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Efficient Markov Chain Monte Carlo Estimation of Exponential-Family Random Graph models

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Introduction

We have developed efficient Markov chain-based algorithm to perform Maximum Likelihood parameter estimation for probability distributions with intractable normalizing constants

ERGMs are exponential family of probability distributions for dependent network data

$$\pi(x,\theta) = \frac{1}{k}\exp\left(\sum_A \theta_A z_A(x)\right)$$

$$k = \sum_x \exp\left(\sum_A \theta_A z_A(x)\right)$$

$z_A(x)$ are networks statistics (e.g. number of ties, triangles, stars ..)

Robins G, Snijders T, Wang P, Handcock M, & Pattison P (2007) Recent developments in exponential random graph (p*) models for social networks. *Social Networks* 29(2):192-215.

Introduction

We want to find MLE of the model parameters θ

$$E_{\pi(\theta)}\left(z_A(x)\right) = z_A(x_{obs})$$

$E_{\pi(\theta)}(z_A(x)) = \sum_x z_A(x)\pi(x,\theta)$ are expected statistics

Metropolis-Hastings algorithm may be used to compute $E_{\pi(\theta)}(z_A(x))$ and to generate **simulated data** $x(\theta)$

And we want to solve inverse problem: find $\theta(x_{obs})$

Lehmann, E.L., Casella, G. Theory of point estimation (2006)

Existing estimation approaches

1) Bayesian
2) Geyer-Thompson MCMCMLE
3) Method of Moments
   (Stochastic approximation)

- Iteratively update θ_A
- At many different θ_A values perform MCMC simulations to draw simulated data $x(\theta_A)$

⬇

MLE is computationally expensive

We can find MCMCMLE without MCMC simulation

Metropolis-Hastings algorithm

Given the state *x* the state *x'* is proposed with probability $q(x \rightarrow x')$

Acceptance probability $\alpha(x \rightarrow x', \theta_A) = \min\left\{1, \frac{q(x' \rightarrow x)\pi(x', \theta_A)}{q(x \rightarrow x')\pi(x, \theta_A)}\right\}$

Transition probability $P(x \rightarrow x', \theta_A) = q(x \rightarrow x')\alpha(x \rightarrow x', \theta_A)$

The algorithm generates a Markov chain x_t that converges to $\pi(x, \theta)$
if the algorithm step *t* is larger then the burn-in time

Metropolis N, Rosenbluth AW, Rosenbluth MN, Teller AH, & Teller E Equation of state calculations by fast computing machines. *The journal of chemical physics* 21, 1087-1092 (1953)
Hastings WK, Monte Carlo sampling methods using Markov chains and their applications. *Biometrika* 57, 97-109 (1970)

New approaches for MLE

I can show that for simulated networks drawn from $\pi(x,\theta)$ MLE may be found from Equilibrium Expectation (EE):

$$\mathrm{E}_{\pi(\theta)}\left(dz_A(x,\theta)\right) = 0$$

$$dz_A(x,\theta) = \sum_{x'} P(x \to x',\theta)\,(z_A(x') - z_A(x))$$

The left part may be computed by Monte Carlo integrations, without time consuming MCMC simulation

New approaches for MLE

If observed network x_{obs} is large then one sample is enough

$$\sum_{x'} P(x_{obs} \to x', \hat{\theta})\left(z_A(x') - z_A(x_{obs})\right) = 0$$

But may be used also for small networks

If we have data samples iid from $\pi(x, \theta)$: $x_{S_1}, x_{S_2}, .., x_{S_n}$

$$E_{\pi(\theta)}(dz_A(x,\theta)) = \frac{1}{n}\sum_i dz_A(x_{S_i}, \theta)$$

Very fast MLE !

