differential network analysis and graph classification

a glocal approach

giuseppe jurman

fondazione bruno kessler

Bringing Maths to Life
naples, 19–21 oct 2015

1. introduction
2. background
3. him distance
4. (bio)-applications

introduction

COMMENTARY | INSIGHT

NATURE PHYSICS | VOL. 8 | JANUARY 2012 | www.nature.com/naturephysics

The network takeover

Albert-László Barabási

Reductionism, as a paradigm, is expired, and complexity, as a field, is tired. Data-based mathematical models of complex systems are offering a fresh perspective, rapidly developing into a new discipline: network science.

By simultaneously looking at the World Wide Web and genetic networks, Internet and social systems, it led to the discovery that despite the many differences in the nature of the nodes and the interactions between them, the networks behind most complex systems are governed by a series of fundamental laws that determine and limit their behaviour.

Molecular Systems Biology 8; Article number 565; doi:10.1038/msb.2011.99

Citation: *Molecular Systems Biology* 8:565

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www.molecularsystemsbiology.com

REVIEW

Differential network biology

Trey Ideker^{1,2,*} and Nevan J Krogan^{3,4,5,*}

during a cellular or adaptive response. Here, we review the technological developments and experimental designs that have enabled differential network mapping at very large scales and highlight biological insight that has been derived from this type of analysis. We argue that differential network mapping, which allows for the interrogation of previously unexplored interaction spaces, will become a standard mode of network analysis in the future, just as

differential network analysis

VS.

differential network analysis

example 1: static networks comparison

doi:10.1016/j.jmb.2007.03.013

J. Mol. Biol. (2007) 369, 1126–1139

JMB

Available online at www.sciencedirect.com

ScienceDirect

The Identification of Similarities between Biological Networks: Application to the Metabolome and Interactome

Adrian P. Cootes¹, Stephen H. Muggleton² and Michael J.E. Sternberg^{1*}

the subgraph. We examined whether considering network context improved subgraph comparison and applied this technique to the comparison of pairs of metabolic and protein–protein interaction networks. We also explored two different methods for calculating the statistical significance of similar subgraphs and the suitability of each for analysing various types of biological networks. In this way, we identified similar subgraphs in pairs of metabolic

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example 2: dynamic networks comparison

The Annals of Applied Statistics
2010, Vol. 4, No. 1, 94–123
DOI: 10.1214/09-AOAS308
© Institute of Mathematical Statistics, 2010

ESTIMATING TIME-VARYING NETWORKS

BY MLADEN KOLAR, LE SONG¹, AMR AHMED AND ERIC P. XING²

Carnegie Mellon University

- gene expression from microarray
- 588 developmental genes
- 58 go categories (nodes)
- links are keller gene interactions
- 66 time points
 - embryonic (1–30) larval (31–40)
 - pupal (41–58) adult (59–66)

the problem

the problem

need for a

quantitative measure
of network difference

background

network comparison

indirect

vector of network indicators

- degree distribution
- node correlation
- path lengths
- diameter
- clustering
- ...

direct

$d(\text{graph}, \text{graph})$

- edit distances
- maxcommonsbg distances
- ζ functions of volume differences
- spectral measures
- ...

network comparison

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- degree distribution
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direct

$d(\text{graph}, \text{graph})$

- edit distances
- spectral measures

local and global metrics

$$d(\text{graph}_1, \text{graph}_2)$$

edit distances

spectral distances

$f(\text{insert}, \text{delete})$

$f(\text{spec}_1, \text{spec}_2)$

local

global

edges have same importance

isospectral graphs coincide

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edit distances spectral distances

Solution:

$f(\text{insert, delete})$ $f(\text{spec}, \text{spec})$

local global

edges have same importance *local spectral graphs coincide*

glocal distance

him distance

- $\mathcal{N}_1, \mathcal{N}_2$ simple networks on N nodes
- corresponding adjacency matrices $A^{(1)}$ and $A^{(2)}$, with $a_{ij}^{(1)}, a_{ij}^{(2)} \in \mathcal{F}$
- unweighted: $\mathcal{F} = \mathbb{F}_2 = \{0, 1\}$, weighted: $\mathcal{F} = [0, 1] \subseteq \mathbb{R}$

- $\mathbb{I}_N = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ & \vdots & \ddots & \\ 0 & 0 & \cdots & 1 \end{pmatrix}$

