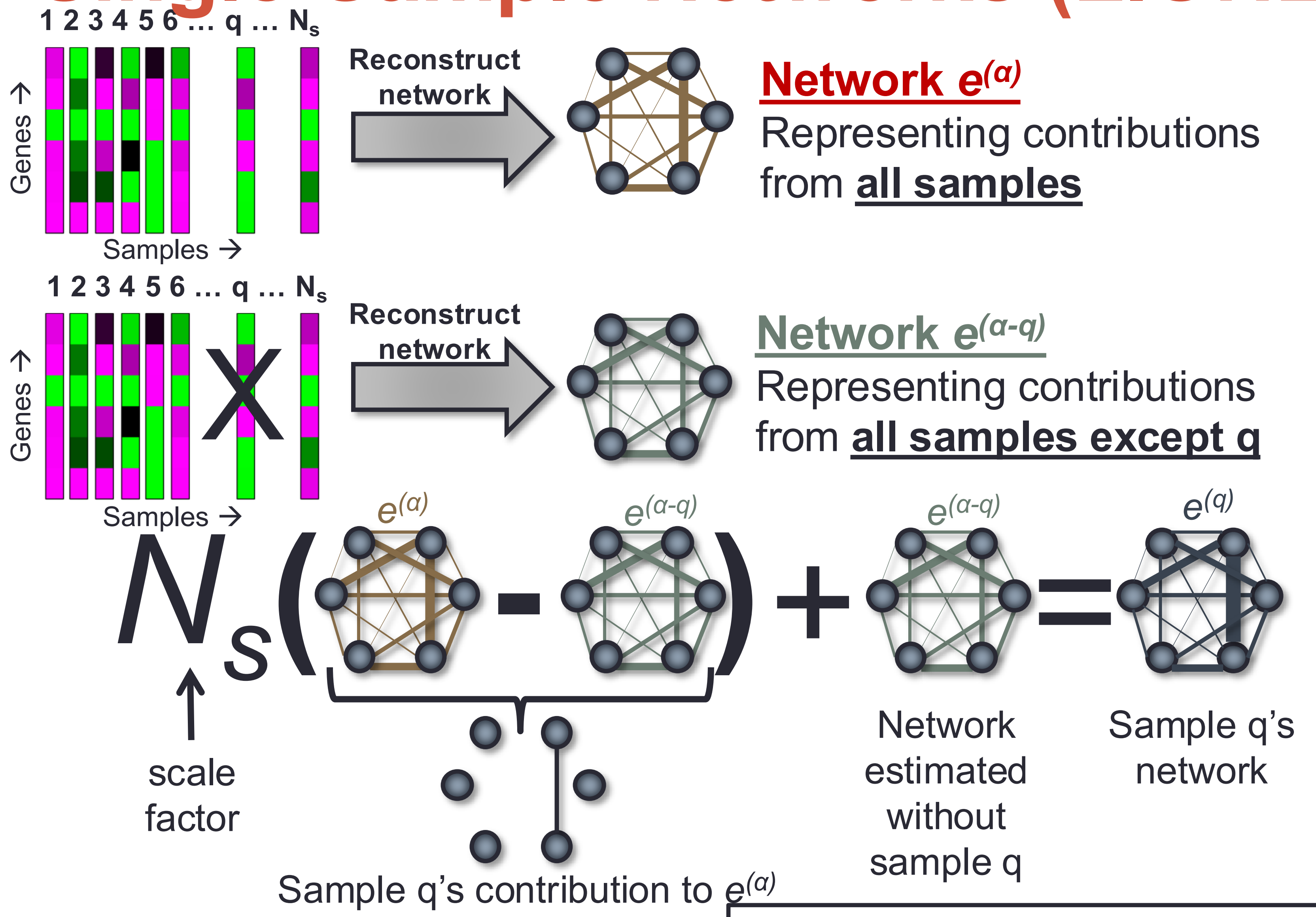
Pearson Correlation, Mutual Information, CLR, PANDA, etc.

One Network

Represents information from all the input samples

Linear Interpolation to Obtain Network Estimates for Single Samples (LIONESS)

Single-Sample Networks (LIONESS)



Reconstruct network

Network $e^{(\alpha)}$

Representing contributions from **all samples**

Reconstruct network

Network $e^{(\alpha-q)}$

Representing contributions from **all samples except q**

$e^{(\alpha)}$ $e^{(\alpha-q)}$ $e^{(\alpha-q)}$ $e^{(q)}$

scale factor

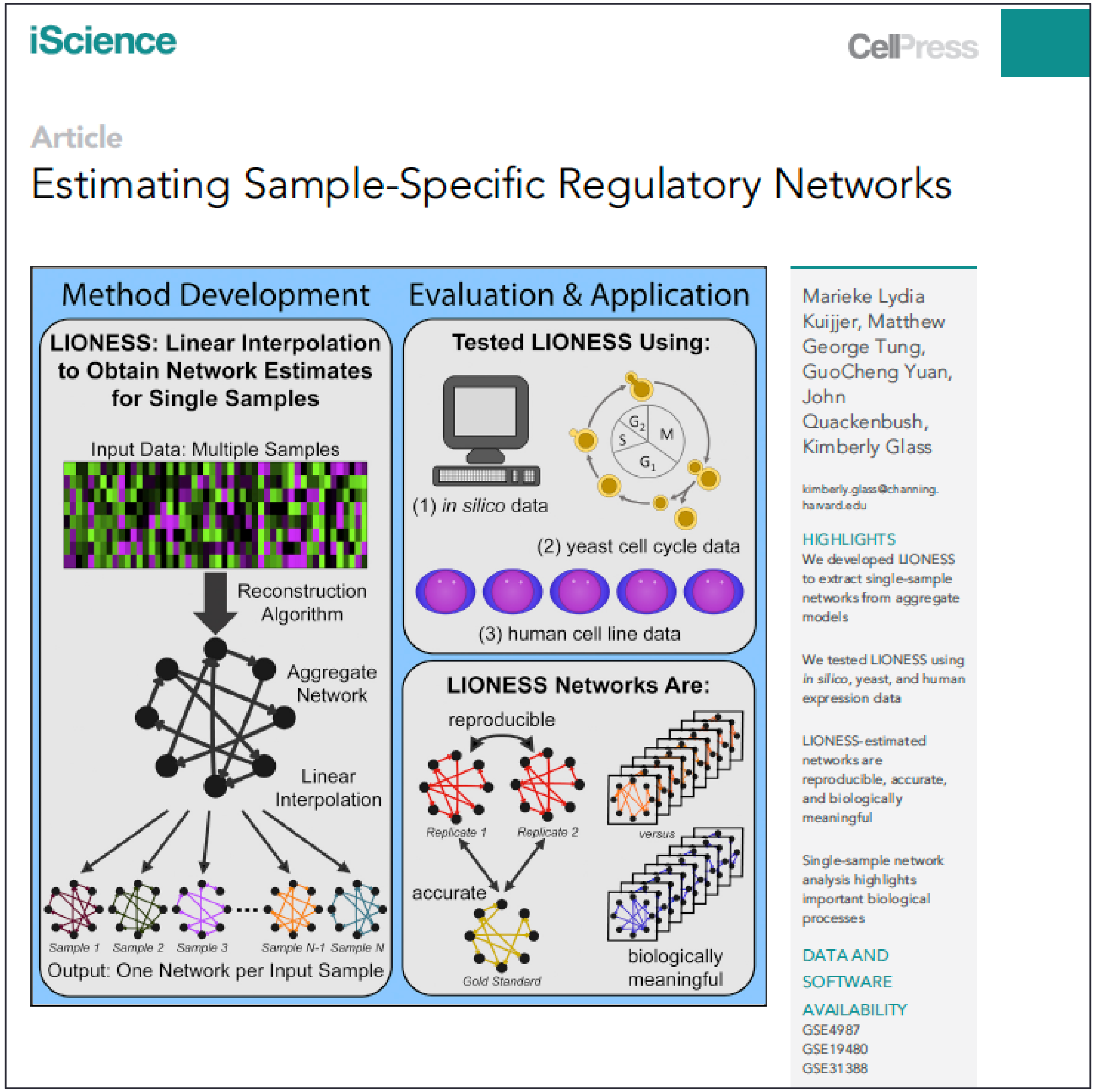
Sample q's contribution to $e^{(\alpha)}$

