# Sparse random graphs with exchangeable point processes

### François Caron

Department of Statistics, Oxford

Research seminar in Statistics and Mathematics Vienna University of Economics and Business May 8, 2015

Joint work with Emily Fox (U. Washington)



F. Caron 1/57

Exchangeable matrices and their limitations

Statistical network models using exchangeable random measures

Exchangeability and sparsity properties

Special case: Generalized gamma process

Posterior characterization & Inference

Experimental results

F. Caron 2 / 57

#### Outline

#### Introduction

Exchangeable matrices and their limitations

Statistical network models using exchangeable random measures

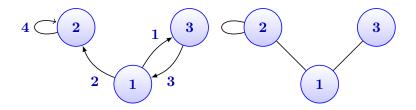
Exchangeability and sparsity properties

Special case: Generalized gamma process

Posterior characterization & Inference

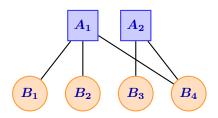
Experimental result

F. Caron 3 / 57



- Multi-edges directed graphs
  - Emails
  - Citations
  - WWW
- ► Simple graphs
  - Social network
  - ▶ Protein-protein interaction

F. Caron 4/57



- ► Bipartite graphs
  - Scientists authoring papers
  - ► Readers reading books
  - ▶ Internet users posting messages on forums

Customers buying items

F. Caron 5 / 57

- Build a statistical model of the network to
  - ► Find interpretable structure in the network
  - Predict missing edges
  - Predict connections of new nodes

F. Caron 6 / 57

- Properties of real world networks
  - Sparsity

Dense graph:  $n_e = \Theta(n^2)$ Sparse graph:  $n_e = o(n^2)$ 

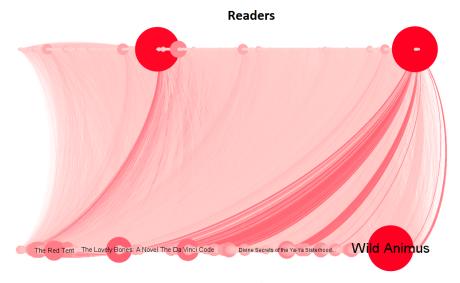
with  $n_e$  the number of edges and n the number of nodes

Power-law degree distributions

[Newman, 2009, Clauset et al., 2009]

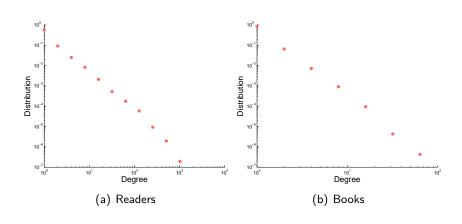
## Book-crossing community network

5 000 readers, 36 000 books, 50 000 edges



## Book-crossing community network

Degree distributions on log-log scale



F. Caron 9 / 57

## Outline

Introduction

#### Exchangeable matrices and their limitations

Statistical network models using exchangeable random measures

Exchangeability and sparsity properties

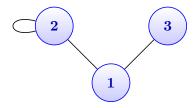
Special case: Generalized gamma process

Posterior characterization & Inference

Experimental results

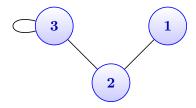
F. Caron 10 / 57

- Statistical network modeling
- Probabilistic symmetry: exchangeability
- Ordering of the nodes is irrelevant



F. Caron 11/57

- Statistical network modeling
- Probabilistic symmetry: exchangeability
- Ordering of the nodes is irrelevant

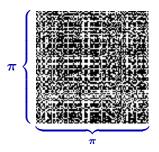


F. Caron 12 / 57

- Graphs usually represented by a discrete structure
- lacktriangle Adjacency matrix  $X_{ij} \in \{0,1\}, (i,j) \in \mathbb{N}^2$
- Joint exchangeability

$$(X_{ij}) \stackrel{d}{=} (X_{\pi(i)\pi(j)})$$

for any permutation  $\pi$  of  $\mathbb N$ 



F. Caron 13 / 5'

► Aldous-Hoover representation theorem

$$(X_{ij})=(F(U_i,U_j,U_{\{ij\}}))$$

where  $U_i, U_{\{ij\}}$  are uniform random variables and F is a random function from  $[0,1]^3$  to  $\{0,1\}$ 

► Several network models fit in this framework (e.g. stochastic blockmodel, infinite relational model, etc.)