- 1_N unitary, 0_N null
- $\mathcal{E}_N$ empty network (adjacency matrix 0_N)
- $\mathcal{F}_N$ the clique (adjacency matrix $1_N - \mathbb{I}_N$)

nb: directed networks are bipartitely represented

(normalized) hamming distance

Thus we define the distance $D(x, y)$ between two points x and y as the number of coordinates for which x and y are different. This is the same as the

evaluating the presence/absence of matching links

$$H(\mathcal{N}_1, \mathcal{N}_2) = \frac{\text{Hamming}(\mathcal{N}_1, \mathcal{N}_2)}{\text{Hamming}(\mathcal{E}_N, \mathcal{F}_N)} = \frac{1}{N(N-1)} \sum_{1 \leq i \neq j \leq N} |A_{ij}^{(1)} - A_{ij}^{(2)}|,$$

$A^{(1)} = A^{(2)}$

$A^{(1)} + A^{(2)} = 1_N - \mathbb{I}_N = \begin{pmatrix} 0 & 1 & \cdots & 1 \\ 1 & 0 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 0 \end{pmatrix}$

ipsen-mikhailov distance

Journal STATISTICS
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2013, Paris, 2013
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doi:10.1007/978-1-4020-6900-9_127

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An introduction to
spectral distances in networks

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^bINdE, University of Trento, Trento, Italy

PHYSICAL REVIEW E 66, 046109 (2002)

Evolutionary reconstruction of networks

Mads Ipsen^{*} and Alexander S. Mikhailov

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

(Received 9 November 2001; revised manuscript received 21 May 2002; published 14 October 2002)

l_2 integrated difference of the laplacian spectral densities

$$\text{IM}(\mathcal{N}_1, \mathcal{N}_2) = \sqrt{\int_0^\infty [\rho_{\mathcal{N}_1}(\omega, \bar{\gamma}) - \rho_{\mathcal{N}_2}(\omega, \bar{\gamma})]^2 d\omega}$$

ipsen-mikhailov distance: the gory details

- balls_and_springs net model

$$\ddot{x}_i + \sum_{j=1}^N A_{ij}(x_i - x_j) = 0 \quad \text{for } i = 0, \dots, N-1$$

- its vibrational frequencies are the square root of the laplacian eigenvalues

$$\omega_i = \sqrt{\lambda_i}, \text{ for } \lambda_i \in \text{spec}_L = \text{spec}_{D-A}$$

- spectral density as sum of lorentz distributions

$$\rho(\omega, \gamma) = K \sum_{i=1}^{N-1} \frac{\gamma}{(\omega - \omega_i)^2 + \gamma^2}$$

- K normalization constant defined by

$$\int_0^\infty \rho(\omega, \gamma) d\omega = 1$$

- γ common width chosen as $\overline{\gamma}$, the unique solution of

$$\int_0^\infty [\rho_{\mathcal{E}_N}(\omega, \gamma) - \rho_{\mathcal{F}_N}(\omega, \gamma)]^2 d\omega = 1$$

hamming-ipsen-mikhailov distance

normalized euclidean product metric of H and IM

$$\text{HIM}_\xi(\mathcal{N}_1, \mathcal{N}_2) = \frac{1}{\sqrt{1+\xi}} \sqrt{H^2(\mathcal{N}_1, \mathcal{N}_2) + \xi \cdot \text{IM}^2(\mathcal{N}_1, \mathcal{N}_2)} \text{ for } \xi \in [0, +\infty)$$

$\xi = 1$ and omitted as default

the cartesian $[0, 1] \times [0, 1]$ space with H and IM as axes

h/im space

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$$P(A, \mathcal{E}_4) = (0.33, 0.66), \text{ HIM}(A, \mathcal{E}_4) = 0.52$$

(non-bio) examples (i)

the gulf dataset

- kansas event data system
- political events between pairs of (202) countries
"pessimist comment", "meet", "formal protest",
"military engagement"
- regarding gulf region / arabian peninsula
- 15 apr 79 – 31 mar 99 (240 mo)
- translated into 240 unweighted undirected nets with 202 nodes
- computed all $\frac{240 \times 239}{2}$ him distances

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classic metric multidimensional scaling

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- first gulf war months ● (jul 90 - apr 91) cluster together away from other months
- Special months ● February 1998, iraq disarmament crisis: not formal war, but war-like relationships

classic metric multidimensional scaling

(non-bio) examples (ii)

the international trade dataset

- trade flows 1948–2000, all world
- 13 south american countries

- for each year, build a weighted directed net with 13 nodes
- links are export flows, flow volume as weight

