Ranking paths

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2.2. Path ranking

3. Modules

Summary

Network as a computer: Ranking paths to find flows

Dusko Pavlovic

Oxford University and Kestrel Institute

CSR, Moscow June 2008

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- 1. Paths and cost
- 2.1. Dynamics and ranking
- 2.2. Path ranking
- 3. Modules, concept networks

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Introduction

Definition

A network is an annotated graph

$$\mathsf{A} = \left(\mathsf{R} \stackrel{\varphi}{\leftarrow} \mathsf{E} \stackrel{\delta}{\underset{\mathcal{Q}}{\Rightarrow}} \mathsf{N}\right)$$

where

- N is a finite set of nodes,
- E is a finite set of edges (or links),
- *R* is an ordered rig of *rates* (e.g. \mathbb{R}_+).

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Definition

A network is an annotated graph

$$\mathsf{A} = \left(\mathsf{R} \stackrel{\varphi}{\leftarrow} \mathsf{E} \stackrel{\delta}{\underset{\mathcal{Q}}{\Rightarrow}} \mathsf{N}\right)$$

where

- N is a finite set of nodes,
- E is a finite set of edges (or links),
- *R* is an ordered rig of *rates* (e.g. \mathbb{R}_+).

Notation

▶
$$i \xrightarrow[v]{} j$$
 denotes $e \in E$ such that
 $\delta(e) = i, \ \varrho(e) = j \text{ and } \varphi(e) = v$

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- protein interactions, gene regulation, metabolism,
- food webs, populations,

Networks are used to model

traffic, distribution systems,

neural nets,

social groups

Web, Internet

probabilistic grammars (generative, phonological)

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Problem and objective

Networks get large and complex.

Problem

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Problem Networks get large and complex.

Objective Simplify them...

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... by clustering similar nodes

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... by extracting functional modules



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Problem and objective

Problem of the Web

Data structures and semantics vary from node to node.

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Problem and objective

Problem of the Web

Data structures and semantics vary from node to node.

Solutions

- the Semantic Web
- search, latent semantics
 - extract structure from network
 - concepts = communities = modules

Ranking paths

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Approach

Notation

Given a network
$$A = \left(R \stackrel{\varphi}{\leftarrow} E \stackrel{\delta}{\xrightarrow{\varphi}} N\right)$$
, define

• total flow
$$A_{ij} = \sum_{i \to i} \varphi(e)$$

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Notation

Given a network
$$A = \left(R \stackrel{\varphi}{\leftarrow} E \stackrel{\delta}{\underset{o}{\Rightarrow}} N \right)$$
, define

• total flow
$$A_{ij} = \sum_{i \to j} \varphi(e)$$

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Approach

Notation

Given a network
$$A = \left(R \stackrel{\varphi}{\leftarrow} E \stackrel{\delta}{\underset{o}{\Rightarrow}} N \right)$$
, define

- total flow $A_{ij} = \sum_{\substack{e \ i \to j}} \varphi(e)$
- Flow distribution Φ_{ij} = A_{ij}/A_i, where A_{••} = Σ_{ij} A_{ij}
- ► flow bias $\Upsilon_{ij} = \Phi_{ij} \Phi_{i\bullet} \Phi_{\bullet j}$ where $\Phi_{i\bullet} = \sum_k \Phi_{ik}$ and $\Phi_{\bullet j} = \sum_k \Phi_{kj}$.

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Cohesion and adhesion

Definition

Cohesion of $U \subseteq N$ is the total flow bias between its members

$$\operatorname{Coh}(U) = \sum_{i,i\in U} \Upsilon_{ij}$$

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Cohesion and adhesion

Definition

Cohesion of $U \subseteq N$ is the total flow bias between its members

$$\mathsf{Coh}(U) = \sum_{i,j \in U} \Upsilon_{ij}$$

Adhesion of $U \subseteq N$ is the total flow bias of its members and nonmembers

$$\mathsf{Adh}(U) = \sum_{i \in U, j \notin U} \Upsilon_{ij} + \Upsilon_{ji}$$

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Modularity

Definition

Modularity of $U \subseteq N$ is the difference of its cohesion and its adhesion

Mdu(U) = Coh(U) - Adh(U)

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Modularity

Definition

Modularity of $U \subseteq N$ is the difference of its cohesion and its adhesion

$$\mathsf{Mdu}(U) = \mathsf{Coh}(U) - \mathsf{Adh}(U)$$

Idea Find modules by maximizing modularity.