[Hoover, 1979, Aldous, 1981, Lloyd et al., 2012]

14 / 57

F. Caron

Corollary of A-H theorem

Exchangeable random graphs are either empty or dense

▶ To quote the survey paper of Orbanz and Roy

"the theory [...] clarifies the limitations of exchangeable models. It shows, for example, that most Bayesian models of network data are inherently misspecified"

► Give up exchangeability for sparsity? e.g. preferential attachment model

F. Caron

#### Outline

Introduction

Exchangeable matrices and their limitations

Statistical network models using exchangeable random measures

Exchangeability and sparsity properties

Special case: Generalized gamma process

Posterior characterization & Inference

Experimental result

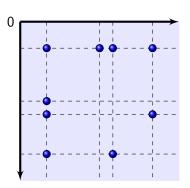
F. Caron 16 / 57

- ightharpoonup Representation of a graph as a (marked) point process over  $\mathbb{R}^2_+$
- Representation theorem by Kallenberg for jointly exchangeable point processes on the plane
- Construction based on a completely random measure
- Properties of the model
  - Exchangeability
  - Sparsity
  - Power-law degree distributions (with exponential cut-off)
  - Interpretable parameters and hyperparameters
  - Reinforced urn process construction
- Posterior characterization
- Scalable inference

lacktriangle Undirected graph represented as a point process on  $\mathbb{R}^2_+$ 

$$Z = \sum_{i,j} z_{ij} \delta_{( heta_i, heta_j)}$$

with  $heta_i \in \mathbb{R}$ ,  $z_{ij} \in \{0,1\}$  with  $z_{ij} = z_{ji}$ 



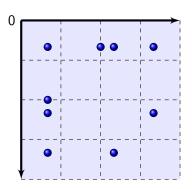
F. Caron 18 / 57

Joint exchangeability

Let  $A_i = [h(i-1), hi]$  for  $i \in \mathbb{N}$  then

$$(Z(A_i \times A_j)) \stackrel{d}{=} (Z(A_{\pi(i)} \times A_{\pi(j)}))$$

for any permutation  $\pi$  of  $\mathbb N$  and any h>0



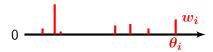
F. Caron 19 / 57

- ► Kallenberg derived a de Finetti style representation theorem for jointly and separately exchangeable point processes on the plane
- Representation via random transformations of unit rate Poisson processes and uniform variables
- ► Continuous-time equivalent of Aldous-Hoover for binary variables
- Our construction will fit into this framework

## Completely random measures

- lacktriangle Nodes are embedded at some location  $oldsymbol{ heta}_i \in \mathbb{R}_+$
- lacktriangle To each node is associated some sociability parameter  $w_i$
- ▶ Homogeneous completely random measure on  $\mathbb{R}_+$

$$W = \sum_{i=1}^\infty w_i \delta_{ heta_i} \quad W \sim \mathsf{CRM}(
ho, \lambda).$$



Lévy measure  $u(dw,d\theta)=
ho(dw)\lambda(d\theta)$  with  $\lambda$  the Lebesgue measure

[Kingman, 1967]

F. Caron

## Completely random measures

- ullet Lévy measure  $u(dw,d heta)=
  ho(dw)\lambda(d heta)$  with  $\lambda$  the Lebesgue measure
- ho is a measure on  $\mathbb{R}_+$  such that

$$\int_0^\infty (1 - e^{-w})\rho(dw) < \infty. \tag{1}$$

which implies that  $W([0,T]) < \infty$  for any  $T < \infty$ .

$$\int_0^\infty 
ho(dw) = \infty \Longrightarrow$$
 Infinite number of jumps in any interval  $[0,T]$ 

"Infinite activity CRM"

$$\int_0^\infty 
ho(dw) < \infty \Longrightarrow$$
 Finite number of jumps in any interval  $[0,T]$ 

"Finite activity CRM"