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- raising economy in the 50s/60s
- suffering in the 70s/mid 80s
- growth again in the late 80s/90s

classic metric multidimensional scaling

(bio)-applications

d. melanogaster development dataset (i/ii)

- [kolar *et al*, ann appl stat, 2010] & [arbeitman *et al*, science, 2002]
- 588 developmental genes on 66 time points, expression from microarray
- 4 stages: embryonic (1–30), larval (31–40), pupal (41–58), adult (59–66)
- 66 nets N_i on 588 genes, links are keller gene interactions
- compute $\text{him}(N_i, N_1)$

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- compute $\text{him}(N_i, N_1)$

quantitatively confirming the original qualitative observations

embryonic and adult stages have closer profiles

d. melanogaster development dataset (ii/ii)

developmental stages discrimination

multidimensional scaling of
all mutual him distances

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embryonic 1-30

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adult 59-66

d. melanogaster development dataset (ii/ii)

developmental stages discrimination

multidimensional scaling of
all mutual him distances

embryonic 1-30

larval 31-40

pupal 41-58

adult 59-66

- discrimination via machine learning
- use support vector machine with him kernel
- $k(x, y) = e^{-\gamma \cdot \text{HIM}_{\xi}^2(x, y)}$
- 5-fold cross validation
- embryonic & adult vs larval & pupal: accuracy 0.97
- embryonic vs adult: accuracy 1

meg biomag 2010 competition 1 dataset

original data

- 4 subjects, meg data
- fix a cross at the center of the screen and at regular intervals a cue indicated which direction they had to covertly attend the next 2500ms
- brain activity recorded from 500ms before cue offset to 2500ms after cue offset through 274 sensors at 300Hz
- a total of 128 trials per condition were collected
- 256 total trials per subject.

processed data

- raw signals independently decomposed, multitaper frequency transformation 5-40 hz, 2 hz bin width
- a coherence network built for each trial, rescaled to get eigenvalues in $[-1, 1]$
- network deconvolution procedure as in [feizi *et al*, nat biotech, 2013]
- elastic net linear regression via lasso, mixed l1l2 algorithm
- final dataset: 252 covariance networks on 274 nodes, equally distributed between label "right" and "left"
- classification setup: 100 montecarlo resampling, stratified training (84+84) and test (42+42)

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l-svm	0.72 (0.02)
him ₀ -svm	0.74 (0.03)
him _{+∞} -svm	0.48 (0.05)
him-svm	0.63 (0.04)
rf	0.70 (0.02)

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acks to m cristoforetti (fbk) and t furlanello (ucla)

- tumor-infiltrating T cells are important prognostic indicator
- 84 neuroblastoma patients from OPBG
- cell density of CD3/4/8 assessed in tumor cell Nests and in surrounding fibrovascular Septa
- for INSS stages (1, 2, 4, 4S) and COG-risk groups (low/intermediate and high), a correlation network was generated with Spearman correlation coefficient

t lymphocytes & neuroblastoma

Oncotarget 4:8, e1019881; September 2015; © 2015 Taylor & Francis Group, LLC

ORIGINAL RESEARCH

Tumor-infiltrating T lymphocytes improve clinical outcome of therapy-resistant neuroblastoma

Marco Mina^{1,2}, Renata Boldrin^{1,2}, Arianna Citti², Paolo Romania³, Valerio D'Alicandro², Mareta De Ioris², Aurora Castellano², Cesare Furlanello¹, Franco Locatelli^{1,3}, and Dorianna Fruci^{1,2}

¹Fondazione Bruno Kessler, Povo, Italy; ²Pediatric Hematology/Oncology Department IRCCS Ospedale Pediatrico Bambino Gesù, Rome, Italy; ³University of Pavia, Pavia, Italy

*These authors contributed equally to this work

Keywords: clinical outcome, correlation network analysis, neuroblastoma, prognostic marker, T cells, tumor-infiltrating T lymphocytes

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Oncotarget 6:9, e1019881, September 2015; © 2015 Taylor & Francis Group, LLC

