

**Belief Propagation** 



Conclusion

### Bayesian inference of cascades on networks

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NIPS Montreal, Dec 2015 A. Ingrosso, J. Bindi, L. Dall'Asta

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Belief Propagation

 $P(\mathbf{x}^T | \lambda, \mu)$ 

Conclusion

The patient zero or index case problem

### The patient zero or index case problem

#### INPUT





Belief Propagation



Conclusion

The patient zero or index case problem

### The *patient zero* or *index case* problem



#### INPUT

- A contact network in a community:
  - Hospital wards [Vanhems'13]
  - Livestock Surveillance [Bajardi'12]
  - Many others, e.g.: Sexual contacts [Rocha'10], Proximity in a closed environment [Isella'10]

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- An epidemic *snapshot* at time t = T
  - $\circ \ {\sf Susceptible}$
  - Infected
  - Recovered



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### The patient zero or index case problem



#### INPUT

- A contact network in a community:
  - Hospital wards [Vanhems'13]
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  - Many others, e.g.: Sexual contacts [Rocha'10], Proximity in a closed environment [Isella'10]
- An epidemic *snapshot* at time t = T
   Susceptible
  - Infected
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### OUTPUT

• Find the *source* node at time t = 0

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## **Related Problems**

### INPUTS

- Various types of observations: time and space scattered and noisy
- Unknown epidemic "age" *T*
- Time-evolving networks
- Multiple sources

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# **Related Problems**

### INPUTS

- Various types of observations: time and space scattered and noisy
- Unknown epidemic "age" *T*
- Time-evolving networks
- Multiple sources

### OUTPUTS

- Identifying contagion paths and undiscovered positives
- Predicting of future development of an outbreak
- Reconstructing the contact network (from the observation of multiple cascades)







Conclusion

The SIR model on networks

# The (discrete) SIR process on a network

Per-vertex variables  $x_i \in \{\mathbb{S}, \mathbf{I}, \mathbf{R}\}$ . At each *t*, each **infected** node  $x_i^t \in \mathbf{I}$ 

- attempts **contagion** to susceptible neighbors in  $x_i^t \in \mathbb{S}$  with probability  $\lambda$ . If successful,  $x_i^{t+1} = \mathbf{I}$
- **attempts recovery** with probability  $\mu$ . If successful,  $x_i^{t+1} = \mathbf{R}$







Conclusion

The SIR model on networks

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SIR Markov Chain  

$$P\left(\mathbf{x}^{t+1}|\mathbf{x}^{t}\right) = \prod_{i} P\left(x_{i}^{t+1}|\mathbf{x}^{t}\right),$$

$$P(x_{i}^{t+1} = \mathbb{S}|\mathbf{x}^{t}) = \mathbb{I}[x_{i}^{t} = \mathbb{S}] \prod_{j \in \partial i} (1 - \lambda \mathbb{I}[x_{j}^{t} = \mathbf{I}])$$

$$P(x_{i}^{t+1} = \mathbf{I}|\mathbf{x}^{t}) = \mathbb{I}[x_{i}^{t} = \mathbf{I}](1 - \mu) + \mathbb{I}[x_{i}^{t} = \mathbb{S}](1 - \prod_{j \in \partial i} (1 - \lambda \mathbb{I}[x_{j}^{t} = \mathbf{I}]))$$

$$P(x_{i}^{t+1} = \mathbf{R}|\mathbf{x}^{t}) = \mathbb{I}[x_{i}^{t} = \mathbf{I}]\mu + \mathbb{I}[x_{i}^{t} = \mathbf{R}]$$

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The problem and classical approaches				

### Approaches

■ Topological centrality measures [Shah'10], [Comin'11], [Zhu'12]



Belief Propagation

 $P\left(\mathbf{x}^{T}|\boldsymbol{\lambda},\boldsymbol{\mu}\right)$ 

Conclusion

The problem and classical approaches

# Approaches

- Topological centrality measures [Shah'10], [Comin'11], [Zhu'12]
- **Bayesian** inference: compute  $P(\mathbf{x}^0 | \mathbf{x}^T)$ 
  - "Brute-Force" Monte Carlo (variant: use soft compatibility [Antulov-Fantulin'14])
  - Naive Bayes
  - Belief Propagation

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P(x<sup>0</sup>|x<sup>T</sup>) ○●○○ ○○○ Belief Propagation