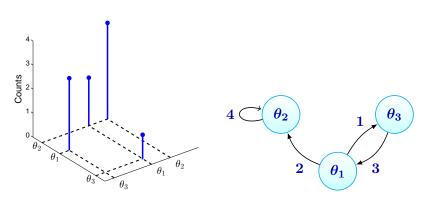
F. Caron 22 / 57

# Model for multi-edges directed graphs

Multigraph represented by an atomic measure on  $\mathbb{R}^2_+$ 

$$D = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} n_{ij} \delta_{(\theta_i, \theta_j)},$$

where  $n_{ij}$  counts the number of directed edges from node  $heta_i$  to node  $heta_j$ .

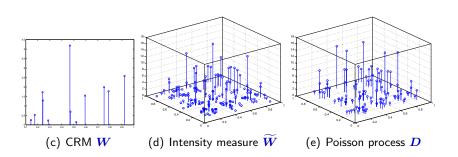


F. Caron 23 / 57

## Model for multi-edges directed graphs

▶ Conditional Poisson process with intensity measure  $\widetilde{W} = W \times W$  on the product space  $\mathbb{R}^2_+$ :

$$D \mid W \sim \mathsf{PP}(W \times W)$$



F. Caron 24 / 57

# Model for multi-edges directed graphs

 $lackbox{egin{aligned} \blacktriangleright\ By\ construction,\ for\ any\ bounded\ intervals\ A\ and\ B\ of\ \mathbb{R}_+,\ \widetilde{W}(A imes B)=W(A)W(B)<\infty \end{aligned}}$ 

lacktriangle Finite number of counts over  $A imes B \subset \mathbb{R}^2_+$ 

$$D(A \times B) < \infty$$

F. Caron 25 / 57

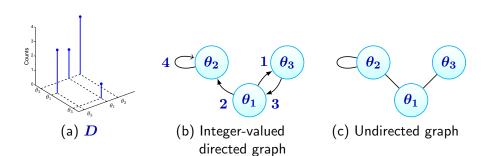
## Model for undirected graphs

Point process

$$Z = \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} z_{ij} \delta_{(\theta_i, \theta_j)},$$

with the convention  $z_{ij}=z_{ji}\in\{0,1\}$ 

 $lackbox{ Constructed from }D$  by setting  $z_{ij}=z_{ji}=1$  if  $n_{ij}+n_{ji}>0$  and  $z_{ij}=z_{ji}=0$  otherwise



F. Caron 26 / 57

## Model for undirected graphs

Hierarchical model

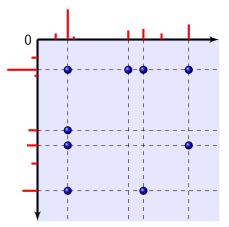
$$\begin{split} W &= \sum_{i=1}^{\infty} w_i \delta_{\theta_i} & W \sim \mathsf{CRM}(\rho, \lambda) \\ D &= \sum_{ij} n_{ij} \delta_{(\theta_i, \theta_j)} & D \sim \mathsf{PP}\left(W \times W\right) \\ Z &= \sum_{ij} \min(n_{ij} + n_{ji}, 1) \delta_{(\theta_i, \theta_j)} \end{split}$$

F. Caron 27 / 57

## Model for undirected graphs

▶ Equivalent direct formulation for  $i \leq j$ 

$$\Pr(z_{ij}=1\mid w)=\left\{egin{array}{ll} 1-\exp(-2w_iw_j) & i
eq j\ 1-\exp(-w_i^2) & i=j \end{array}
ight.$$
 and  $z_{ji}=z_{ij}$ 



F. Caron 28 / 57

### Outline

Introduction

Exchangeable matrices and their limitations

Statistical network models using exchangeable random measures

## Exchangeability and sparsity properties

Special case: Generalized gamma process

Posterior characterization & Inference

Experimental results

F. Caron 29 / 57

Properties: Exchangeability

## Exchangeability

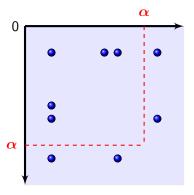
Let h>0 and  $A_i=[h(i-1),hi],\,i\in\mathbb{N}.$  By construction,

$$(Z(A_i \times A_j)) \stackrel{d}{=} (Z(A_{\pi(i)} \times A_{\pi(j)}))$$

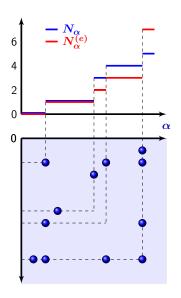
for any permutation  $\pi$  of  $\mathbb{N}$ .