Network estimated without sample q

Sample q's network

$$\boxed{N_s\left(e_{ij}^{(\alpha)} - e_{ij}^{(\alpha-q)}\right) + e_{ij}^{(\alpha-q)} = e_{ij}^{(q)}}$$

Single-Sample Networks (LIONESS)



iScience

CellPress

Article

Estimating Sample-Specific Regulatory Networks

Marieke Lydia Kuijjer, Matthew George Tung, GuoCheng Yuan, John Quackenbush, Kimberly Glass

kimberly.glass@channing.harvard.edu

HIGHLIGHTS

We developed LIONESS to extract single-sample networks from aggregate models

We tested LIONESS using *in silico*, yeast, and human expression data

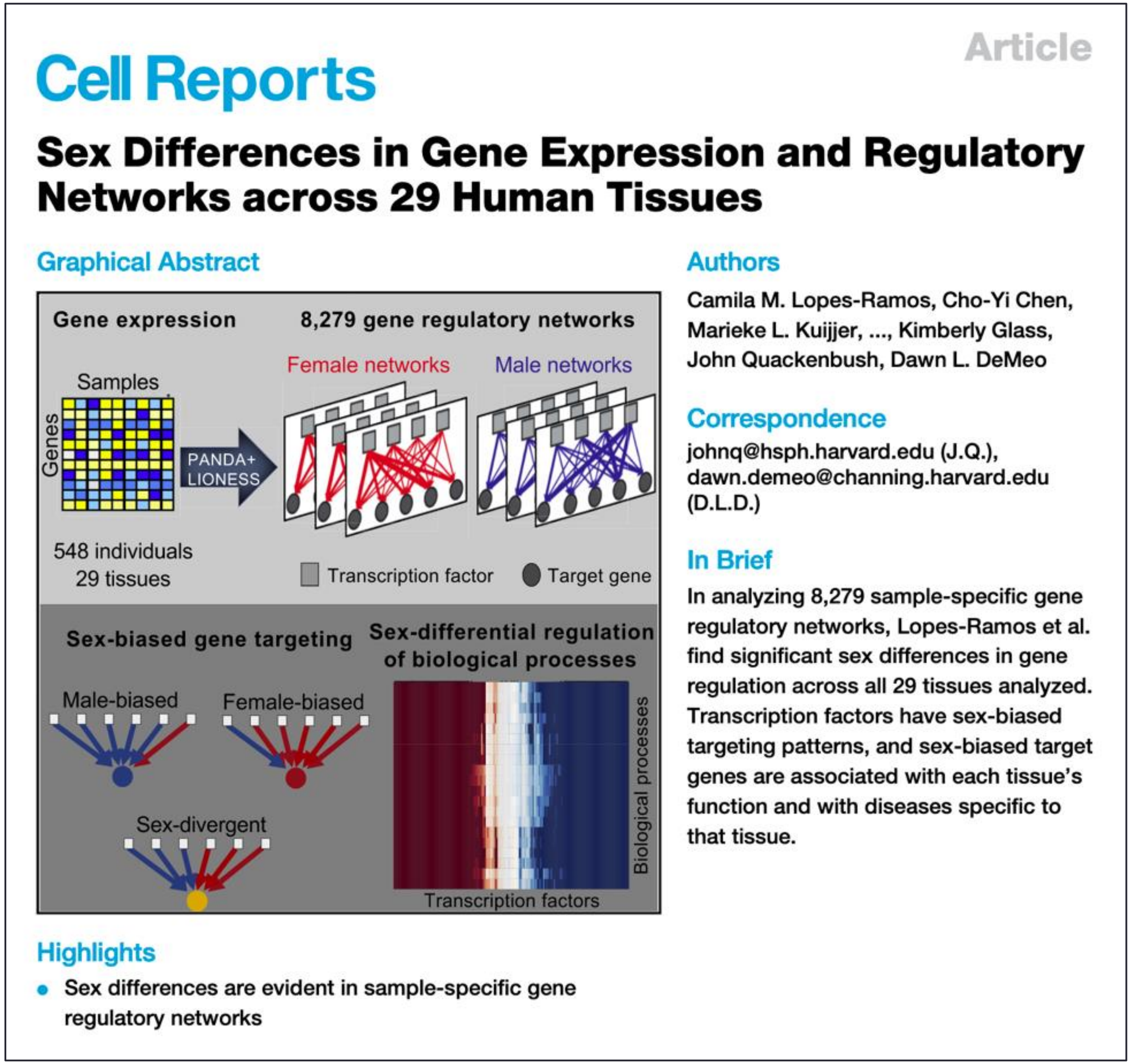
LIONESS-estimated networks are reproducible, accurate, and biologically meaningful

Single-sample network analysis highlights important biological processes

DATA AND SOFTWARE AVAILABILITY

GSE4987
GSE19480
GSE31388

Sex Differences in Twenty-Nine Tissues



Cell Reports

Article

Sex Differences in Gene Expression and Regulatory Networks across 29 Human Tissues

Graphical Abstract

Authors

Camila M. Lopes-Ramos, Cho-Yi Chen, Marieke L. Kuijjer, ..., Kimberly Glass, John Quackenbush, Dawn L. DeMeo

Correspondence

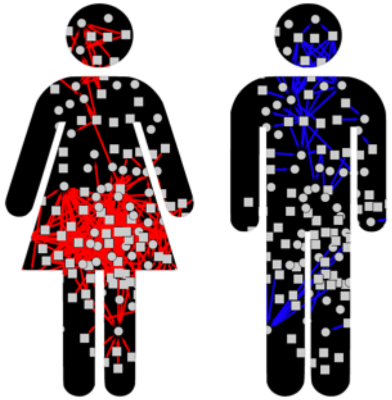
johnq@hsph.harvard.edu (J.Q.), dawn.demeo@channing.harvard.edu (D.L.D.)