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- for INSS stages (1, 2, 4, 4S) and COG-risk groups (low/intermediate and high), a correlation network was generated with Spearman correlation coefficient

multidimensional scaling of him distances

gradual disruption of the correlation structure associated with a drift towards poor outcome, with largest difference between stages 4 and 4S

hepatocellular carcinoma mirna dataset

- 482 paired (cancerous/non cancerous) samples, 241 patients [budhu *et al*, hepatology, 2008], [volinia *et al.*, gen res, 2010]
- ohio state ccc microRNA array 2.0: 11520 probes, 250 human + 200 mouse miRNA
- preprocessed dataset hcc: 240+240 paired samples, 210 human miRNA (210 ♂ + 30 ♀).
- hcc is partitioned into 4 subsets, sex/disease phenotypes (MT, FT, MnT, FnT).
- 4 Pearson co-expression weighted networks are inferred

multidimensional scaling him distances

- orthogonal separations for the two phenotypes
- different development in male and female: FT closer to MnT rather than to MT and FnT
- largest distance detected between MnT and FnT

stability in network inference

net reliability when gold standard not available

stability in network inference

net reliability when gold standard not available

n

n_1

n_2

n_3

n_4

n_5

stability in the hcc dataset

same algorithm (CLR), different resampling with 95% bootstrap students confidence intervals

stability in the hcc dataset

same algorithm (CLR), different resampling with 95% bootstrap students confidence intervals

stability in the hcc dataset

same resampling (4-fold CV), different algorithms with 95% bootstrap students confidence intervals

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● M much stabler than F ● T stability similar to nT ● F LOO worse than M k10 fold ● aracne best alg for both cohorts

implementations

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ReNette WebServices

This is a web-interface for network analysis. It supports inference methods, quantitative network distance and network stability analysis.

Network Distance

A quantitative analysis of differences between networks. Three methods are available, one based on an edit distance, another based on a spectral distance and a product metric combining contributions from edit and spectral distances.

[View details >](#)

Network Distance Video Tutorial

Network Distance

Network Inference

Network Stability

Network Statistics

My process list

Process stats last 5 min

- Active Processes: 0
- Scheduled Processes: 0
- Registered Processes: 12

If you use ReNette please cite:
Stability Indicators in Network
Reconstruction, M. Filosi, G. Ventrone,
S. Riccardonna, G. Juman, G. Furlanello,
PloS one, 01/2014

nettools@CRAN

<http://renette.fbk.eu>

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nettools: A Network Comparison Framework

A collection of network inference methods for co-expression networks, quantitative network distances and a novel framework for network stability analysis.

Version: 1.0.1
Depends: R (≥ 2.14.1), methods
Imports: parallel, rcosSolve, dplyr, WGCNA, mini, Matrix, minerva, combinator, igraph
Published: 2014-09-12
Author: Michele Filosi [aut, cre], Roberto Ventrone [aut], Samantha Riccardonna [aut], Giuseppe Juman [ctb], Cesare Furlanello [ctb]
Maintainer: Michele Filosi <filosi@fbk.eu>
License: CC BY-NC-SA 4.0
NeedsCompilation: no
Materials: README
CRAN checks: nettools results

Downloads:

Reference manual: [nettools.pdf](#)
Package source: [nettools_1.0.1.tar.gz](#)
Windows binaries: [nettools_1.0.1.zip](#), r-release: [nettools_1.0.1.zip](#), r-oldrel: [nettools_1.0.1.zip](#)

OS X Snow Leopard binaries: r-release: not available, r-oldrel: not available
OS X Mavericks binaries: r-release: not available

OPEN ACCESS Freely available online

Stability Indicators in Network Reconstruction

Michele Filosi^{1,2*}, Roberto Visintainer^{1*}, Samantha Riccadonna³, Giuseppe Jurman^{1*}, Cesare Furlanello¹

1 MBISA/Center for Information and Communication Technology, Fondazione Bruno Kessler, Trento, Italy, **2** CIBIO, University of Trento, Trento, Italy, **3** Department of Computational Biology, Research and Innovation Centre, Fondazione Edmund Mach (FEM), San Michele all'Adige, Italy

RESEARCH ARTICLE

A Null Model for Pearson Coexpression Networks

Andrea Gobbi, Giuseppe Jurman*

Fondazione Bruno Kessler, Trento, Italy

more info on research & publications:

acknowledgments

joint work with

cesare
furlanello

michele
filosi

roberto
visintainer

samantha
riccadonna

MPBA
PREDICTIVE MODELS FOR BIOMEDICINE & ENVIRONMENT

thank you
for the attention!

question time now