F. Caron 30 / 57

- $W(\mathbb{R}_+)=\infty$ , so infinite number of edges on  $\mathbb{R}^2_+$
- ightharpoonup Restrictions  $D_{\alpha}$  and  $Z_{\alpha}$  of D and Z, respectively, to the box  $[0, \alpha]^2$ .
- $lacktriangleright N_lpha$  number of nodes, and  $N_lpha^{(e)}$  number of edges



F. Caron 31/57



F. Caron 32 / 57

#### Definition

(Regular variation) Let  $W \sim \text{CRM}(\rho, \lambda)$ . The (infinite-activity) CRM is said to be *regularly varying* if the tail Lévy intensity verifies

$$\int_{x}^{\infty} \rho(dw) \overset{x\downarrow 0}{\sim} \ell(1/x) x^{-\sigma}$$

for  $\sigma \in (0,1)$  where  $\ell$  is a slowly varying function satisfying  $\lim_{t \to \infty} \ell(at)/\ell(t) = 1$  for any a>0.

F. Caron 33 / 57

Assume ho 
eq 0 and  $\mathbb{E}[W([0,1])] < \infty$ .

#### **Theorem**

Let  $N_{\alpha}$  be the number of nodes and  $N_{\alpha}^{(e)}$  the number of edges in the undirected graph restriction,  $Z_{\alpha}$ . Then

$$N_{\alpha}^{(e)} = \left\{ \begin{array}{ll} \Theta\left(N_{\alpha}^{2}\right) & \text{if $W$ is finite-activity} \\ o\left(N_{\alpha}^{2}\right) & \text{if $W$ is infinite-activity} \\ O\left(N_{\alpha}^{2/(1+\sigma)}\right) & \text{if $W$ is regularly varying}^{1} \text{ with } \sigma \in (0,1) \end{array} \right.$$

almost surely as  $\alpha \to \infty$ .

F. Caron 34 / 57

<sup>&</sup>lt;sup>1</sup>with  $\lim_{t\to\infty}\ell(t)>0$ 

### Outline

Introduction

Exchangeable matrices and their limitations

Statistical network models using exchangeable random measures

Exchangeability and sparsity properties

Special case: Generalized gamma process

Posterior characterization & Inference

Experimental result

F. Caron 35 / 57

## Generalized Gamma Process

Lévy intensity

$$\frac{1}{\Gamma(1-\sigma)}w^{-1-\sigma}e^{-\tau w}$$

with  $\sigma \in (-\infty,0]$  and  $\tau > 0$  or  $\sigma \in (0,1)$  and  $\tau \geq 0$ 

- Special cases:
  - Gamma process ( $\sigma = 0$ )
  - ▶ Stable process  $(\tau = 0, \sigma \in (0, 1))$
  - ▶ Inverse Gaussian process  $(\sigma = 1/2, \tau > 0)$
- ▶ Infinite activity for  $\sigma > 0$
- lacktriangle Regularly varying for  $\sigma \in (0,1)$
- Exact sampling of the graph via an urn process
- Power-law degree distribution

[Brix, 1999, Lijoi et al., 2007]

### Generalized Gamma Process

Sparsity

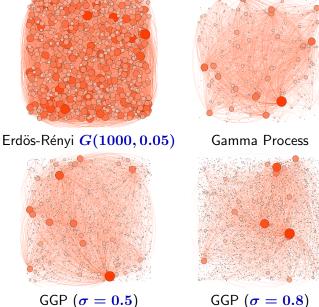
#### Theorem

Let  $N_{\alpha}$  be the number of nodes and  $N_{\alpha}^{(e)}$  the number of edges in the undirected graph restriction,  $Z_{\alpha}$ . Then

$$N_{\alpha}^{(e)} = \left\{ \begin{array}{ll} \Theta\left(N_{\alpha}^{2}\right) & \text{if } \sigma < 0 \\ o\left(N_{\alpha}^{2}\right) & \text{if } \sigma \in [0,1), \tau > 0 \\ O\left(N_{\alpha}^{2/(1+\sigma)}\right) & \text{if } \sigma \in (0,1), \tau > 0 \end{array} \right.$$