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Finding network modules boils down to evaluating

• modularity Mdu(U) = Coh(U) - Adh(U)

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Finding network modules boils down to evaluating

modularity Mdu(U) = Coh(U) – Adh(U)
 which is induced by

• flow bias
$$\Upsilon : N \times N \longrightarrow [-1, 1]$$

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Finding network modules boils down to evaluating

- modularity Mdu(U) = Coh(U) Adh(U)
 which is induced by
- flow bias $\Upsilon : N \times N \longrightarrow [-1, 1]$

which is induced by

• flow distribution $\Phi : N \times N \longrightarrow [0, 1],$

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Finding network modules boils down to evaluating

- modularity Mdu(U) = Coh(U) Adh(U)
 which is induced by
- flow bias $\Upsilon : N \times N \longrightarrow [-1, 1]$

which is induced by

• flow distribution $\Phi : N \times N \longrightarrow [0, 1]$,

which is induced by

• flow $\varphi : E \longrightarrow R$

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Problems

flows unknown

- network dynamics unknown
- modules disjoint and hard to compute

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Problems

•	flows unknown
	Step 1: use cost and paths to estimate flows
	network dynamics unknown
	Step 2: use Markovian and ranking methods
•	modules disjoint and hard to compute

Step 3: parametrize modularity

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Cost instead of flow

Modified definition

A network is a labelled graph

$$A = \left(R \stackrel{\gamma}{\leftarrow} E \stackrel{\delta}{\underset{\varrho}{\Rightarrow}} N \right)$$

where the **cost** γ determines the likely flow φ

$$arphi(e) = 2^{-\gamma(e)}$$

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Cost instead of flow

Modified definition

A network is a labelled graph

$$\mathsf{A} = \left(\mathsf{R} \stackrel{\gamma}{\leftarrow} \mathsf{E} \stackrel{\delta}{\underset{\varrho}{\Rightarrow}} \mathsf{N}\right)$$

where the **cost** γ determines the likely flow φ

$$arphi(e)~=~2^{-\gamma(e)}$$

The estimated total flow $i \rightarrow j$ in A is now thus

$$A_{ij} = \sum_{\substack{i = j \ i o j}} 2^{-\gamma(e)}$$

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Definition

Given

• network
$$A = (R \stackrel{\gamma}{\leftarrow} E \stackrel{\delta}{\Rightarrow} N),$$

- cutoff value $v \in R$, and
- length penalty $d \in R$,

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Definition

Given

• network
$$A = (R \stackrel{\gamma}{\leftarrow} E \stackrel{\delta}{\Rightarrow} N),$$

- cutoff value $v \in R$, and
- length penalty $d \in R$,

we define the path completion of A as

• network
$$A^{*vd} = \left(R \stackrel{\gamma}{\leftarrow} E^{*vd} \stackrel{\delta}{\underset{\varrho}{\Rightarrow}} N \right)$$

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Definition

Given

• network
$$A = (R \stackrel{\gamma}{\leftarrow} E \stackrel{\delta}{\Rightarrow} N),$$

- cutoff value $v \in R$, and
- length penalty $d \in R$,

we define the path completion of A as

• network
$$A^{*vd} = \left(R \stackrel{\gamma}{\leftarrow} E^{*vd} \stackrel{\delta}{\Rightarrow} N \right)$$
 with

► links
$$E^{*vd} = \{a \in E^+ \mid \gamma(a) \le v\}$$

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Definition

Given

• network
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 with

► links
$$E^{*vd} = \{a \in E^+ \mid \gamma(a) \le v\}$$

E⁺ is the set of nonempty paths

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Definition

Given

• network
$$A = (R \stackrel{\gamma}{\leftarrow} E \stackrel{\delta}{\underset{\varrho}{\Rightarrow}} N),$$