MLE for empirical data

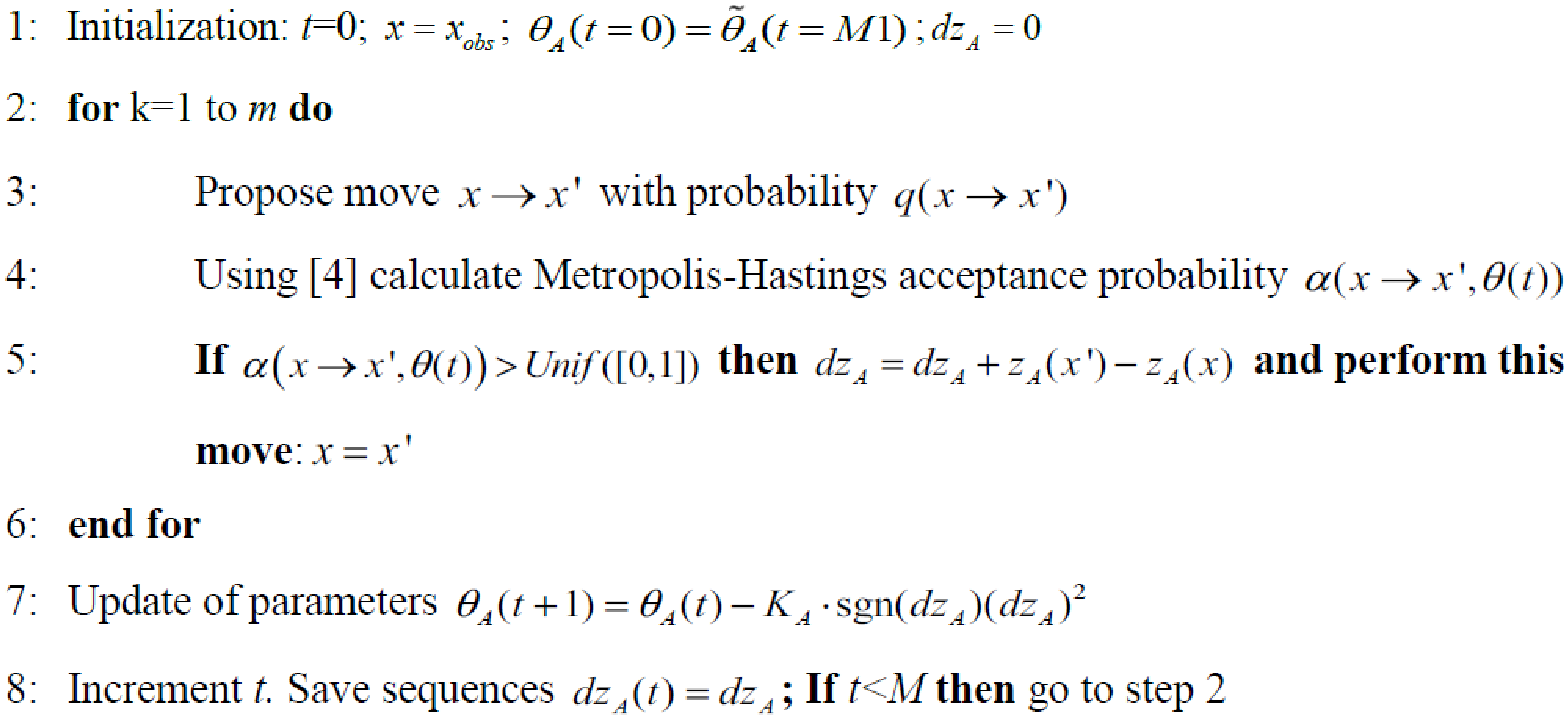
How to apply this methodology for empirical data x_{obs} ?
We can draw simulated data x so that $z_A(x) = z_A(x_{obs})$

$$\left.\begin{array}{l} \sum_{x'} P(x \to x', \theta_A)\left(z_A(x') - z_A(x)\right) = 0 \\ z_A(x) = z_A(x_{obs}) \end{array}\right\} \Rightarrow \quad E_\theta\left(z_A(x)\right) = z_A(x_{obs})$$

We have developed MCMC algorithm to solve this system of equation

EE algorithm for empirical data

MCMC to constrain the values of all the statistics



```
1: Initialization: $t$=0; $x = x_{obs}$; $\theta_A(t=0) = \tilde{\theta}_A(t=M1)$; $dz_A = 0$
2: for k=1 to $m$ do
3:         Propose move $x \to x'$ with probability $q(x \to x')$
4:         Using [4] calculate Metropolis-Hastings acceptance probability $\alpha(x \to x', \theta(t))$
5:         If $\alpha(x \to x', \theta(t)) > Unif([0,1])$ then $dz_A = dz_A + z_A(x') - z_A(x)$ and perform this
           move: $x = x'$
6: end for
7: Update of parameters $\theta_A(t+1) = \theta_A(t) - K_A \cdot \mathrm{sgn}(dz_A)(dz_A)^2$
8: Increment $t$. Save sequences $dz_A(t) = dz_A$; If $t$<$M$ then go to step 2
```

EE algorithm for empirical data

MoM (Snijders 2002) and MCMCMLE (Geyer CJ & Thompson 1992) require many converged outputs of Metropolis-Hastings algorithm