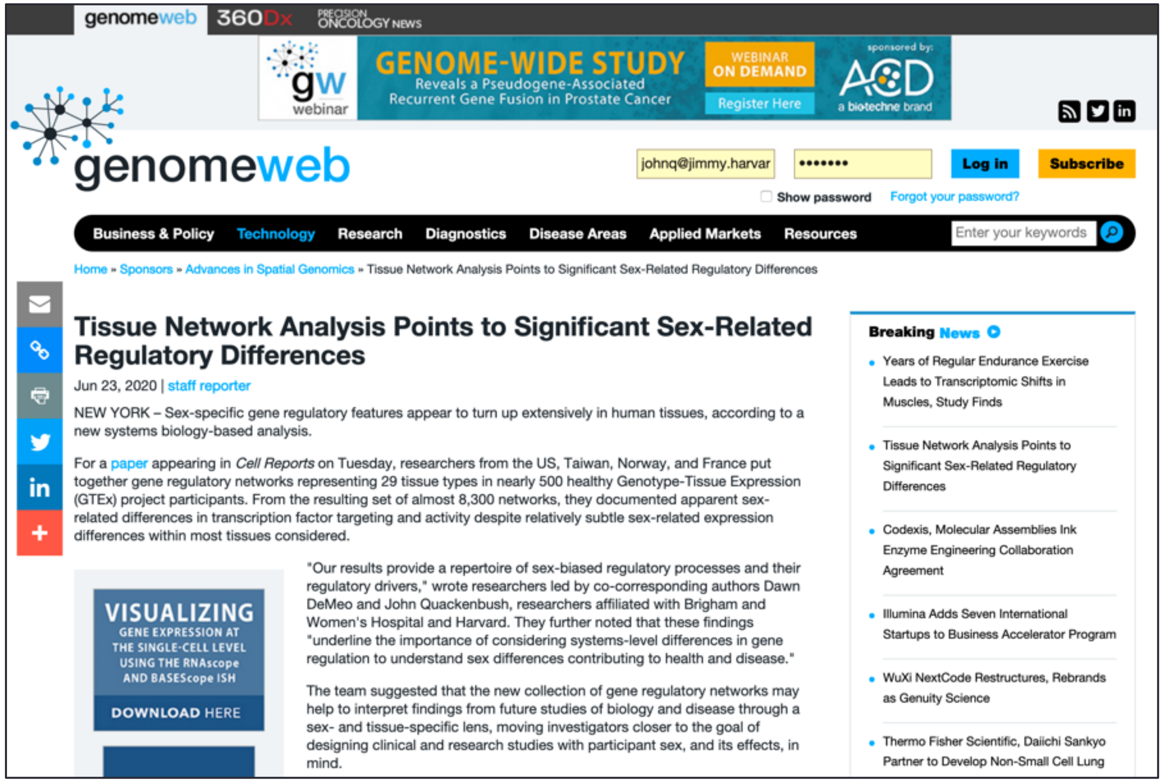
In Brief

In analyzing 8,279 sample-specific gene regulatory networks, Lopes-Ramos et al. find significant sex differences in gene regulation across all 29 tissues analyzed. Transcription factors have sex-biased targeting patterns, and sex-biased target genes are associated with each tissue's function and with diseases specific to that tissue.

Highlights

- Sex differences are evident in sample-specific gene regulatory networks





Home » Sponsors » Advances in Spatial Genomics » Tissue Network Analysis Points to Significant Sex-Related Regulatory Differences

Tissue Network Analysis Points to Significant Sex-Related Regulatory Differences

Jun 23, 2020 | staff reporter

NEW YORK – Sex-specific gene regulatory features appear to turn up extensively in human tissues, according to a new systems biology-based analysis.

For a paper appearing in *Cell Reports* on Tuesday, researchers from the US, Taiwan, Norway, and France put together gene regulatory networks representing 29 tissue types in nearly 500 healthy Genotype-Tissue Expression (GTEx) project participants. From the resulting set of almost 8,300 networks, they documented apparent sex-related differences in transcription factor targeting and activity despite relatively subtle sex-related expression differences within most tissues considered.

"Our results provide a repertoire of sex-biased regulatory processes and their regulatory drivers," wrote researchers led by co-corresponding authors Dawn DeMeo and John Quackenbush, researchers affiliated with Brigham and Women's Hospital and Harvard. They further noted that these findings "underline the importance of considering systems-level differences in gene regulation to understand sex differences contributing to health and disease."

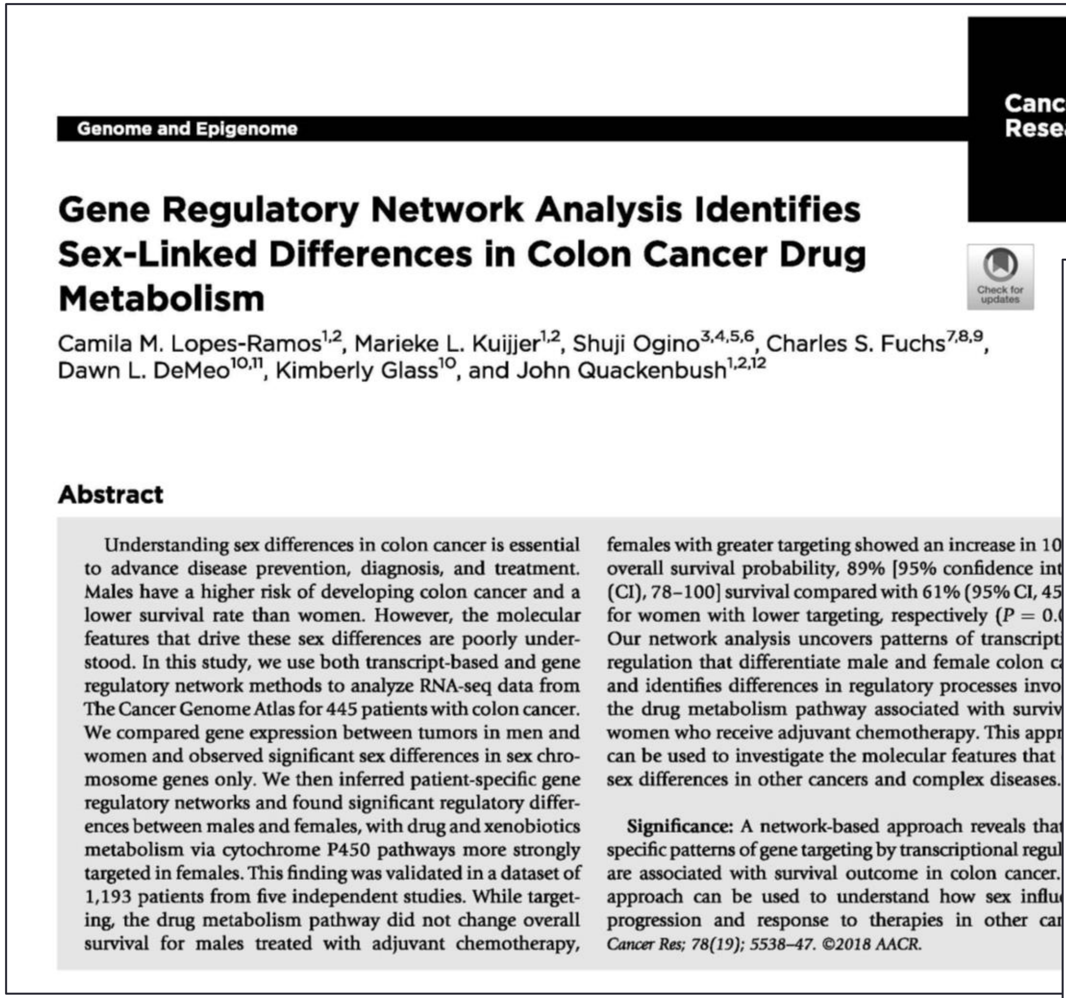
The team suggested that the new collection of gene regulatory networks may help to interpret findings from future studies of biology and disease through a sex- and tissue-specific lens, moving investigators closer to the goal of designing clinical and research studies with participant sex, and its effects, in mind.