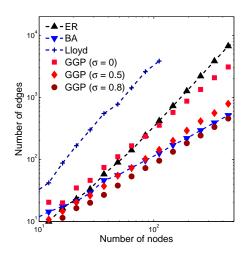
almost surely as  $\alpha \to \infty$ . That is, the underlying graph is sparse if  $\sigma > 0$  and dense otherwise.

F. Caron 37 / 57



F. Caron

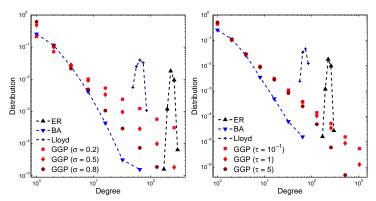
GGP ( $\sigma = 0.8$ )



F. Caron 39 / 57

#### Power-law degree distributions

- ▶ Power-law like behavior providing a heavy-tailed degree distribution
- ightharpoonup Higher power-law exponents for larger  $\sigma$
- ightharpoonup The parameter au tunes the exponential cut-off in the tails.



F. Caron 40 / 57

F. Caron 41/57

### Outline

Introduction

Exchangeable matrices and their limitations

Statistical network models using exchangeable random measures

Exchangeability and sparsity properties

Special case: Generalized gamma process

Posterior characterization & Inference

Experimental result

F. Caron 42 / 57

#### Posterior characterization

Conditional distribution of  $W_{\alpha}$  given  $D_{\alpha}$ .

#### **Theorem**

Let  $(\theta_1,\ldots,\theta_{N_{\alpha}})$ ,  $N_{\alpha}\geq 0$ , be the set of support points of  $D_{\alpha}$  such that  $D_{\alpha}=\sum_{1\leq i,j\leq N_{\alpha}}n_{ij}\delta_{(\theta_i,\theta_j)}$ . Let  $m_i=\sum_{j=1}^{N_{\alpha}}(n_{ij}+n_{ji})>0$  for  $i=1,\ldots,N_{\alpha}$ . The conditional distribution of  $W_{\alpha}$  given  $D_{\alpha}$  is equivalent to the distribution of

$$w_* \sum_{i=1}^{\infty} \widetilde{P}_i \delta_{\widetilde{ heta}_i} + \sum_{i=1}^{N_{lpha}} w_i \delta_{ heta_i}$$

where  $\widetilde{\theta}_i \sim \mathrm{Unif}([0,\alpha])$ , and  $(\widetilde{P}_i)|w_* \sim \mathrm{PK}(\rho|w_*)$  are from a Poisson-Kingman distribution . The weights  $(w_1,\ldots,w_{N_\alpha},w_*)$  are jointly dependent conditional on  $D_\alpha$ , with  $p(w_1,\ldots,w_{N_\alpha},w_*|D_\alpha) \propto$ 

$$\left[\prod_{i=1}^{N_{\alpha}} w_i^{\ m_i}\right] e^{-\left(\sum_{i=1}^{N_{\alpha}} w_i + \mathbf{w_*}\right)^2} \left[\prod_{i=1}^{N_{\alpha}} \rho(w_i)\right] \times g_{\alpha}^*(\mathbf{w_*})$$

where  $g_{lpha}^*$  is the probability density function of the random variable  $W_{lpha}^*=W_{lpha}([0,lpha]).$ 

[Prünster, 2002, James, 2002, James et al., 2009]