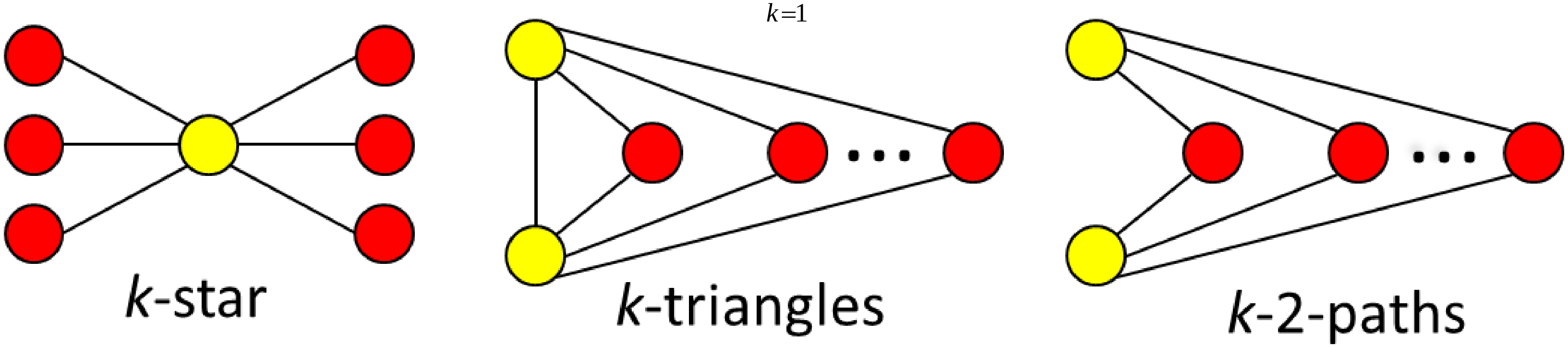
EE algorithm does not need such outputs. Instead it generates one converged output

EE algorithm is similar to Metropolis-Hastings algorithm, but allows Monte Carlo simulation to be performed while constraining the values of statistics $z_A(x)$ and in such a way that the EE condition is satisfied

Tests and applications

Networks statistics typical for social networks

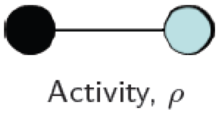
$$z_{AT}(x) = 3T_1(x) + \sum_{k=1}^{N-3} (-1)^k T_{k+1}(x) / \lambda^k$$



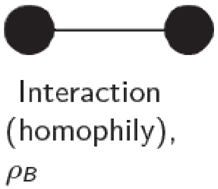
$$z_{AS}(x) = \sum_{k=2}^{N-1} (-1)^k S_k(x) / \lambda^{k-2}$$

$$z_{A2P}(x) = U_1(x) - \frac{2U_2(x)}{\lambda} + \sum_{k=3}^{N-2} (-1)^{k-1} U_k(x) / \lambda^{k-1}$$

Node attributes



$$z_\rho = \sum_{i,j} a_i x_{ij}$$



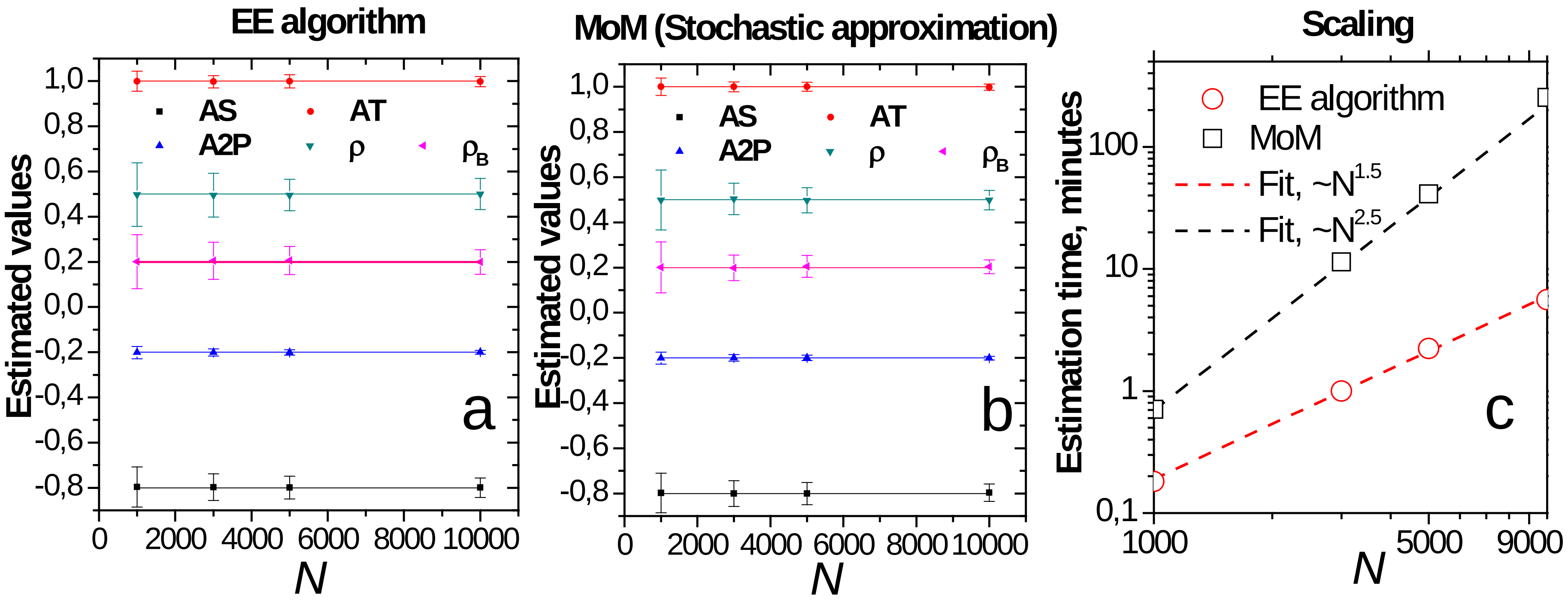
$$z_{\rho_B} = \sum_{i,j} x_{ij} a_i a_j$$