Breaking News

- Years of Regular Endurance Exercise Leads to Transcriptomic Shifts in Muscles, Study Finds
- Tissue Network Analysis Points to Significant Sex-Related Regulatory Differences
- Codexis, Molecular Assemblies Ink Enzyme Engineering Collaboration Agreement
- Illumina Adds Seven International Startups to Business Accelerator Program
- WuXi NextCode Restructures, Rebrands as Genuity Science
- Thermo Fisher Scientific, Daiichi Sankyo Partner to Develop Non-Small Cell Lung

Camila Lopes-Ramos

Sexual Differences in Colorectal Cancer



Genome and Epigenome

Cancer Research

Gene Regulatory Network Analysis Identifies Sex-Linked Differences in Colon Cancer Drug Metabolism

Camila M. Lopes-Ramos[1,2], Marieke L. Kuijjer[1,2], Shuji Ogino[3,4,5,6], Charles S. Fuchs[7,8,9], Dawn L. DeMeo[10,11], Kimberly Glass[10], and John Quackenbush[1,2,12]

Abstract

Understanding sex differences in colon cancer is essential to advance disease prevention, diagnosis, and treatment. Males have a higher risk of developing colon cancer and a lower survival rate than women. However, the molecular features that drive these sex differences are poorly understood. In this study, we use both transcript-based and gene regulatory network methods to analyze RNA-seq data from The Cancer Genome Atlas for 445 patients with colon cancer. We compared gene expression between tumors in men and women and observed significant sex differences in sex chromosome genes only. We then inferred patient-specific gene regulatory networks and found significant regulatory differences between males and females, with drug and xenobiotics metabolism via cytochrome P450 pathways more strongly targeted in females. This finding was validated in a dataset of 1,193 patients from five independent studies. While targeting, the drug metabolism pathway did not change overall survival for males treated with adjuvant chemotherapy,
females with greater targeting showed an increase in 10
overall survival probability, 89% [95% confidence int
(CI), 78–100] survival compared with 61% (95% CI, 45
for women with lower targeting, respectively ($P = 0.$
Our network analysis uncovers patterns of transcripti
regulation that differentiate male and female colon c
and identifies differences in regulatory processes invo
the drug metabolism pathway associated with surviv
women who receive adjuvant chemotherapy. This appr
can be used to investigate the molecular features that
sex differences in other cancers and complex diseases.

Significance: A network-based approach reveals that
specific patterns of gene targeting by transcriptional regul
are associated with survival outcome in colon cancer.
approach can be used to understand how sex influe
progression and response to therapies in other can

Cancer Res; 78(19); 5538–47. ©2018 AACR.

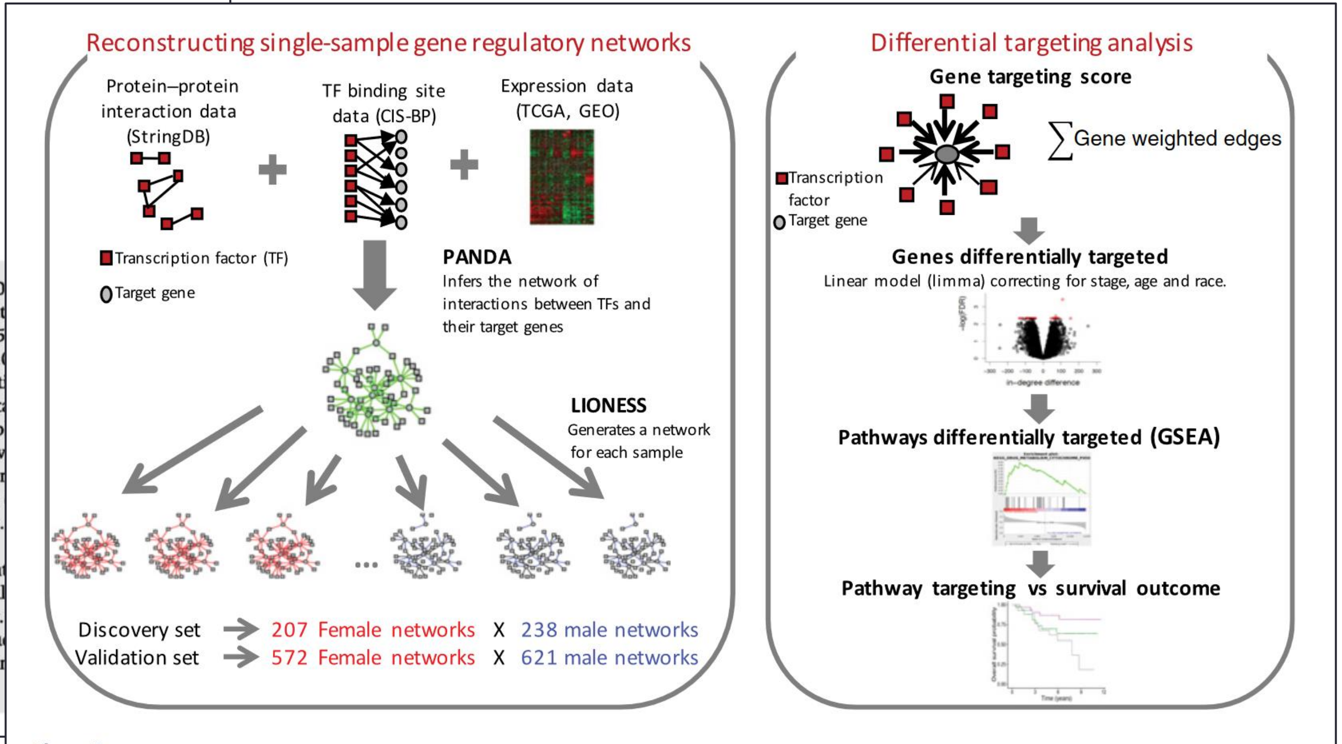
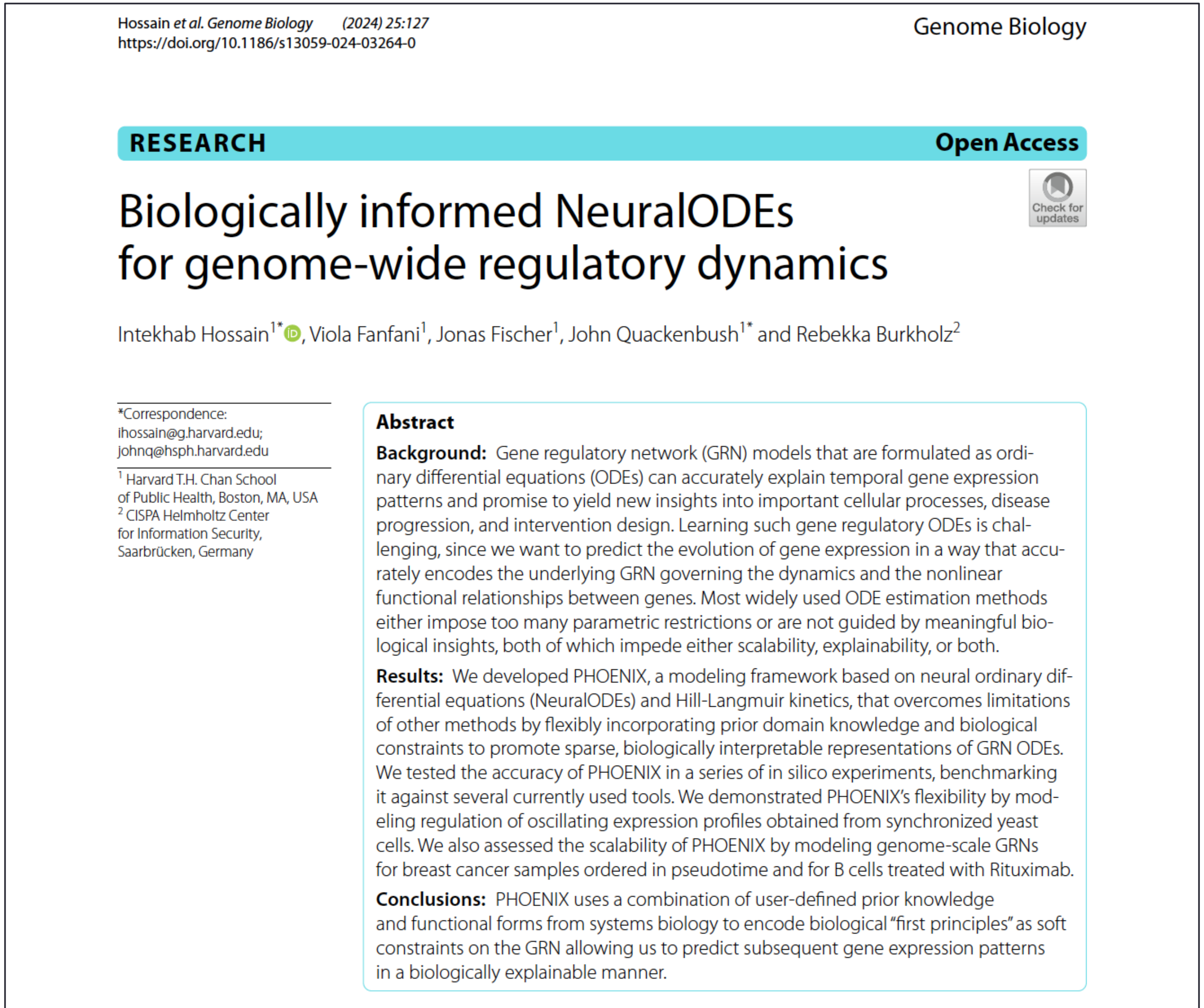


