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A node-similarity based algorithm for tree generation and evolution

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Received 6 August 2015; Accepted 28 September 2015; Published online 1 September 2016

Abstract

In present study we proposed a node-similarity based algorithm for tree generation and evolution. In this algorithm, we assume that each isolated node is a node set at the beginning, two node sets with the greatest similarity tend to connect into a new node set firstly. Repeat this procedure, until all isolated nodes are combined into a tree. Pearson correlation measure, cosine measure, and (negative) Euclidean distance measure (the three measures are for interval attributes), contingency correlation measure (for nominal attributes), or Jaccard coefficient measure (for binary attributes) were used as the between-node similarity. In this way, all connections are sequentially generated and it thus forms the evolution process of a spanning tree of maximum likelihood. The similarity value of a connection can be considered as the weight of the connection. Matlab codes of the algorithm are provided.

Keywords tree; generation; evolution; node similarity; algorithm.

Network Biology ISSN 2220-8879 URL: http://www.iaees.org/publications/journals/nb/online-version.asp RSS: http://www.iaees.org/publications/journals/nb/rss.xml E-mail: networkbiology@iaees.org Editor-in-Chief: WenJun Zhang Publisher: International Academy of Ecology and Environmental Sciences

1 Introduction

Early in 1998, Watts and Strogatz developed a method for generating random graphs. Barabasi and Albert (1999) proposed a general mechanism for network evolution. Cancho and Sole (2001) algorithm can generate a variety of complex networks with diverse degree distributions. Fath et al. (2007) defined a step-by-step procedure for constructing an ecological network. Zhang (2011, 2012b, 2012c, 2012d, 2015a, 2016) proposed a series of methods and models for network generation and evolution. So far, research on network generation and evolution is still fewer. In present study, we will propose a node-similarity based algorithm for tree generation and evolution. Matlab codes of the algorithm are presented for further use.

2 Algorithm

Suppose there are *m* isolated nodes (or objects, etc.) and *n* attributes. The raw data matrix is $a=(a_{ij})_{m\times n}$. In the generation/evolution of a tree, I assume that in a set of isolated nodes (node sets), two nodes (node sets) with the greatest similarity tend to connect firstly. Pearson correlation measure, cosine measure, and (negative)

Euclidean distance measure (the three measures are for interval attributes), contingency correlation measure (for nominal (1, 2, 3...) attributes), or Jaccard coefficient measure (for binary (0, 1) attributes) can be used as the between-node similarity.

Pearson correlation measure is (Zhang, 2011, 2016; Zhang et al., 2014; Zhang, 2012b, c; Zhang and Li, 2015)

$$r_{ij} = \sum_{k=1}^{n} ((a_{ik} - a_{ib})(a_{jk} - a_{jb})) / (\sum_{k=1}^{n} (a_{ik} - a_{ib})^2 \sum_{k=1}^{n} (a_{jk} - a_{jb})^2)^{1/2}$$

i, *j*=1, 2,...,*m*

where $-1 \le r_{ij} \le 1$, $a_{ib} = \sum_{k=1}^{n} a_{ik}/n$, $a_{jb} = \sum_{k=1}^{n} a_{jk}/n$, $i, j=1, 2, \dots, m$.

Cosine measure is (Zhang, 2007; Zhang, 2012a)

$$r_{ij} = \sum_{k=1}^{n} a_{ik} a_{jk} / (\sum_{k=1}^{n} a_{ik}^2 \sum_{k=1}^{n} a_{jk}^2)^{1/2}$$

i, *j*=1, 2,...,*m*

Euclidean distance measure is (Zhang, 2007, 2012a)

$$d_{ij} = \left(\sum_{k=1}^{n} (a_{ik} - a_{jk})^2\right)^{1/2}$$

Its negative value is used as the similarity measure

 $r_{ij} = -d_{ij}$

Contingency correlation measure is (Zhang, 2007, 2012b; Zhang et al., 2014):

$$r_{ij}=2(h/(s(p-1)))^{1/2}-1$$
 $i, j=1, 2, \dots, m$

where $-1 \le r_{ij} \le 1$, and

$$h = s_{..} (\sum_{i=1}^{p} \sum_{j=1}^{p} s_{ij}^{2} / (s_{i}, s_{j}) - 1)$$

$$s_{..} = \sum_{i=1}^{p} s_{i}, \quad s_{i} = \sum_{j=1}^{p} s_{ij}, \quad n_{.j} = \sum_{i=1}^{p} s_{ij}$$

where there are *p* available nominal values, i.e., t_1 , t_2 ,..., t_p , for attributes *i* and *j*, s_{kl} is the number of attributes of node *i* takes value t_k and node *j* takes value t_l , k, l = 1, 2, ..., p.