$$z_{Match} = \sum_{i,j} x_{ij} \delta_{a_i, a_j}$$

Snijders T.A., Pattison P.E., Robins G.L., Handcock M.S., New specifications for exponential random graph models, *Sociological Methodology* **36**(1), 99-153 (2006)

Tests and applications

We use EE algorithm to estimate parameters of ERGMs



With EE algorithm the estimation time grows with number of nodes *N* almost linear

Snijders, Tom AB. Markov chain Monte Carlo estimation of exponential random graph models, Journal of Social Structure, 1-40 (2002)

Tests and applications. Biological networks

Arabidopsis Interactome Mapping Consortium. Science, 333(6042):601–607, 2011.

C. von Mering, et al. Comparative assessment of large-scale data sets of protein–protein interactions. Nature, 417(6887):399–403, 2002

T. Rolland et al. A proteome-scale map of the human interactome network. Cell, 159(5):1212–1226, 2014.

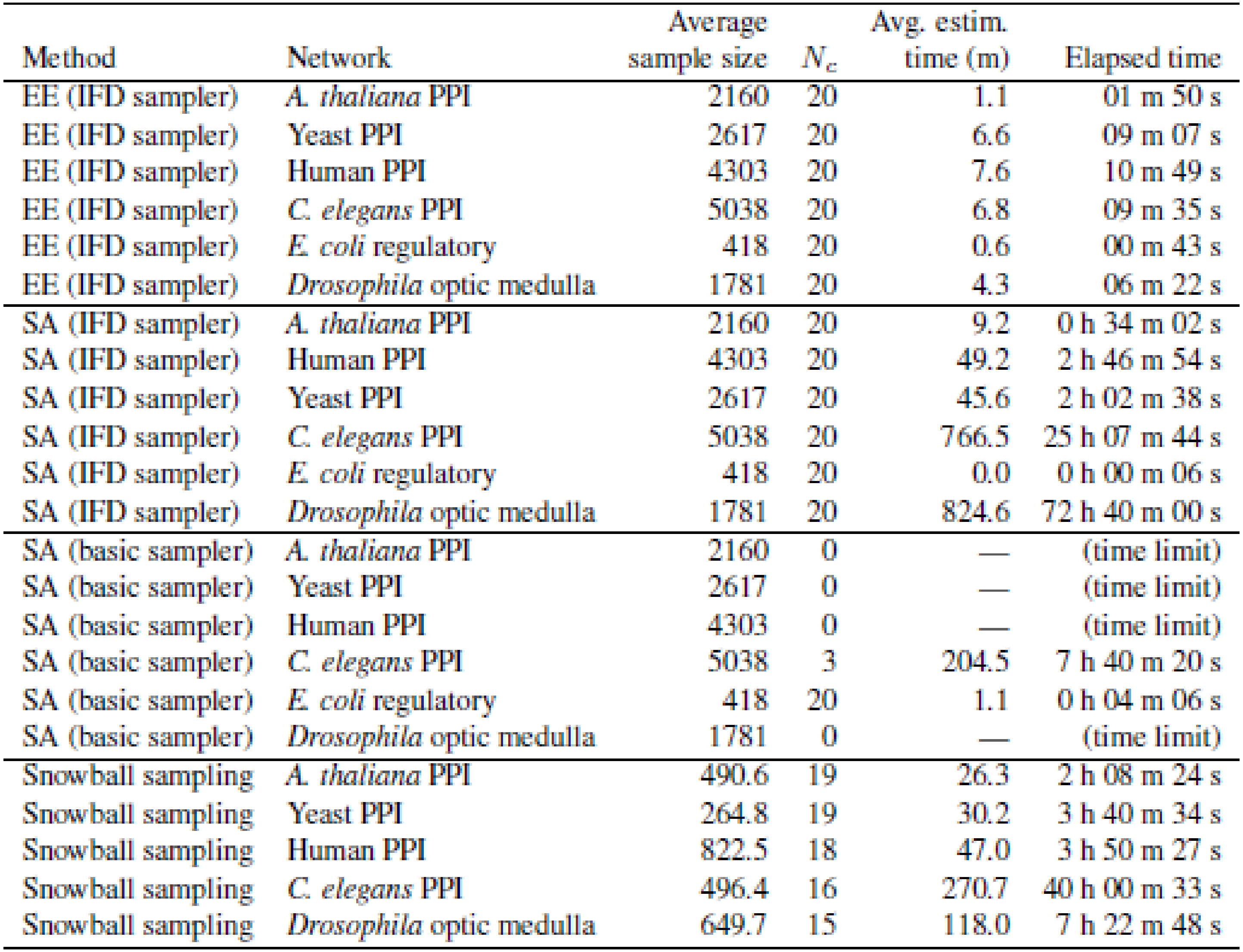
X.-T. Huang, et al An integrative C. elegans protein–protein interaction network with reliability assessment based on a probabilistic graphical model. Molecular BioSystems, 12(1):85–92, 2016.

S.-y. Takemura, et al. A visual motion detection circuit suggested by Drosophila connectomics. Nature, 500(7461):175–181, 2013

S. S. Shen-Orr et al, Network motifs in the transcriptional regulation network of Escherichia coli. Nature Genetics, 31(1):64–68, 2002.

Stivala, A. D., Koskinen, J. H., Rolls, D. A., Wang, P., & Robins, G. L. (2016). Snowball sampling for estimating exponential random graph models for large networks. *Social Networks*, *47*, 167-188.

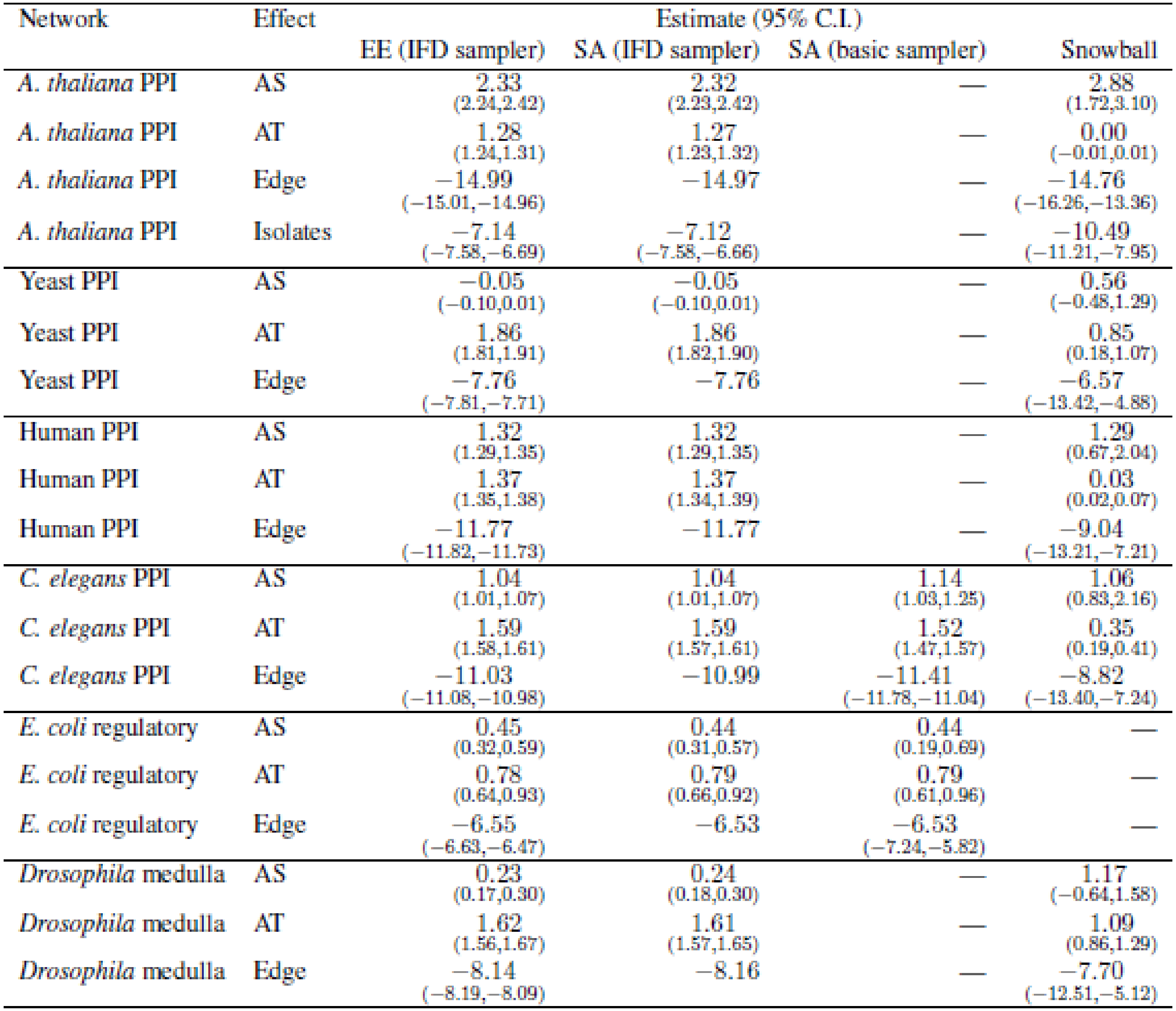
Tests and applications. Biological networks