Figure 1.
Study workflow. Overview of the approach used to reconstruct single-sample gene regulatory networks and to perform differential targeting analysis.

Camila Lopes-Ramos

Pardon me, do you have the pseudo-time course?

PHOENIX: A NeuralODE Solver



Hossain *et al. Genome Biology* (2024) 25:127
https://doi.org/10.1186/s13059-024-03264-0

Genome Biology

RESEARCH **Open Access**

Biologically informed NeuralODEs for genome-wide regulatory dynamics

Intekhab Hossain[1*], Viola Fanfani[1], Jonas Fischer[1], John Quackenbush[1*] and Rebekka Burkholz[2]

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[2] CISPA Helmholtz Center for Information Security, Saarbrücken, Germany

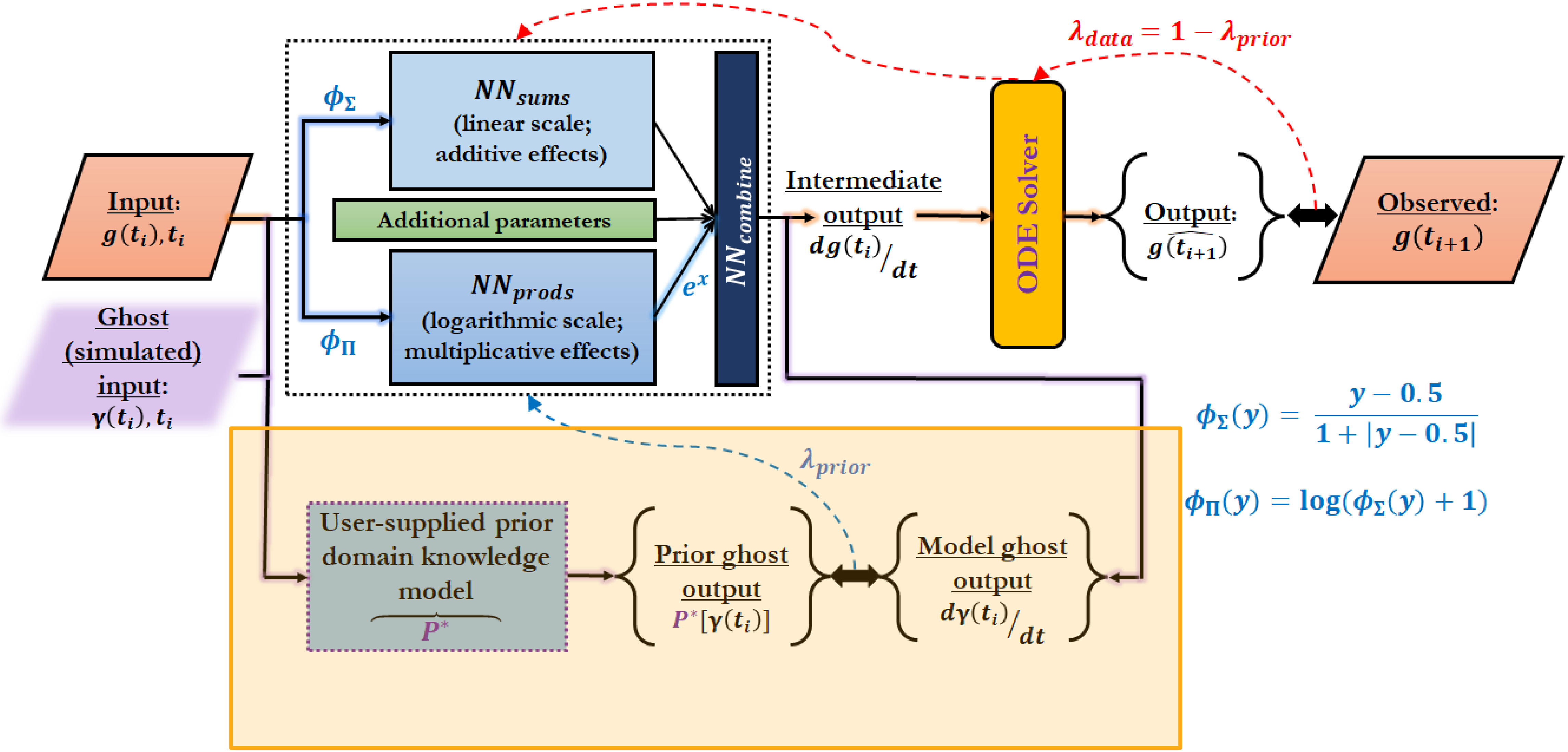
Abstract

Background: Gene regulatory network (GRN) models that are formulated as ordinary differential equations (ODEs) can accurately explain temporal gene expression patterns and promise to yield new insights into important cellular processes, disease progression, and intervention design. Learning such gene regulatory ODEs is challenging, since we want to predict the evolution of gene expression in a way that accurately encodes the underlying GRN governing the dynamics and the nonlinear functional relationships between genes. Most widely used ODE estimation methods either impose too many parametric restrictions or are not guided by meaningful biological insights, both of which impede either scalability, explainability, or both.

Results: We developed PHOENIX, a modeling framework based on neural ordinary differential equations (NeuralODEs) and Hill-Langmuir kinetics, that overcomes limitations of other methods by flexibly incorporating prior domain knowledge and biological constraints to promote sparse, biologically interpretable representations of GRN ODEs. We tested the accuracy of PHOENIX in a series of in silico experiments, benchmarking it against several currently used tools. We demonstrated PHOENIX's flexibility by modeling regulation of oscillating expression profiles obtained from synchronized yeast cells. We also assessed the scalability of PHOENIX by modeling genome-scale GRNs for breast cancer samples ordered in pseudotime and for B cells treated with Rituximab.