- cutoff value $v \in R$, and
- length penalty $d \in R$,

we define the path completion of A as

• network
$$A^{*vd} = \left(R \stackrel{\gamma}{\leftarrow} E^{*vd} \stackrel{\delta}{\Rightarrow}_{\varrho} N \right)$$
 with

► links
$$E^{*vd} = \{a \in E^+ \mid \gamma(a) \le v\}$$

E⁺ is the set of nonempty paths

• cost
$$\gamma(i_0 \xrightarrow{a_1} i_1 \xrightarrow{a_2} \cdots \xrightarrow{a_n} i_n) = (n-1)d + \gamma(a_1) + \cdots + \gamma(a_n).$$

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Simple network dynamics

forward: probability that traffic at *i* flows to *j*

$$A_{ij}^{\triangleright} = \frac{A_{ij}}{A_{i\bullet}}$$
 where

$$A_{i\bullet} = \sum_{k=1}^{N} A_{ik}$$

backward: probability that traffic at *j* flows from *i*

$$A_{ij}^{\triangleleft} = \frac{A_{ij}}{A_{\bullet j}}$$
 where
 $A_{\bullet j} = \sum_{k=1}^{N} A_{kj}$

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Simple node ranking

pull rank (reputation): probability that the traffic arrives at j

$$r_j^{\triangleright} = \sum_{k=1}^N r_k^{\triangleright} A_{kj}^{\diamond}$$

push rank (promotion): probability that the traffic departs from i

$$r_i^{\triangleleft} = \sum_{k=1}^N A_{ik}^{\triangleleft} r_k^{\triangleleft}$$

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Simple pull rank: Reputation

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Simple push rank: Promotion

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One-hop dynamics

forward out: probability that traffic at *i* flows to a hub *j*

$$A_{ij}^{\blacktriangleright} = A_{ij}^{\flat} \cdot \Phi_{j\bullet}$$
 where
 $\Phi_{i} = \sum_{k} A_{jk}$

$$\Phi_{j\bullet} = \frac{\sum_{k} A_{jk}}{\sum_{\ell k} A_{\ell k}}$$

backward in: probability that traffic at *j* flows from an authority *i*

$$A_{ij}^{\blacktriangleleft} = \Phi_{\bullet i} \cdot A_{ij}^{\triangleleft} \text{ where}$$
$$\Phi_{\bullet i} = \frac{\sum_{k} A_{ki}}{\sum_{k \ell} A_{k\ell}}$$

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One-hop ranking

pull-out rank: probability that traffic arrives to a hub j

$$r_j^{\blacktriangleright} = \sum_{k=1}^N r_k^{\blacktriangleright} A_{kj}^{\blacktriangleright}$$

push-in rank: probability that traffic departs from an authority i

$$r_i^{\blacktriangleleft} = \sum_{k=1}^N A_{ik}^{\blacktriangle} r_k^{\bigstar}$$

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Pull-out rank

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Push-in rank

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Unibased flow

If the traffic from *j* to *k* is only driven by

- ▶ *j*'s push r_i^{\triangleright} , and by
- ► k's pull r_k^{\blacktriangleleft} ,

which are assumed to be mutually independent

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Summary

Unibased flow

If the traffic from *j* to *k* is only driven by

- ▶ *j*'s push r_i^{\triangleright} , and by
- ► k's pull r_k^{\blacktriangleleft} ,

which are assumed to be mutually independent, then

expected unbiased flow from j to k is

$$\begin{array}{rcl} \stackrel{\scriptstyle \blacktriangleright}{}_{jk} & = & r_{j}^{\scriptscriptstyle \bullet} r_{k}^{\scriptscriptstyle \bullet} \\ & = & \sum_{i\ell} A_{ij}^{\scriptscriptstyle \bullet} r_{i\ell}^{\scriptscriptstyle \bullet} A_{k\ell} \\ & = & \sum_{i\ell} \frac{A_{ij} A_{j\bullet} A_{\bullet k} A_{k\ell}}{A_{i\bullet} A_{\bullet \bullet}^{2} A_{\bullet \ell}} r_{i\ell}^{\scriptscriptstyle \bullet} \end{array}$$