 $P\left(\mathbf{x}^{T}|\boldsymbol{\lambda},\boldsymbol{\mu}\right)$ 

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The problem and classical approaches

# Naive Bayes (1/3)

- Assume the following naive MF structure for the distribution  $P\left(\mathbf{x}^{T}|\mathbf{x}^{0}\right) \simeq \prod_{i} P\left(x_{i}^{T}|\mathbf{x}^{0}\right)$
- Marginals P (x<sub>i</sub><sup>T</sup> | x<sup>0</sup>) can be computed either with MC or with Dynamical Message-Passing [Lokhov, Mézard & al.'14]

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- Then maximize over  $\mathbf{x}^0$  the likelihood  $P(\mathscr{O}|\mathbf{x}^0) \simeq \prod_i P(\mathbf{x}_i^T = \mathscr{O}_i | \mathbf{x}^0)$

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- Note that Naive MF can easily be replaced by e.g.:
  - $P\left(\mathbf{x}^{T}|\mathbf{x}^{0}\right) \simeq \prod_{\langle ij \rangle} \frac{P\left(\mathbf{x}_{i}^{T}, \mathbf{x}_{j}^{T}|\mathbf{x}^{0}\right)}{P\left(\mathbf{x}_{i}^{T}|\mathbf{x}^{0}\right)P\left(\mathbf{x}_{j}^{T}|\mathbf{x}^{0}\right)} \prod_{i} P\left(\mathbf{x}_{i}^{T}|\mathbf{x}^{0}\right) \text{ [Lokhov, Mézard & al.'14, maybe]}$

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Naive Bayes (2/3)



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# Naive Bayes (2/3)



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# Naive Bayes (2/3)



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 $P\left(\mathbf{x}^{T}|\boldsymbol{\lambda},\boldsymbol{\mu}\right)$ 

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Naive Bayes (3/3)



• Sites  $x_i^T$  and  $x_k^T$  interact e.g. through  $x_i^{T-1}$ 

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Naive Bayes (3/3)



- Sites  $x_i^T$  and  $x_k^T$  interact e.g. through  $x_i^{T-1}$
- Interactions between surface (t = T) variables are long-range



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Naive Bayes (3/3)



- Sites  $x_i^T$  and  $x_k^T$  interact e.g. through  $x_i^{T-1}$
- Interactions between surface (t = T) variables are long-range
- The real problem is not to compute  $P\left(x_i^T, x_j^T | \mathbf{x}^0\right)$  accurately but to give a "functional" parametrization of  $P\left(\mathbf{x}^T | \mathbf{x}^0\right)$

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Naive Bayes (3/3)



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- [Note: to recover the MRF independence property one should fix full columns/trajectories x<sub>i</sub><sup>0:T</sup>]

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Conclusion

A static representation of SIR

### Parametrization of trajectories

• We will assume for simplicity  $\mu = 1$ . The case  $\mu < 1$  is similar.

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### Parametrization of trajectories

- We will assume for simplicity  $\mu = 1$ . The case  $\mu < 1$  is similar.
- Single site trajectories, e.g. **x**<sub>i</sub> = SSS**IRRRRR** can be parametrized by a single *infection time t*<sub>i</sub>

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**Belief** Propagation

 $P(\mathbf{x}^T | \lambda, \mu)$ 

- We can divide the process in two parts:
  - First, stochastic "delays" s<sub>ij</sub> ∈ {0,∞} for all (ij) ∈ E are extracted independently with probabilities P (s<sub>ij</sub> = 0) = λ

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  - **1** Afterwards, all  $t_i \neq 0$  can be computed **deterministically** with the following self-consisting equations

$$t_i = 1 + \min_{j \in \partial i} \left\{ t_j + s_{ji} \right\}$$

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• Key: stochastic parameters are *independent* 

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Belief Propagation



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### A factorized distribution

$$\mathscr{P}(\mathbf{t}|\mathbf{x}^{0}) = \sum_{\mathbf{s}} \mathscr{P}(\mathbf{t}|\mathbf{s}, \mathbf{x}^{0}) \mathscr{P}(\mathbf{s})$$

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## A factorized distribution

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#### Define

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## A factorized distribution

$$\mathscr{P}(\mathbf{t}|\mathbf{x}^{0}) = \sum_{\mathbf{s}} \mathscr{P}(\mathbf{t}|\mathbf{s}, \mathbf{x}^{0}) \mathscr{P}(\mathbf{s})$$