Conclusions: PHOENIX uses a combination of user-defined prior knowledge and functional forms from systems biology to encode biological "first principles" as soft constraints on the GRN allowing us to predict subsequent gene expression patterns in a biologically explainable manner.

PHOENIX: No Free Lunch



Input: $g(t_i), t_i$

Ghost (simulated) input: $\gamma(t_i), t_i$

ϕ_Σ

ϕ_Π

NN_{sums} (linear scale; additive effects)

Additional parameters

NN_{prods} (logarithmic scale; multiplicative effects)

e^x

$NN_{combine}$

Intermediate output $dg(t_i)/dt$

ODE Solver

$\lambda_{data} = 1 - \lambda_{prior}$

Output: $\widehat{g(t_{i+1})}$

Observed: $g(t_{i+1})$

λ_{prior}

User-supplied prior domain knowledge model $\overbrace{\qquad}^{}$ P^*

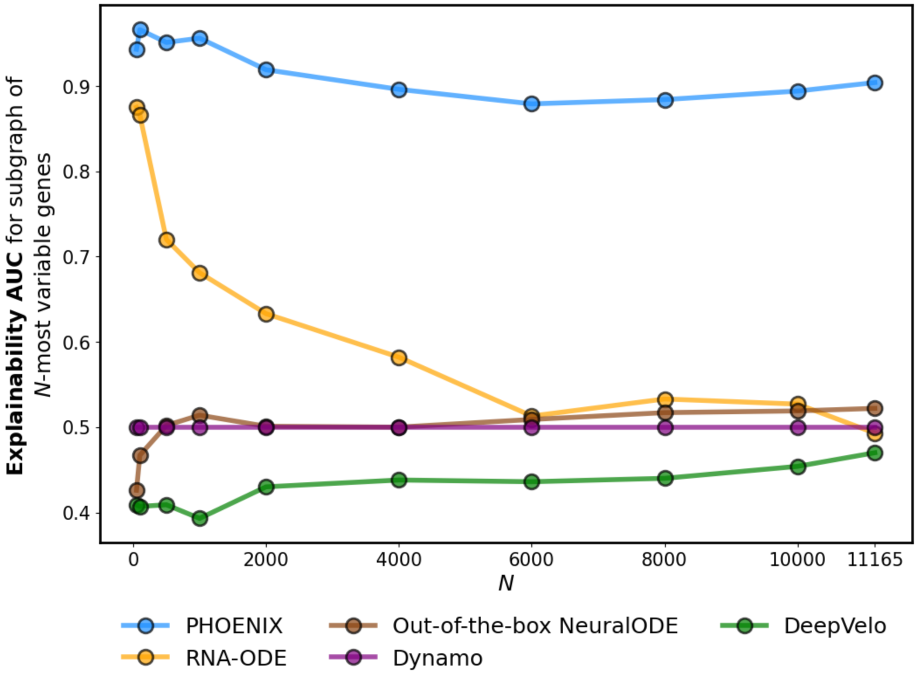
Prior ghost output $P^*[\gamma(t_i)]$

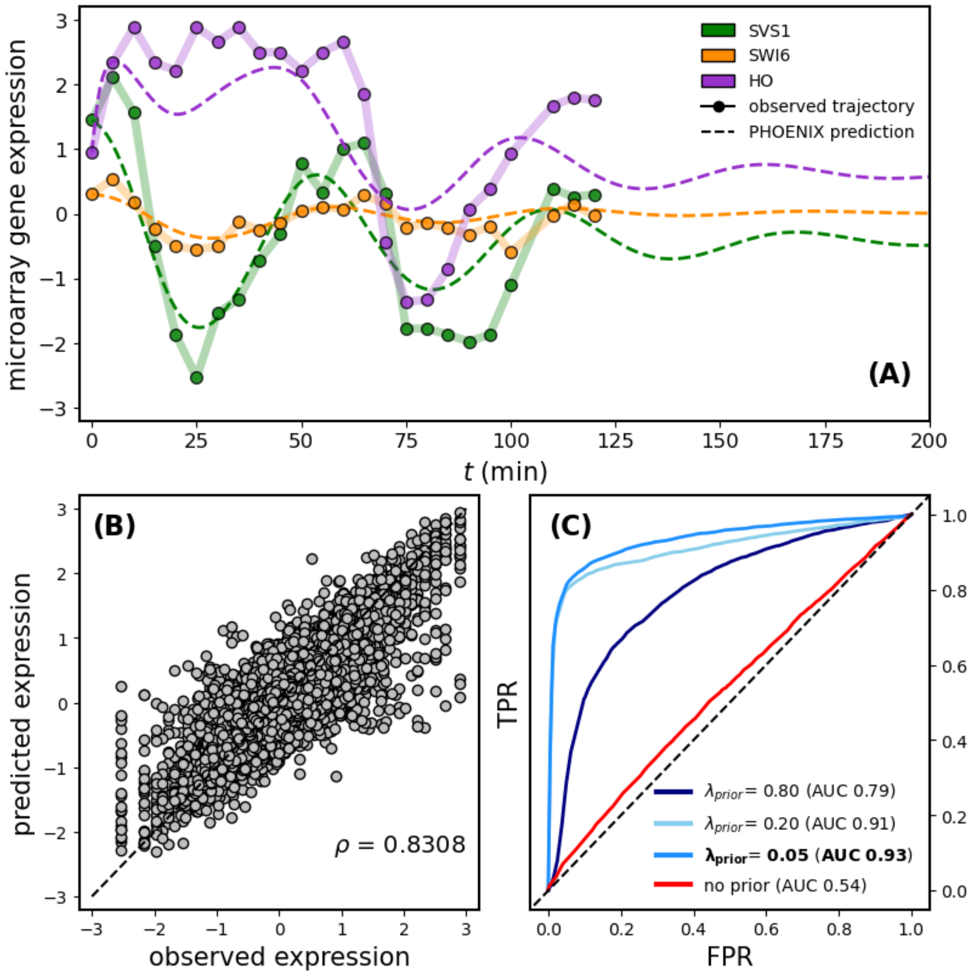
Model ghost output $d\gamma(t_i)/dt$

$$\phi_\Sigma(y) = \frac{y - 0.5}{1 + |y - 0.5|}$$

$$\phi_\Pi(y) = \log(\phi_\Sigma(y) + 1)$$

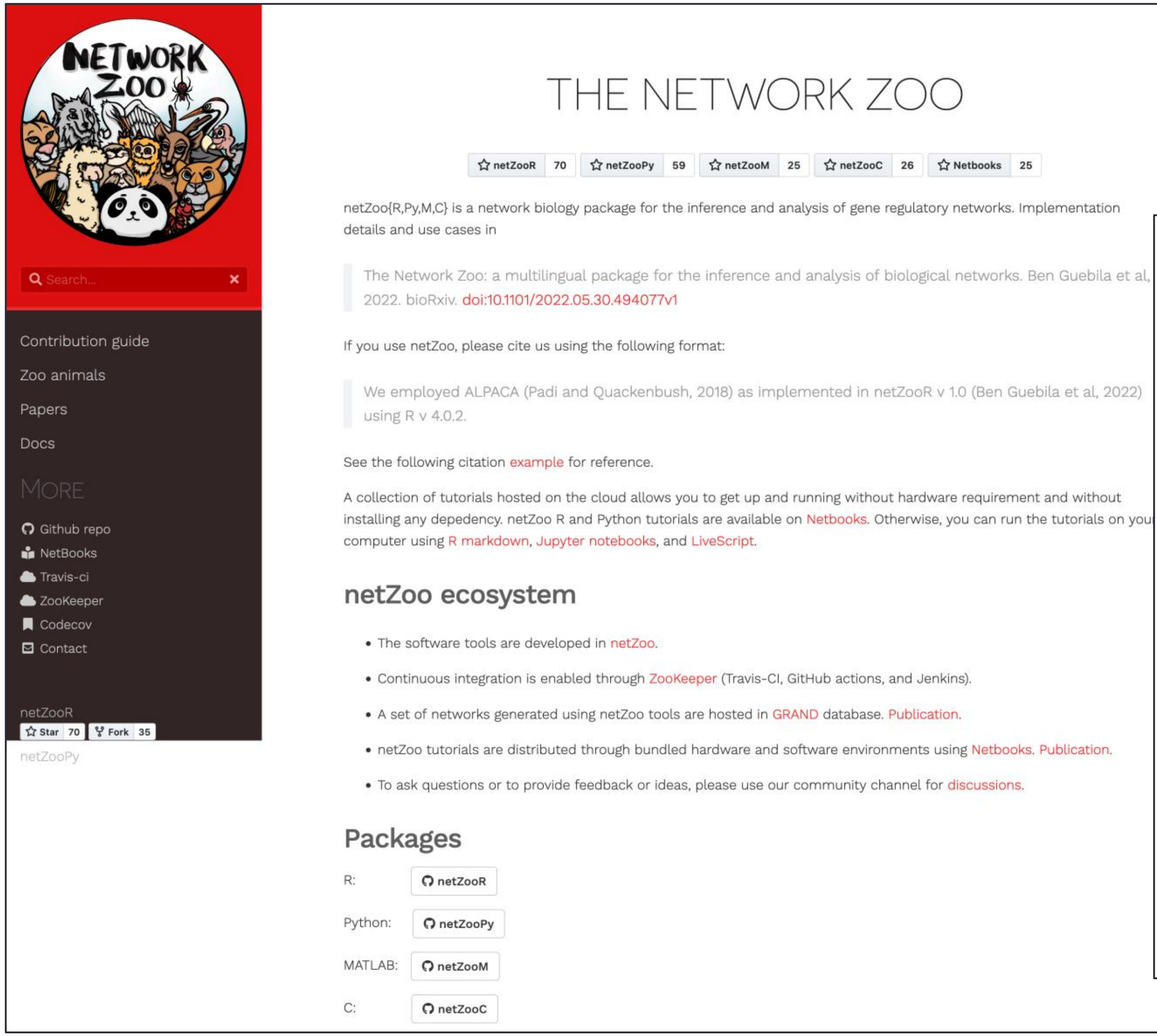
PHOENIX: Scales to the Genome and is Explainable





How do I maximize my impact as a scientist?

netZoo: An integrated platform



THE NETWORK ZOO

netZoo{R,Py,M,C} is a network biology package for the inference and analysis of gene regulatory networks. Implementation details and use cases in