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Idea: capture path dynamics

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Definition

Given

• path complete network $A = \left(R \stackrel{\gamma}{\leftarrow} E \stackrel{\delta}{\Rightarrow} N \right)$

we define

• path network
$$\widehat{A} = \left(R \stackrel{\widehat{\gamma}}{\leftarrow} \widehat{E} \stackrel{\widehat{\delta}}{\Rightarrow} \widehat{N} \right)$$
, with

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• path network
$$\widehat{A} = \left(R \stackrel{\widehat{\gamma}}{\leftarrow} \widehat{E} \stackrel{\widehat{\delta}}{\Rightarrow} \widehat{N} \right)$$
, with

• nodes $\widehat{N} = E$

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Definition

Given

▶ path complete network $A = \left(R \stackrel{\gamma}{\leftarrow} E \stackrel{\delta}{\Rightarrow} N \right)$

we define

▶ path network
$$\widehat{A} = \left(R \stackrel{\widehat{\gamma}}{\leftarrow} \widehat{E} \stackrel{\widehat{\delta}}{\Rightarrow}_{\widehat{\rho}} \widehat{N} \right)$$
, with

• nodes
$$\widehat{N} = E$$

► links
$$\widehat{E} = \sum_{a,b\in E} \widehat{E}_{ab}$$
, where $\widehat{E}_{ab} = \begin{cases} i & f_0 \\ a & f_1 \\ f_1 & f_2 \\ f_1 & f_1 \\ f_1 & f_2 \\ f_2 & f_1 \\ f_1 & f_2 \\ f_2 & f_2 \\ f_1 & f_2 \\ f_2 & f_2 \\ f_1 & f_2 \\ f_2 & f_2 \\ f_1 & f_2 \\ f_1 & f_2 \\ f_2 & f_2 \\ f_1 & f_2 \\ f_2 & f_2 \\ f_3 & f_3 \\ f_4 & f_4 \\ f_5 & f_5 \\ f_5 & f_$

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Given

• path complete network $A = \left(R \stackrel{\gamma}{\leftarrow} E \stackrel{\delta}{\Rightarrow} N \right)$

we define

• path network
$$\widehat{A} = \left(R \stackrel{\widehat{\gamma}}{\leftarrow} \widehat{E} \stackrel{\widehat{\delta}}{\underset{\widehat{\rho}}{\Rightarrow}} \widehat{N} \right)$$
, with

• nodes
$$\widehat{N} = E$$

► links
$$\widehat{E} = \sum_{a,b\in E} \widehat{E}_{ab}$$
, where $\widehat{E}_{ab} = \begin{cases} 1 & j \\ j & k \\ \ell & f_1 \\ \ell & f_1 \end{cases}$
► cost $\widehat{\gamma}(f) = \gamma(f_0) + \gamma(b) + \gamma(f_1) - \gamma(a) + 2d \le v$

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Dynamics of path selection

attraction: probability that traffic through a will traverse b

repulsion: probability that traffic through *b* is diverted away from *a*

$$\widehat{A}_{ab}^{\triangleleft} = \frac{\widehat{A}_{ab}}{\widehat{A}_{\bullet b}} \text{ where}$$
$$\widehat{A}_{\bullet b} = \sum_{x} A_{xb}$$

$$\widehat{A}_{ab}^{\flat} = \frac{\widehat{A}_{ab}}{\widehat{A}_{aullet}}$$
 where

$$\widehat{A}_{a\bullet} = \sum_{x} A_{ax}$$

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path pull: probability that traffic traverses b

$$\widehat{r}_{b}^{\diamond} = \sum_{a} \widehat{r}_{a}^{\diamond} \widehat{A}_{ab}^{\diamond}$$

path push: probability that traffic is diverted from a

$$\widehat{r}_{a}^{\triangleleft} = \sum_{b \in \widehat{N}} \widehat{A}_{ab}^{\triangleleft} \widehat{r}_{b}^{\triangleleft}$$