#### Define

$$\mathscr{Q} = \frac{1}{Z} \prod_{i} \phi_{i} \prod_{i,j} \boldsymbol{\omega}_{ij}$$

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## A factorized distribution

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#### Define

$$\mathscr{Q} = \frac{1}{Z} \prod_{i} \phi_{i} \prod_{i,j} \boldsymbol{\omega}_{ij}$$

Then 
$$\mathscr{P}(\mathbf{t}|\mathbf{x}^{0}) = \sum_{s} \mathscr{Q}(\mathbf{t}, \mathbf{s}, \mathbf{x}^{0})$$

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# Adding priors

•  $\mathbf{x}^T$  depends **deterministically** on t:  $P(\mathbf{x}^T | \mathbf{t}) = \prod_i \xi_i(t_i, x_i^T)$  where  $\xi_i(t_i, x_i^T)$  is the indicator function of

$$\left(x_{i}^{T} = \mathbb{S}, t_{i} > T\right) \lor \left(x_{i}^{T} = \mathbf{I}, t_{i} = T\right) \lor \left(x_{i}^{T} = \mathbf{R}, t_{i} < T\right)$$

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•  $\mathbf{x}^{0}$  have a prior concentrated on single-seed initial conditions:  $P(\mathbf{x}^{0}) = \prod_{i} \gamma_{i} (x_{i}^{0})$  with  $\gamma_{i} (x_{i}^{0} = \mathbf{I})$  very small.

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- $\mathbf{x}^{0}$  have a prior concentrated on single-seed initial conditions:  $P(\mathbf{x}^{0}) = \prod_{i} \gamma_{i} (x_{i}^{0})$  with  $\gamma_{i} (x_{i}^{0} = \mathbf{I})$  very small.
- Finally, we can write the **posterior** distribution  $P(\mathbf{x}^0|\mathbf{x}^T) \propto \sum_{\mathbf{t}} P(\mathbf{x}^T|\mathbf{t}) P(\mathbf{t}|\mathbf{x}^0) P(\mathbf{x}^0)$  as

$$P\left(\mathbf{x}^{0}|\mathbf{x}^{T}\right) \propto \sum_{\mathbf{t}} \sum_{\mathbf{s}} \prod_{ij} \phi_{ij} \prod_{i} \phi_{i} \xi_{i} \gamma_{i}$$
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Belief Propagation



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## **Belief Propagation**

$$P\left(\mathbf{x}^{0}|\mathbf{x}^{T}\right) \propto \sum_{\mathbf{t}} \sum_{\mathbf{s}} \left[\prod_{ij} \phi_{ij} \prod_{i} \phi_{i} \xi_{i} \gamma_{i}\right] = \sum_{\mathbf{t}} \sum_{\mathbf{s}} Q\left(\mathbf{x}^{0}, \mathbf{t}, \mathbf{s}\right)$$

Single-instance RS cavity equations / Belief Propagation

- Fixed-point equation  $\mathbf{m} = F_{BP}(\mathbf{m})$  for a vector  $\mathbf{m}$  (called *cavity* marginals or messages) that is solved by iteration.
  - On a fixed point (approximate) marginals  $P(t_i | \mathbf{x}^T)$  or  $P(x_i^0 | \mathbf{x}^T)$  can be computed.
  - Fast: each iteration is often linear in the number of edges, needed number of iterations is usually logarithmic
  - Exact if the *factor graph* is acyclic



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### Results on random graphs

N 
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 1000,  $k$   $=$  4,  $\lambda$   $=$  0.5,  $\mu$   $=$  0.5,  $\gamma$   $=$  10<sup>-6</sup>



**unknown**  $T - t_0 = 10$ , 60% observed nodes

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### Results on random graphs RRG $N = 1000, k = 4, \mu = 0.5, T - t_0 = 10$ and preferential attachment $\langle k \rangle = 4, N = 1000, T - t_0 = 5$



- Belief Propagation
- Dynamic message-passing [Lokhov, Mézard, Ohta & Zdeborová'14]
- Jordan centrality [Zhu & Ying'12]

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### Time-evolving networks

• Temporal networks can be analyzed by using a modified  $\omega_{ii}$ 



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Conclusion

## Inference of parameters

■ The likelihood of  $\lambda, \mu$  can be computed as:  $P(\mathbf{x}^T | \lambda, \mu) = \sum_{t, g, x^0} P(\mathbf{x}^T | \mathbf{t}, \mathbf{g}) P(\mathbf{t}, \mathbf{g} | \mathbf{x}^0, \lambda, \mu) P(\mathbf{x}^0)$ 