> The Network Zoo: a multilingual package for the inference and analysis of biological networks. Ben Guebila et al, 2022. bioRxiv. doi:10.1101/2022.05.30.494077v1

If you use netZoo, please cite us using the following format:

> We employed ALPACA (Padi and Quackenbush, 2018) as implemented in netZooR v 1.0 (Ben Guebila et al, 2022) using R v 4.0.2.

See the following citation example for reference.

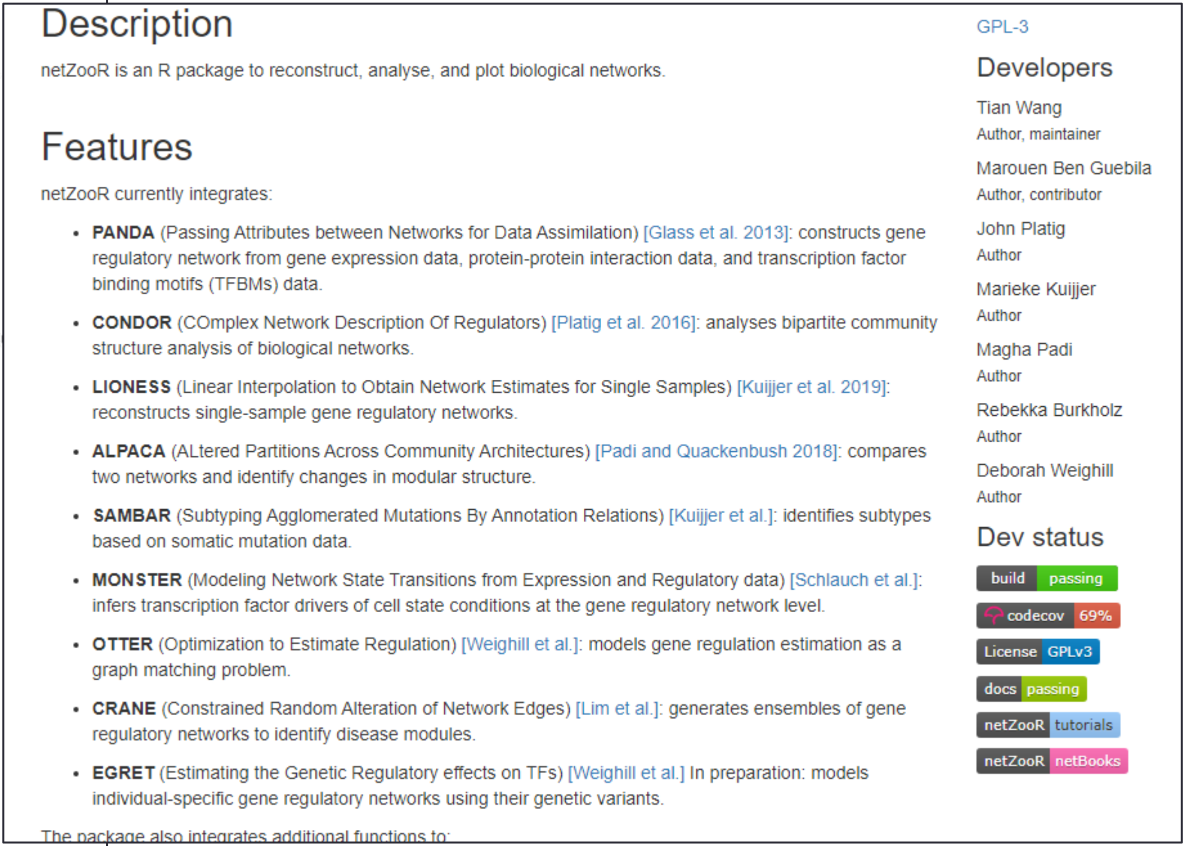
A collection of tutorials hosted on the cloud allows you to get up and running without hardware requirement and without installing any depedency. netZoo R and Python tutorials are available on Netbooks. Otherwise, you can run the tutorials on you computer using R markdown, Jupyter notebooks, and LiveScript.

netZoo ecosystem

- The software tools are developed in netZoo.
- Continuous integration is enabled through ZooKeeper (Travis-CI, GitHub actions, and Jenkins).
- A set of networks generated using netZoo tools are hosted in GRAND database. Publication.
- netZoo tutorials are distributed through bundled hardware and software environments using Netbooks. Publication.
- To ask questions or to provide feedback or ideas, please use our community channel for discussions.