F. Caron 43 / 57

# Posterior inference for undirected graphs

- Let  $\phi = (\alpha, \sigma, \tau)$  with flat priors
- ▶ We want to approximate

$$p(w_1,\ldots,w_{N_{\alpha}},w_*,\phi|(z_{ij})_{1\leq i,j\leq N_{\alpha}})$$

- ▶ Latent count variables  $\overline{n}_{ij} = n_{ij} + n_{ji}$
- Markov chain Monte Carlo sampler
  - 1. Update the weights  $(w_1, \ldots, w_{N_{\alpha}})$  given the rest using an Hamiltonian Monte Carlo update
  - 2. Update the total mass  $w_*$  and hyperparameters  $\phi = (\alpha, \sigma, \tau)$  given the rest using a Metropolis-Hastings update
  - 3. Update the latent counts  $(\overline{n}_{ij})$  given the rest from a truncated Poisson distribution

F. Caron 44 / 57

### Outline

Introduction

Exchangeable matrices and their limitations

Statistical network models using exchangeable random measures

Exchangeability and sparsity properties

Special case: Generalized gamma process

Posterior characterization & Inference

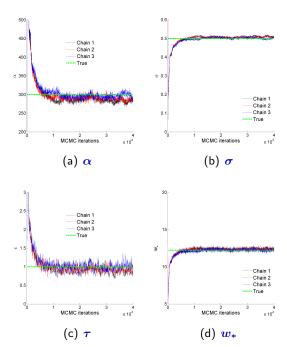
#### Experimental results

F. Caron 45 / 57

#### Simulated data

- ▶ Simulation of a GGP graph with  $\alpha = 300, \sigma = 1/2, \tau = 1$
- ▶ 13,995 nodes and 76,605 edges
- MCMC sampler with 3 chains and 40,000 iterations
- ► Takes 10min on a standard desktop with Matlab

F. Caron 46 / 57



F. Caron 47 / 57

#### Simulated data

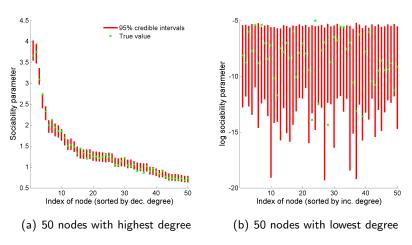


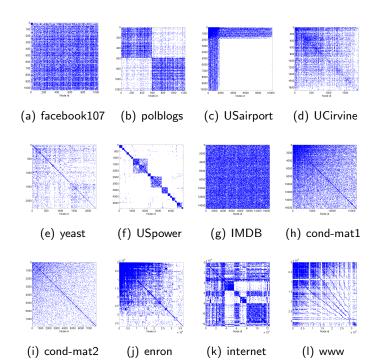
Figure: 95 % posterior intervals of (a) the sociability parameters  $w_i$  of the 50 nodes with highest degree and (b) the log-sociability parameter  $\log w_i$  of the 50 nodes with lowest degree. True values are represented by a green star.

F. Caron 48 / 57

#### Real network data

- Assessing the sparsity of the network
- We aim at reporting  $\Pr(\sigma \geq 0|z)$  based on a set of observed connections (z)
- ▶ 12 different networks
- $\sim 1,000 300,000$  nodes and 10,000 1,000,000 edges