Jaccard coefficient measure is (Zhang, 2015b)

$$r_{ii} = (e - (c + b))/(e + c + b)$$
 $i, j = 1, 2, \dots, m$

where $-1 \le r_{ij} \le 1$, *c* is the number of node pairs of 1 for attribute *i* but not for *j*; *b* is the number of node pairs of 1 for attribute *j* but not for *i*; *e* is the number of node pairs of 1 for both attribute *i* and attribute *j*.

Between-node similarity matrix, $r=(r_{ij})_{m\times m}$, is a symmetric matrix, i.e., r=r'.

Calculate the similarity between node sets. Suppose there are two node sets, A and B. The similarity between A and B is defined as the greatest similarity between A and B

$$r_{AB}=max r_{ij}, \quad i \in A, j \in B$$

At the start, *m* isolated nodes (or objects, etc.) are *m* node sets respectively. In all of node sets, choose two node sets with the maximal r_{AB} to combine into a new node set, and the corresponding nodes, *i* and *j*, with the maximal r_{ij} , are connected. Repeat this procedure, until *m* isolated nodes are eventually combined into a tree. In this way, all connections are sequentially generated, and thus form the evolution process of a spanning tree (a more general network can be further generated from the spanning tree by adding more connections).

The following are Matlab codes of the algorithm

% Reference: Zhang WJ, Li X. 2016. A node-similarity based algorithm for tree generation and evolution. Selforganizology, 3(2): choice=input('Input a number to choose similarity measure (1: Pearson linear correlation; 2: Cosine measure; 3: (Negative) Euclidean distance; 4: Contingency correlation; 5: Jaccard coefficient): '); a=load(str); m=size(a,1);for i=1:m-1 for j=i+1:m ix=a(i,:); jx=a(j,:); if (choice==1) str='Pearson correlation'; ixbar=mean(ix); jxbar=mean(jx); aa=sum((ix-ixbar).*(jx-jxbar)); bb=sum((ix-ixbar).^2); cc=sum((jx-jxbar).^2); r(i,j)=aa/sqrt(bb*cc); end if (choice==2) str='Cosine measure'; aa=sum(ix.*jx); bb=sum(ix.^2); $cc=sum(jx.^2);$ r(i,j)=aa/sqrt(bb*cc); end if (choice==3) str='(Negative) Euclidean distance'; r(i,j)=-sqrt(sum((ix-jx).^2)); end if (choice==4) str='Contingency correlation'; xx=[ix;jx]; pn=1;tt(1)=xx(1);for kk=1:max(size(xx)) jj=0; for ii=1:pn