Method	Network	Average sample size	N_c	Avg. estim. time (m)	Elapsed time
EE (IFD sampler)	*A. thaliana* PPI	2160	20	1.1	01 m 50 s
EE (IFD sampler)	Yeast PPI	2617	20	6.6	09 m 07 s
EE (IFD sampler)	Human PPI	4303	20	7.6	10 m 49 s
EE (IFD sampler)	*C. elegans* PPI	5038	20	6.8	09 m 35 s
EE (IFD sampler)	*E. coli* regulatory	418	20	0.6	00 m 43 s
EE (IFD sampler)	*Drosophila* optic medulla	1781	20	4.3	06 m 22 s
SA (IFD sampler)	*A. thaliana* PPI	2160	20	9.2	0 h 34 m 02 s
SA (IFD sampler)	Human PPI	4303	20	49.2	2 h 46 m 54 s
SA (IFD sampler)	Yeast PPI	2617	20	45.6	2 h 02 m 38 s
SA (IFD sampler)	*C. elegans* PPI	5038	20	766.5	25 h 07 m 44 s
SA (IFD sampler)	*E. coli* regulatory	418	20	0.0	0 h 00 m 06 s
SA (IFD sampler)	*Drosophila* optic medulla	1781	20	824.6	72 h 40 m 00 s
SA (basic sampler)	*A. thaliana* PPI	2160	0	—	(time limit)
SA (basic sampler)	Yeast PPI	2617	0	—	(time limit)
SA (basic sampler)	Human PPI	4303	0	—	(time limit)
SA (basic sampler)	*C. elegans* PPI	5038	3	204.5	7 h 40 m 20 s
SA (basic sampler)	*E. coli* regulatory	418	20	1.1	0 h 04 m 06 s
SA (basic sampler)	*Drosophila* optic medulla	1781	0	—	(time limit)
Snowball sampling	*A. thaliana* PPI	490.6	19	26.3	2 h 08 m 24 s
Snowball sampling	Yeast PPI	264.8	19	30.2	3 h 40 m 34 s
Snowball sampling	Human PPI	822.5	18	47.0	3 h 50 m 27 s
Snowball sampling	*C. elegans* PPI	496.4	16	270.7	40 h 00 m 33 s
Snowball sampling	*Drosophila* optic medulla	649.7	15	118.0	7 h 22 m 48 s

IFD sampler: Byshkin M, Stivala A, Mira A, Krause R, Robins G, Lomi A, Auxiliary Parameter MCMC for Exponential Random Graph Models J. Stat. Phys. 165: 740-754 (2016)