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Path pull rank

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Path push rank

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Definition

The *node attraction* between j and k is the total attraction of all paths between them:

$$\widehat{r}_{jk} = \sum_{\substack{j \to k \\ b}} \widehat{r}_b$$

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Definition

The *node attraction* between j and k is the total attraction of all paths between them:

$$\widehat{r}_{jk} = \sum_{\substack{j \to k \\ b}} \widehat{r}_b$$

Idea

Estimate the traffic bias as the difference between the node attraction and the unbiased flow

$$\Upsilon_{jk} = \widehat{r_{jk}} - r_{jk}^{\bigstar}$$

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Definition

The attraction dynamics of a network A is the Markov chain $\widehat{A} = (\widehat{A}_{(ij)(k\ell)})_{N^2 \times N^2}$, with the entries

$$\widehat{A}_{(ij)(k\ell)} = \frac{A_{ij}A_{jk}A_{k\ell}}{A_{j\bullet}A_{\bullet\bullet}A_{\bullet\ell}}$$

where
$$A_{i\bullet}A_{\bullet\bullet}A_{\bullet\ell} = \sum_{m,n\in N} A_{im}A_{mn}A_{n\ell}$$
.

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Definition

The attraction dynamics of a network A is the Markov chain $\widehat{A} = (\widehat{A}_{(ij)(k\ell)})_{N^2 \times N^2}$, with the entries

$$\widehat{A}_{(ij)(k\ell)} = \frac{A_{ij}A_{jk}A_{k\ell}}{A_{i\bullet}A_{\bullet\bullet}A_{\bullet\ell}}$$

where
$$A_{i\bullet}A_{\bullet\bullet}A_{\bullet\ell} = \sum_{m,n\in N} A_{im}A_{mn}A_{n\ell}$$
.

Recall

$$A_{(ij)(k\ell)}^{\bigstar} = \frac{A_{ij}A_{j\bullet}A_{\bullet k}A_{k\ell}}{A_{i\bullet}A_{\bullet\bullet}A_{\bullet\bullet}A_{\bullet\ell}}$$
$$r_{jk}^{\bigstar} = \sum_{i,\ell\in\mathbb{N}}A_{(ij)(k\ell)}^{\bigstar}r_{i\ell}^{\bigstar}$$

and

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Proposition

Let a network A be path complete for a sufficiently large cutoff value v.

Then the node attraction \hat{r} is the stationary distribution of the attraction dynamics:

$$\widehat{r}_{jk} = \sum_{i,\ell \in N} \widehat{A}_{(ij)(k\ell)} \widehat{r}_{i\ell}$$

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Corollary

The directed reputation and promotion ranks are the marginals of the node attraction

$$\sum_{k\in N} \widehat{r}_{jk} = r_j^{\bullet}$$
$$\sum_{j\in N} \widehat{r}_{jk} = r_k^{\bullet}$$

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Summary

$$r_{j}^{\bullet} = \operatorname{Prob}\left(\bullet \xrightarrow{\xi} j \mid \xi \in \widehat{A}\right)$$
$$r_{k}^{\bullet} = \operatorname{Prob}\left(k \xrightarrow{\xi} \bullet \mid \xi \in \widehat{A}\right)$$
$$\widehat{r}_{jk} = \operatorname{Prob}\left(j \xrightarrow{\xi} k \mid \xi \in \widehat{A}\right)$$

Interpretation

The mutual information

$$I(r^{\blacktriangleright}; r^{\blacktriangleleft}) = D(\widehat{r} \parallel r^{\blacktriangleright}) = \sum_{j=1}^{N} \sum_{k=1}^{N} \widehat{r}_{jk} \log \frac{\widehat{r}_{jk}}{r_{j}^{\blacktriangleright} r_{k}^{\blacktriangleleft}}$$

quantifies the non-local information processing in A.

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Interpretation

The mutual information

$$I(r^{\blacktriangleright}; r^{\blacktriangleleft}) = D(\widehat{r} \parallel r^{\blacktriangleright}) = \sum_{j=1}^{N} \sum_{k=1}^{N} \widehat{r}_{jk} \log \frac{\widehat{r}_{jk}}{r_{j}^{\blacktriangleright} r_{k}^{\blacktriangleleft}}$$

quantifies the non-local information processing in A.