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if (xx(kk)~=tt(ii)) jj=jj+1; end;
end
if (jj==pn) pn=pn+1;tt(pn)=xx(kk); end;
end
for kk=1:pn
for jj=1:pn
temp(kk,jj)=0;
for ii=1:max(size(ix))
if ((ix(ii)==tt(kk)) & (jx(ii)==tt(jj))) temp(kk,jj)=temp(kk,jj)+1; end; end
end; end
for kk=1:pn
pp=0;
for jj=1:pn pp=pp+temp(kk,jj); end
ni(kk)=pp;
end
for kk=1:pn
pp=0;
for jj=1:pn pp=pp+temp(jj,kk); end
nj(kk)=pp;
end
summ=0;
for kk=1:pn
summ=summ+ni(kk);
end;
xsquare=0;
for kk=1:pn
for jj=1:pn
if (ni(kk)==0 | nj(jj)==0) continue; end
xsquare=xsquare+temp(kk,jj)*temp(kk,jj)/(ni(kk)*nj(jj));
end; end
xsquare=summ*(xsquare-1);
r(i,j)=2*sqrt(xsquare/(summ*(pn-1)))-1;
end
if (choice==5)
str='Jaccard coefficient';
bb=sum((ix==0) & (jx~=0));
cc=sum((ix~=0) & (jx==0));
dd=sum((ix~=0) & (jx~=0));
r(i,j)=(dd-(cc+bb))/(dd+cc+bb);
end
r(j,i)=r(i,j);
end; end
adj=zeros(m);
r0=r;
classid=1;
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u(classid)=0;
classnum(classid)=m;
for i=1:classnum(classid) x(classid,i)=i; end
tree=zeros(m);
disp(['Step Node
                      Node
                               ' str]);
while (classnum(classid)>1)
aa = -1e + 10;
for i=1:classnum(classid)-1
for j=i+1:classnum(classid)
if (r(i,j)>aa) aa=r(i,j); end
end; end
aa1=0:
for i=1:classnum(classid)-1
for j=i+1:classnum(classid)
if (abs(r(i,j)-aa)<=1e-06)
aa1=aa1+1; v(aa1)=i; w(aa1)=j;
temp=-1e+10;
for k=1:m
if (x(classid,k)==i)
for kk=1:m
if (x(classid,kk)==j)
if (r0(k,kk)>temp) temp=r0(k,kk); end
end; end; end; end;
for k=1:m
if (x(classid,k)==i)
for kk=1:m
if (x(classid,kk)==j)
if (abs(r0(k,kk)-temp)<1e-06) tree(k,kk)=classid;
disp([num2str(classid) '
                               ' num2str(k) '
                                                    'num2str(kk) '
                                                                         'num2str(r0(k,kk))]);
adj(k,kk)=1; adj(kk,k)=1;
end;
end; end; end; end
end; end; end
for i=1:classnum(classid) s(i)=0; end
nn1=0;
for i=1:aa1
if ((v(i)~=0) & (w(i)~=0))
nn1=nn1+1;
for j=1:aa1
if ((v(j)==v(i)) | (v(j)==w(i)) | (w(j)==w(i)) | (w(j)==v(i)))
s(v(j))=nn1; s(w(j))=nn1;
if (j \rightarrow i) v(j) = 0; w(j) = 0; end; end
end
v(i)=0; w(i)=0;
end; end
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for i=1:nn1 for j=1:classnum(classid) if (s(j)==i)for k=1:m if (x(classid,k)==j) x(classid+1,k)=i; end end end; end; end for i=1:classnum(classid) if (s(i)==0)nn1=nn1+1;for k=1:m if (x(classid,k)==i) x(classid+1,k)=nn1; end end; end; end; classid=classid+1; u(classid)=aa; classnum(classid)=nn1; for i=1:classnum(classid)-1 for j=i+1:classnum(classid) r(i,j)=-1e+10;for k=1:m if (x(classid,k) == i)for kk=1:m if (x(classid,kk)==j) if (rO(k,kk)>r(i,j)) r(i,j)=rO(k,kk); end end; end; end; end; r(j,i)=r(i,j);end; end; end: fprintf('\nMatrix for tree evolution (elements are step IDs)') tree fprintf('\n') disp([str ' for each step']) corr=u(2:classid) fprintf('\nThe final adjacency matrix\n') adj

3 Application Example

3.1 Analysis of 54 human races and populations and 14 common HLA-DRB1 alleles

Data of the world's 54 human races and populations (nodes) and 14 common HLA-DRB1 alleles (attributes) are from Jia (2001) (Zhang and Qi, 2014; HLA_DRB1.txt; supplementary material). Here I use Pearson correlation measure to generate the tree. The process of tree evolution is listed in Table 1.

The distribution of node degrees of final tree for 54 races and populations are indicated in Table 2, and the corresponding tree graph is drawn for convenient comparison using Java software (Zhang, 2012a), as indicated in Fig. 1.

			Pearson				Pearson	~			Pearson				Pearson
Step	Node	Node	corr.												
1	24	28	0.9817	15	16	15	0.9182	29	39	32	0.8791	43	53	54	0.7374
2	33	35	0.9619	16	20	21	0.9182	30	49	13	0.8753	44	33	37	0.7330
3	28	26	0.9579	17	45	47	0.9181	31	11	10	0.8750	45	2	7	0.7211
4	5	11	0.9545	18	16	14	0.9144	32	44	43	0.8731	46	2	11	0.7065
5	42	44	0.9527	19	49	50	0.9141	33	10	31	0.8707	47	18	32	0.6789
6	45	46	0.9458	20	33	39	0.9136	34	46	48	0.8606	48	2	8	0.6581
7	49	51	0.9413	21	42	40	0.9103	35	5	4	0.8512	49	30	27	0.6562
8	36	40	0.9371	22	15	18	0.9092	36	18	19	0.8458	50	26	31	0.5708
9	33	34	0.9333	23	38	43	0.9082	37	5	1	0.8376	51	7	6	0.5526
10	16	17	0.9328	24	14	12	0.9077	38	1	3	0.8173	52	6	50	0.5353
11	49	52	0.9259	25	25	27	0.8962	39	3	9	0.8062	53	19	21	0.5132
12	46	42	0.9252	26	34	22	0.8915	40	22	23	0.8060				
13	38	41	0.9199	27	12	11	0.8862	41	33	53	0.7828				
14	28	25	0.9185	28	35	40	0.8823	42	29	30	0.7639				

Table 1 The process of tree evolution of world's 54 human races (nodes) and populations.