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Conclusion

## Inference of parameters

■ The likelihood of  $\lambda, \mu$  can be computed as:  $P(\mathbf{x}^T | \lambda, \mu) = \sum_{t, g, \mathbf{x}^0} P(\mathbf{x}^T | \mathbf{t}, \mathbf{g}) P(\mathbf{t}, \mathbf{g} | \mathbf{x}^0, \lambda, \mu) P(\mathbf{x}^0) = Z$ 

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Conclusion

## Inference of parameters

■ The likelihood of  $\lambda, \mu$  can be computed as:  $P(\mathbf{x}^T | \lambda, \mu) = \sum_{t, \mathbf{g}, \mathbf{x}^0} P(\mathbf{x}^T | \mathbf{t}, \mathbf{g}) P(\mathbf{t}, \mathbf{g} | \mathbf{x}^0, \lambda, \mu) P(\mathbf{x}^0) = Z \simeq Z_{Bethe}$ 







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Conclusion

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RRG k = 4, N = 1000

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Conclusion

### Interleaved BP+GA

• We need to maximize the log-likelihood  $\mathscr{L} = \log Z \simeq -f_{Bethe}$  with respect to  $\lambda$  (and/or  $\mu$ ), but

$$\frac{\partial}{\partial \lambda} \left[ f(\mathbf{m}, \lambda) \right] = \nabla_{\mathbf{m}} f \cdot \frac{\partial \mathbf{m}}{\partial \lambda} + \frac{\partial f}{\partial \lambda}$$

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because  $\nabla_{\mathbf{m}} f \equiv 0$  on a FP of BP, as the BP solution is a variational critical point of f.

• Now  $\frac{\partial f}{\partial \lambda}(\mathbf{m}, \lambda) = -\frac{1}{Z} \frac{\partial}{\partial \lambda} \left\{ \sum_{\mathbf{t}, \mathbf{s}} e^{\sum_i \log \psi_i + \sum_{\langle ij \rangle} \log \phi_{ij}} \right\} = -\sum_{\mathbf{t}, \mathbf{s}} \sum_{\langle ij \rangle} \left\{ \frac{\partial}{\partial \lambda} \log \phi_{ij} \right\} \frac{1}{Z} e^{\sum_i \log \psi_i + \sum_{\langle ij \rangle} \log \phi_{ij}} = -\sum_{\langle ij \rangle} \left\langle \frac{\partial}{\partial \lambda} \log \phi_{ij} \right\rangle$ , i.e. the computation of an observable







Conclusion

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- Gradient updates can be interleaved with BP updates to recover the parameters in one single convergence
- Same fixed points as EM but faster

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Conclusion

# Inference of network topology

The same approach can be used to infer single-link parameters from multiple cascades:

$$rac{\partial \log \left( \prod_{\mu=1}^M Z^\mu 
ight)}{\partial \lambda_{ij}} = -\sum_{\mu=1}^M rac{\partial f^\mu}{\partial \lambda_{ij}} = \sum_{\mu=1}^M \left\langle rac{\partial}{\partial \lambda_{ij}} \log \phi_{ij} 
ight
angle_\mu$$

• The factor graph consists in *M* independent (fully-connected  $N \times N$ ) networks that share the matrix  $\lambda$ 

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Conclusion

## Inference of network topology

Karate club network ( $N = 34, \lambda = 0.3, \mu = 0.4, T = 5$ )

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Conclusion

### Inference of network topology

Karate club network ( $N = 34, \lambda = 0.3, \mu = 0.4, T = 5$ )



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Conclusions

# Conclusions

- The Bethe parametrization of the probability space of dynamical trajectories gives great **flexibility!** 
  - Gives a practical solution to the patient-zero problem on real and synthetic networks (exact on acyclic graphs) with many types of observations (incomplete, noisy, etc)
  - Allows to tackle the problem of inferring edges (*ij*) in the supporting network having no direct access to co-infection events x<sub>i</sub><sup>t-1</sup> = I, x<sub>i</sub><sup>t-1</sup> = S and x<sub>i</sub><sup>t</sup> = I.
  - More on: PRL 112(11) 118701 (2014), JSTAT (10), P10016 (2014)

Thank you!

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