E.g, in the extremal cases,

- if *l*(*r*[►]; *r*[◀]) = 0, i.e. *r*[►] and *r*[◀] are independent, all information is generated by the nodes,
- if *I*(*r*[▶]; *r*[◄]) = *H*(*r*) for *r* = *r*[▶] = *r*[◄], all information is generated by the network.

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 Attraction bias is the difference between total attraction and the expected flow

$$\Upsilon_{jk} = \widehat{r}_{jk} - r_{jk}^{\mathbf{M}}$$

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 Attraction bias is the difference between total attraction and the expected flow

$$\Upsilon_{jk} = \widehat{r}_{jk} - r_{jk}^{\mu}$$

Coherence of U ⊆ N is the minimal attraction bias of its members, in either direction

$$\Upsilon(U) = \bigwedge_{i,i\in U} (\Upsilon_{ij} \vee \Upsilon_{ji})$$

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Summary

 Attraction bias is the difference between total attraction and the expected flow

$$\Upsilon_{jk} = \widehat{r}_{jk} - r_{jk}^{\mu}$$

Coherence of U ⊆ N is the minimal attraction bias of its members, in either direction

$$\Upsilon(U) = \bigwedge_{i,j\in U} (\Upsilon_{ij} \vee \Upsilon_{ji})$$

Communities are coherent sets of nodes

$$\mathscr{O}_{\epsilon}A = \{U \subseteq N \mid \Upsilon(U) \ge \epsilon\}$$

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Summary

• Each $\mathcal{O}_{\epsilon}A$, ordered by

 $U \sqsubseteq V \iff U \subseteq V \land \Upsilon(U) \leq \Upsilon(V)$

is a directed complete partial order (dcpo).

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Summary

• Each $\mathcal{O}_{\epsilon}A$, ordered by

 $U \sqsubseteq V \iff U \subseteq V \land \Upsilon(U) \leq \Upsilon(V)$

is a directed complete partial order (dcpo).

• An ϵ -concept is a maximal element of $\mathcal{O}_{\epsilon}(A)$.

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Summary

• Each $\mathscr{D}_{\epsilon}A$, ordered by

 $U \sqsubseteq V \iff U \subseteq V \land \Upsilon(U) \le \Upsilon(V)$

is a directed complete partial order (dcpo).

- An ϵ -concept is a maximal element of $\mathcal{D}_{\epsilon}(A)$.
- $\epsilon_1 \leq \epsilon_2$ implies $\mathscr{D}_{\epsilon_1} A \supseteq \mathscr{D}_{\epsilon_2} A$
 - \mathcal{O}_{ϵ} is easy for large and small ϵ

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Concept modules

Definition

$U \subseteq N$ is an ϵ -concept module if

- ► $\forall i, j \in U$. $\Upsilon(\{i, j\}) \ge \epsilon$, but
- ► $\forall k \in N \setminus U \exists j \in U. \Upsilon(\{k, j\}) < \epsilon.$

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Concept modules

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 $U \subseteq N$ is an ϵ -concept module if

- ► $\forall i, j \in U$. $\Upsilon(\{i, j\}) \ge \epsilon$, but
- ► $\forall k \in N \setminus U \exists j \in U. \Upsilon(\{k, j\}) < \epsilon.$

Let \mathcal{N}^{ϵ} denote the set of ϵ -concept modules in a network A.

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Association networks

Given a path complete network *A*, the induced concept network

$$\mathcal{A}^{\epsilon} = \left(\mathsf{R} \stackrel{\gamma}{\leftarrow} \mathcal{E}^{\epsilon} \stackrel{\delta}{\underset{\varrho}{\Rightarrow}} \mathcal{N}^{\epsilon}
ight)$$

consists of



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- extended the ranking methods to paths
 - path rank is a measure of nonlocal information
 - allows estimating the flow bias to extract modules

Summary

- extended the ranking methods to paths
 - path rank is a measure of nonlocal information
 - allows estimating the flow bias to extract modules
- extracted modules (= communities = concepts)
 - parametric, richer structure for simpler algorithmics
 - concept networks for latent semantics

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Current work

Is this method "real"?

- experimental validation
 - PL networks
 - IMDB
- relate with spectral methods
- algorithmics, convergence...

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