Tests and applications. Biological networks



Network	Effect	Estimate (95% C.I.)			
		EE (IFD sampler)	SA (IFD sampler)	SA (basic sampler)	Snowball
A. thaliana PPI	AS	2.33 (2.24,2.42)	2.32 (2.23,2.42)	—	2.88 (1.72,3.10)
A. thaliana PPI	AT	1.28 (1.24,1.31)	1.27 (1.23,1.32)	—	0.00 (−0.01,0.01)
A. thaliana PPI	Edge	−14.99 (−15.01,−14.96)	−14.97	—	−14.76 (−16.26,−13.36)
A. thaliana PPI	Isolates	−7.14 (−7.58,−6.69)	−7.12 (−7.58,−6.66)	—	−10.49 (−11.21,−7.95)
Yeast PPI	AS	−0.05 (−0.10,0.01)	−0.05 (−0.10,0.01)	—	0.56 (−0.48,1.29)
Yeast PPI	AT	1.86 (1.81,1.91)	1.86 (1.82,1.90)	—	0.85 (0.18,1.07)
Yeast PPI	Edge	−7.76 (−7.81,−7.71)	−7.76	—	−6.57 (−13.42,−4.88)
Human PPI	AS	1.32 (1.29,1.35)	1.32 (1.29,1.35)	—	1.29 (0.67,2.04)
Human PPI	AT	1.37 (1.35,1.38)	1.37 (1.34,1.39)	—	0.03 (0.02,0.07)
Human PPI	Edge	−11.77 (−11.82,−11.73)	−11.77	—	−9.04 (−13.21,−7.21)
C. elegans PPI	AS	1.04 (1.01,1.07)	1.04 (1.01,1.07)	1.14 (1.03,1.25)	1.06 (0.83,2.16)
C. elegans PPI	AT	1.59 (1.58,1.61)	1.59 (1.57,1.61)	1.52 (1.47,1.57)	0.35 (0.19,0.41)
C. elegans PPI	Edge	−11.03 (−11.08,−10.98)	−10.99	−11.41 (−11.78,−11.04)	−8.82 (−13.40,−7.24)
E. coli regulatory	AS	0.45 (0.32,0.59)	0.44 (0.31,0.57)	0.44 (0.19,0.69)	—
E. coli regulatory	AT	0.78 (0.64,0.93)	0.79 (0.66,0.92)	0.79 (0.61,0.96)	—
E. coli regulatory	Edge	−6.55 (−6.63,−6.47)	−6.53	−6.53 (−7.24,−5.82)	—
Drosophila medulla	AS	0.23 (0.17,0.30)	0.24 (0.18,0.30)	—	1.17 (−0.64,1.58)
Drosophila medulla	AT	1.62 (1.56,1.67)	1.61 (1.57,1.65)	—	1.09 (0.86,1.29)
Drosophila medulla	Edge	−8.14 (−8.19,−8.09)	−8.16	—	−7.70 (−12.51,−5.12)

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Tests and applications. Large networks

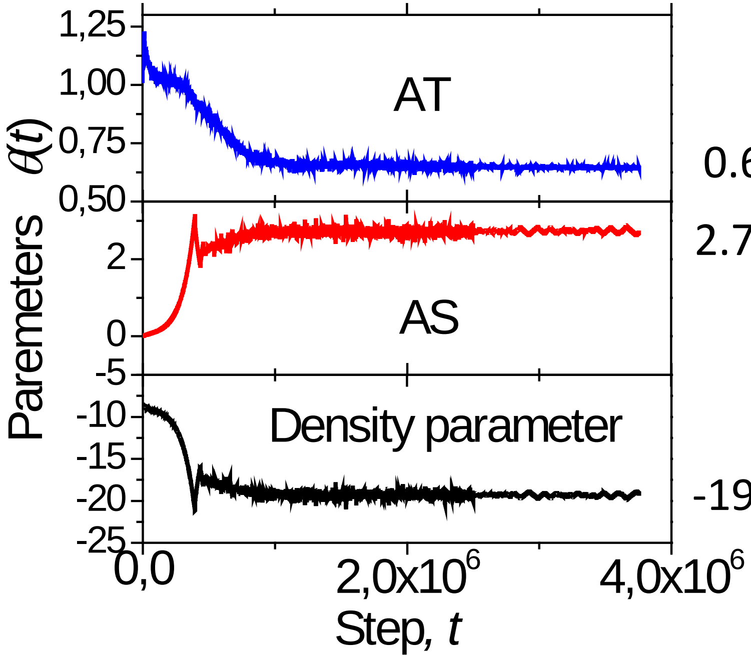
With good scaling we can obtain MLE for large dependent data