Packages

R:	netZooR
Python:	netZooPy
MATLAB:	netZooM
C:	netZooC



Description

netZooR is an R package to reconstruct, analyse, and plot biological networks.

Features

netZooR currently integrates:

- **PANDA** (Passing Attributes between Networks for Data Assimilation) [Glass et al. 2013]: constructs gene regulatory network from gene expression data, protein-protein interaction data, and transcription factor binding motifs (TFBMs) data.
- **CONDOR** (COmplex Network Description Of Regulators) [Platig et al. 2016]: analyses bipartite community structure analysis of biological networks.
- **LIONESS** (Linear Interpolation to Obtain Network Estimates for Single Samples) [Kuijjer et al. 2019]: reconstructs single-sample gene regulatory networks.
- **ALPACA** (ALtered Partitions Across Community Architectures) [Padi and Quackenbush 2018]: compares two networks and identify changes in modular structure.
- **SAMBAR** (Subtyping Agglomerated Mutations By Annotation Relations) [Kuijjer et al.]: identifies subtypes based on somatic mutation data.
- **MONSTER** (Modeling Network State Transitions from Expression and Regulatory data) [Schlauch et al.]: infers transcription factor drivers of cell state conditions at the gene regulatory network level.
- **OTTER** (Optimization to Estimate Regulation) [Weighill et al.]: models gene regulation estimation as a graph matching problem.
- **CRANE** (Constrained Random Alteration of Network Edges) [Lim et al.]: generates ensembles of gene regulatory networks to identify disease modules.
- **EGRET** (Estimating the Genetic Regulatory effects on TFs) [Weighill et al.] In preparation: models individual-specific gene regulatory networks using their genetic variants.

The package also integrates additional functions to:

GPL-3

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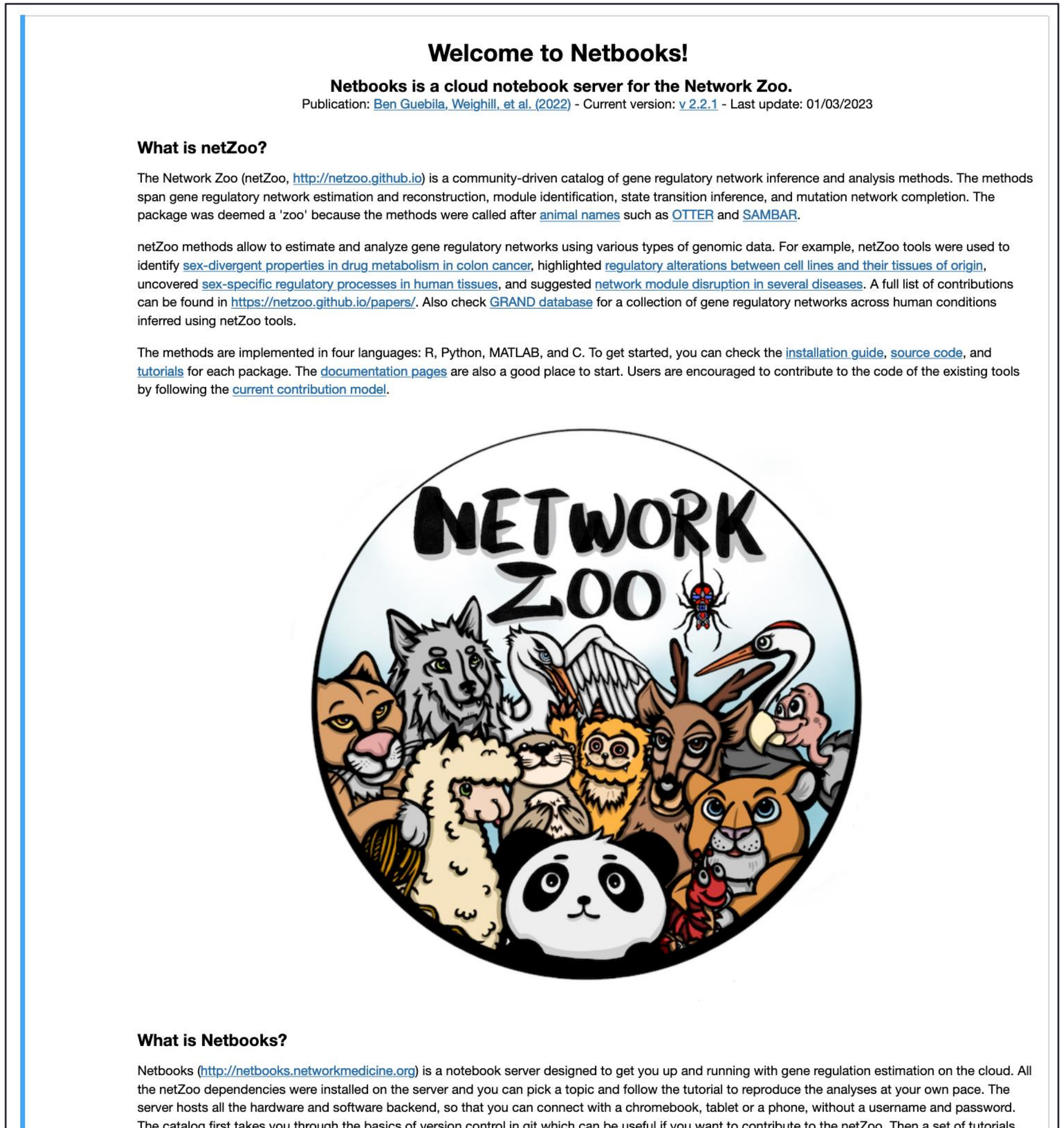
netBooks: Methods in Action



Welcome to Netbooks!

Netbooks is a cloud notebook server for the Network Zoo.

Publication: Ben Guebila, Weighill, et al. (2022) - Current version: v 2.2.1 - Last update: 01/03/2023

What is netZoo?

The Network Zoo (netZoo, http://netzoo.github.io) is a community-driven catalog of gene regulatory network inference and analysis methods. The methods span gene regulatory network estimation and reconstruction, module identification, state transition inference, and mutation network completion. The package was deemed a 'zoo' because the methods were called after animal names such as OTTER and SAMBAR.

netZoo methods allow to estimate and analyze gene regulatory networks using various types of genomic data. For example, netZoo tools were used to identify sex-divergent properties in drug metabolism in colon cancer, highlighted regulatory alterations between cell lines and their tissues of origin, uncovered sex-specific regulatory processes in human tissues, and suggested network module disruption in several diseases. A full list of contributions can be found in https://netzoo.github.io/papers/. Also check GRAND database for a collection of gene regulatory networks across human conditions inferred using netZoo tools.

The methods are implemented in four languages: R, Python, MATLAB, and C. To get started, you can check the installation guide, source code, and tutorials for each package. The documentation pages are also a good place to start. Users are encouraged to contribute to the code of the existing tools by following the current contribution model.

What is Netbooks?

Netbooks (http://netbooks.networkmedicine.org) is a notebook server designed to get you up and running with gene regulation estimation on the cloud. All the netZoo dependencies were installed on the server and you can pick a topic and follow the tutorial to reproduce the analyses at your own pace. The server hosts all the hardware and software backend, so that you can connect with a chromebook, tablet or a phone, without a username and password. The catalog first takes you through the basics of version control in git which can be useful if you want to contribute to the netZoo. Then a set of tutorials

The impediment to action advances action.
What stands in the way becomes the way.

– Marcus Aurelius, *Meditations* 5:20

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