Node IDs from 1 to 54 represent Lahu-China, Dai-China, Yao-China, Guangdong Han-China, Dulong-China, Buyi-China, Thais, Yi-China, Hunan Han-China, Southern Han-China, Singapore Han-Singapore, Pumi-China, Shanghai Han-China, Liaoning Han-China, Shegyang Han-China, Northwest Han-China, Northern Han-China, Manchu-China, Japanese, Hokkaido-Japan, Uighur-China, Kazak-China, Siberian Nivkhs population, Siberian Udegeys population, Siberian Koryaks population, Siberian Eskimo, Siberian Chukchi population, South American Indians Ticuna, South American Indians Terena, Siberian Evenki population, Siberian Kets population, USA whites, Spanish, German, Romanians, Bulgarian, Greek, Polish, Turks, Macedonians, Israeli Arabs, Iranian Jews, Ashkenazi Jews-Germany, Libyan Jews, Moroccan Jews, Ethiopian Jews, Native population-Australia's central desert, Yuendumu Native population-Australia, Kimberley native population-Australia, Cape York native population-Australia, North American blacks, and South African blacks.

Table 2 Node degrees for 54 faces and populations.									
ID	1	2	3	4	5	6	7	8	9
Degree	2	3	2	1	3	2	2	1	1
ID	10	11	12	13	14	15	16	17	18
Degree	2	4	2	1	2	2	3	1	3
ID	19	20	21	22	23	24	25	26	27
Degree	2	1	2	2	1	1	2	2	2
ID	28	29	30	31	32	33	34	35	36
Degree	3	1	2	2	2	5	2	2	1
ID	37	38	39	40	41	42	43	44	45
Degree	1	2	2	3	1	3	2	2	2
ID	46	47	48	49	50	51	52	53	54
Degree	3	1	1	4	2	1	1	2	1

 Table 2 Node degrees for 54 races and populations



Fig. 1 The generated tree of 54 races and populations. Node IDs are explained in Table 1.

3.2 Analysis of 12 Chinese human populations and 17 HLA-DQB1 alleles

Data of the 12 Chinese human populations (nodes) and 17 common HLA-DQB1 alleles (attributes) (12×17; HLA_DQB1.txt; supplementary material) are from Geng et al. (1995), Chang et al. (1997), Mizuki et al. (1997, 1998), et al. Use Pearson cosine measure and results to generate the tree. The process of tree evolution is as follows

Step	Node	Node	Cosine measure
1	7	8	0.9764
2	6	10	0.97057
3	6	4	0.94927
4	10	5	0.94407
5	10	7	0.93692
6	4	3	0.92891
7	11	12	0.92311
8	3	2	0.90887
9	7	1	0.85977
10	6	11	0.78742
11	8	9	0.75927

where the node IDs from 1 to 12 represent Tibetan, Uighur, Kazak, Xingjiang Han, Taiwanese, Hong Kong,

The corresponding tree is indicated in Fig. 2.



Fig. 2 The generated tree of 12 Chinese populations. Node IDs are explained in text.

4 Discussion

The present algorithm is based on similarity between nodes. The node sets with greater similarity tend to connect than that with less similarity. The final tree achieved is thus a spanning tree with maximum likelihood. The similarity value of a connection can be considered as the weight of the connection.

Considering the generality of such mechanism of tree generation in nature, it is expected to be a general method for tree generation. This algorithm can produce connections sequentially, thus can reflect the process of tree evolution. Further studies or applications on the algorithm are expected in the future.

Acknowledgment

We are thankful to the support of High-Quality Textbook *Network Biology* Project for Engineering of Teaching Quality and Teaching Reform of Undergraduate Universities of Guangdong Province (2015.6-2018.6), from Department of Education of Guangdong Province, Discovery and Crucial Node Analysis of Important Biological and Social Networks (2015.6-2020.6), from Yangling Institute of Modern Agricultural Standardization, and Project on Undergraduate Teaching Reform (2015.7-2017.7), from Sun Yat-sen University, China.

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