Livemocha was a social network for language learning

104103 nodes and 2193083 ties

Output of EE algorithm with IFD sampler (in 12 hours)

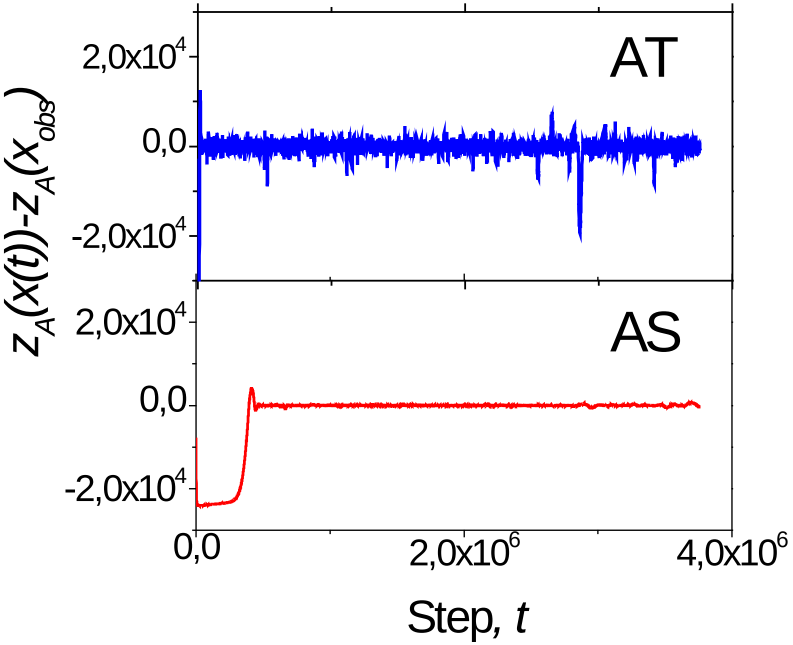
Statistics is constrained to the observed values



0.6242

2.7917

-19.531



Zafarani and H. Liu. Social computing data repository at ASU, 2009

Livmocha network datasets, konect.uni-koblenz.de

Tests and applications. Large networks

Livemocha

Networks with 104103 nodes and 2193083 ties

Both convergence tests are passed

Our convergence test

$$\left.\begin{aligned} &\theta_A(t)\ \text{converge} \\ &\left|\frac{\overline{z_A(x)-z_A(x_{obs})}}{SD(z_A(x)-z_A(x_{obs}))}\right|<0.1 \end{aligned}\right\}$$

⬇

$$\left.\begin{aligned} &\sum_{x'} P(x\to x',\theta_A)\big(z_A(x')-z_A(x)\big)=0 \\ &z_A(x)=z_A(x_{obs}) \end{aligned}\right\} \Rightarrow \quad E_{\pi(\theta)}\big(z_A(x)\big)=z_A(x_{obs})$$

t-ratio convergence test

$$t_A=\frac{E_{\pi(\theta)}\big(z_A(x)\big)-z_A(x_{obs})}{SD_{\pi(\theta)}\big(z_A(x)\big)}$$

$$|t_A|<0.3$$

⬇

Snijders T, Journal of Social Structure (2002): 1-40

More presentations

- Complex Networks, March 20-24, 2017, Dubrovnik, Croatia
- Sunbelt INSNA Conference, May 30-June 4, 2017, Beijing, China
- Cambridge Networks Day, 13th June 2017, Cambridge, UK
- PASC17, June 26 - 28, 2017, Lugano, Switzerland
- International Conference on Monte Carlo Methods and Applications, July 3-7, 2017, Montreal, Canada
- International Conference on Computational Social Science, July 10-13, 2017, Cologne, Germany
- Third European Conference on Social Networks, September 26 to 29, 2017, Mainz, Germany
- 2nd Australian Social Network Analysis Conference, 28-29 November 2017, Sydney, Australia

The code will be available free of charge

www.sonarcenter.eco.usi.ch

Hidden bonus slides

New approaches for MLE

The expected network statistics:

$$E_{\pi(\theta)}(z_A(x)) = \sum_x z_A(x)\pi(x,\theta)$$

The expectation must be taken with respect to $\pi(x,\theta)$

If on step *t* the chain is in state *x* what is the expected network statistics on the next step x′?

The expected network statistics:

$$\sum_{x'} z_A(x')P(x \to x',\theta)$$

The expectation must be taken with respect to $P(x \to x',\theta)$