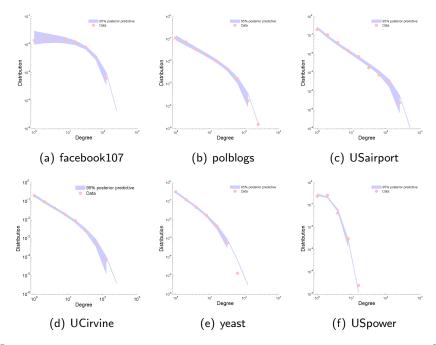
F. Caron 49 / 57



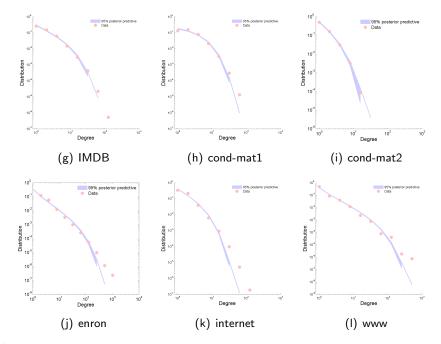
# Real network data

Name	Nb nodes	Nb edges	Time	$ \Pr(\sigma>0 z) $	99% CI <i>σ</i>
			(min)		
facebook107	1,034	26,749	1	0.00	[-1.06, -0.82]
polblogs	1,224	16,715	1	0.00	[-0.35, -0.20]
USairport	1,574	17,215	1	1.00	$[\ 0.10,\ 0.18]$
UCirvine	1,899	13,838	1	0.00	[-0.14, -0.02]
yeast	2,284	6,646	1	0.28	[-0.09, 0.05]
USpower	4,941	6,594	1	0.00	[-4.84, -3.19]
IMDB	14,752	38,369	2	0.00	[-0.24, -0.17]
cond-mat1	16,264	47,594	2	0.00	[-0.95, -0.84]
cond-mat2	7,883	8,586	1	0.00	[-0.18, -0.02]
Enron	36,692	183,831	7	1.00	$[\ 0.20,\ 0.22]$
internet	124,651	193,620	15	0.00	[-0.20, -0.17]
www	325,729	1,090,108	132	1.00	[0.26, 0.30]

F. Caron 51/57



F. Caron 52 / 57



F. Caron 53 / 57

#### Conclusion

- Statistical network models
- ► Build on exchangeable random measures
- Sparsity and power-law properties
- Scalable inference
- ► Similar construction for bipartite graphs
- ► Extensions to more structured models: low-rank, block-model, covariates, dynamic networks,etc
- Matlab code available

http://www.stats.ox.ac.uk/~caron/code/bnpgraph/

F. Caron 54 / 57

# Bibliography I



Aldous, D. J. (1981).

Representations for partially exchangeable arrays of random variables. Journal of Multivariate Analysis, 11(4):581-598.



Barabási, A. L. and Albert, R. (1999).

Emergence of scaling in random networks.

Science, 286(5439):509-512.



Brix, A. (1999).

Generalized gamma measures and shot-noise Cox processes.

Advances in Applied Probability, 31(4):929–953.



Caron, F. (2012).

Bayesian nonparametric models for bipartite graphs.

In NIPS.



Caron, F. and Fox, E. B. (2014).

Sparse graphs using exchangeable random measures.

Technical report. arXiv:1401.1137.



Clauset, A., Shalizi, C. R., and Newman, M. E. J. (2009).

Power-law distributions in empirical data.

SIAM review, 51(4):661-703.

F. Caron 55 / 57

## Bibliography II



Hoover, D. N. (1979).

Relations on probability spaces and arrays of random variables.

Preprint, Institute for Advanced Study, Princeton, NJ.



James, L. F. (2002).

Poisson process partition calculus with applications to exchangeable models and bayesian nonparametrics.

arXiv preprint math/0205093.



James, L. F., Lijoi, A., and Prünster, I. (2009).

Posterior analysis for normalized random measures with independent increments. *Scandinavian Journal of Statistics*, 36(1):76–97.



Kallenberg, O. (1990).

 $\label{prop:exchangeable} \mbox{Exchangeable random measures in the plane}.$ 

Journal of Theoretical Probability, 3(1):81–136.



Kallenberg, O. (2005).

Probabilistic symmetries and invariance principles. Springer.



Kingman, J. (1967).

Completely random measures.

Pacific Journal of Mathematics, 21(1):59-78.

F. Caron 56 / 57

# Bibliography III



Lijoi, A., Mena, R. H., and Prünster, I. (2007).

Controlling the reinforcement in Bayesian non-parametric mixture models.

Journal of the Royal Statistical Society: Series B (Statistical Methodology), 69(4):715–740.



Lloyd, J., Orbanz, P., Ghahramani, Z., and Roy, D. (2012).

Random function priors for exchangeable arrays with applications to graphs and relational data.

In NIPS, volume 25, pages 1007-1015.



Newman, M. (2009).

Networks: an introduction.

OUP Oxford.



Orbanz, P. and Roy, D. M. (2015).

Bayesian models of graphs, arrays and other exchangeable random structures.

IEEE Trans. Pattern Anal. Mach. Intelligence (PAMI), 37(2):437–461.



Prünster, I. (2002).

Random probability measures derived from increasing additive processes and their application to Bayesian statistics.

PhD thesis, University of Pavia.

F. Caron 57 / 57