# Article

# A statistical simulation method for causality inference of Boolean variables

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# Abstract

In present study, a statistical simulation method for causality inference of Boolean variables was proposed. First, I used statistical simulation to generate artificial data of two Boolean variables with known independent and dependent variables. A law was drawn from the simulation analysis of the artificial data. For a set of data of two Boolean variables, a randomization method was proposed and used to test the statistical significance of the Boolean correlation measure (point correlation, quartile correlation, or Jaccard correlation, etc.). The causality inference was then conducted to observed data based on the law. Finally, the statistical significance of was used to determine the statistic significance of the causality. Full Matlab codes were presented also.

**Keywords** causality inference; correlation; Boolean variables; randomization; statistical simulation; non-parametric statistics.

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## **1** Introduction

Causality inference is a frontier area in science. So far few successful theories have been made in causality inference of variables. Causality will result in correlation between two variables. We can conduct causality inference only the two variables are correlated with each other. Theories and applications of correlations have been well studied, including that in network biology (Qi and Zhang, 2003; Kuang and Zhang, 2011; Huang and Zhang, 2012; Jiang and Zhang, 2015a, b; Zhang, 2007, 2011b, 2012a, 2014-2018, 2021; Zhang and Zhang, 2019; Xin and Zhang, 2020). There are many correlation measures, among which Pearson correlation, Spearman correlation, etc., are for interval variables, and point correlation, Jaccard coefficient, etc., are for Boolean (binary) variables. In addition to the methods of parametrical statistics, statisticall simulation (randomization) methods are widely used to make statistical inferences (Solow, 1993; Manly, 1997; Zhang and Schoenly, 1999; Zhang, 2010, 2011a). In present study, a statistical simulation (randomization) method for causality inference of Boolean variables was proposed. Full Matlab codes were presented also.

# 2 Correlations and Statistic Tests

Causality will result in correlation between two variables. We can conduct causality inference only the two variables are correlated with each other. There are many correlation measures, among which Pearson correlation, Spearman correlation, etc., are for interval variables, and point correlation, Jaccard coefficient, etc., are for Boolean (binary) variables (Qi and Zhang, 2003; Zhang, 2007, 2012a, 2014, 2015, 2016, 2017, 2018, 2021).

# 2.1 Correlation measures of Boolean variables

There are a lot of correlation measures for Boolean variables. Here I use five representative ones as follows.

# 2.1.1 Point correlation

Suppose there are *n* pairs of Boolean data. The point correlation between Boolean variables *x* and *y* is (Qi and Zhang, 2003; Zhang, 2007, 2012a, 2015, 2016, 2017, 2018, 2021; Zhang et al., 2014)

$$r=(ad-bc)/((a+b)(c+d)(a+c)(b+d))^{1/2}$$

where  $-1 \le r \le 1$ , both variable *x* and variable *y* take values 0 or 1. *a* is number of both variable *x* and variable *y* take value 0, *b* is number of variable *x* takes 0 and variable *y* takes 1, *c* is number of variable *x* takes 1 and variable *y* takes 0, and *d* is number of both variable *x* and variable *y* take value 1. n=a+b+c+d. A greater and positive *r* means a positive point correlation between variables *x* and *y*; a greater and negative *r* means a negative point correlation between variables *x* and *y*.

2.1.2 Quartile correlation

Quartile correlation is defined by (Zhang, 2016, 2018):

$$r = \sin((a+d-(b+c))/(a+b+c+d)*\pi/2)$$

where  $-1 \le r \le 1$ ; *a*, *b*, *c* and *d* follow the definitions above.

2.1.3 Cosine correlation

Cosine correlation is defined by (Zhang, 2016, 2018):

$$r = (a^{2*}d^2/((a+b)(a+c)(b+d)(c+d)))^{1/2}$$

where  $0 \le r \le 1$ ; *a*, *b*, *c* and *d* follow the definitions above. 2.1.4 Cosine+ correlation

$$r=(a^2/((a+b)(a+c)))^{1/2}$$

where  $0 \le r \le 1$ ; *a*, *b*, and *c* follow the definitions above.

2.1.5 Jaccard correlation

Jaccard correlation is defined by (Qi and Zhang, 2003; Zhang, 2007, 2012a, 2014, 2015, 2016, 2017, 2018, 2021):

$$r = (d - (c + b))/(d + c + b)$$

where  $-1 \le r \le 1$ ; *b*, *c* and *d* follow the definitions above.

#### 2.2 Detection of correlation between two Boolean variables

Following the principle of randomization methods (Manly, 1997; Solow, 1993; Zhang, 2007, 2010, 2011a; Zhang and Schoenly, 1999), here I propose a method to test the statistical significance of the Boolean correlation measures as described above. Suppose that there are n pairs of observed data for two Boolean variables x and y, as demonstrated bellow:

We assume that there are  $n_x$  and  $n_y$  of 1 in vector x and vector y respectively. First, calculate the practical correlation r of x and y. Second, randomly re-assign  $n_x$  and  $n_y$  of 1 in x and y respectively, and calculate the theoretical correlation r of re-arranged x and y. Repeat the procedure s times, and find the times of absolute theoretical correlations greating than the absolute practical correlation, w. If w/s < p, here p=0.01, 0.001, etc., then we conclude that the practical correlation r between x and y is statistically significant at the statistical level p.

#### **3** Causality Inference of Two Boolean Variables

There is a possible causality between two Boolean variables if their correlation is statistically significant. To exploit the general law of causality and correlation, we need to construct the artificial data of two Boolean variables, known the independent variable, x, and dependent variable, y.

# 3.1 Causality principle of Boolean variables

Suppose that the significant correlation between two Boolean variables x and y is confirmed. We assume that there is likely a causality between two Boolean variables x and y, and furthermore, x is the independent variable and y is the dependent variable. In a set of sample data, as demonstrated above, x=1 will most likely result in y=1 at a greater probability. And, y=1 that have not been resulted from x=1 occurs occasionally at a smaller probability and meet x=0 or x=1. The latter stochastic y=1 is produced from the stochasticity of variable y and the dependence of y on other unknown variables.

## 3.2 Relationship between causality and statistic parameters

#### 3.2.1 Statistical simulation

From the Boolean correlation measures above, it is apparent that the only valuable parameters for causality inference are b and c. The parameters, a and d, are not able to provide any valuable information on the inference of between-variable causality. I try to find the deterministic relationship between (b, c) and causality by statistical simulation.

To avoid infinity (Inf, value/0) or non-value (NaN, 0/0), only quartile correlation is used in the simulation. In a simulation, construct the data of independent variable x and dependent variable y following the method above. Second, calculate the quartile correlation r, and b, c. Repeat the procedure many times, each time construct the new data of independent variable x and dependent variable y with random data sizes and dependency probabilities and dependency errors, etc., and record r, and b, c. Finally, calculate the mean r, mean b and mean c, and test the statistic difference between mean b and mean c. Meanwhile, calculate the Pearson correlation between absolute r and c>b (c>b: 1;  $c\leq b$ : 0) and the Pearson correlation between absolute r and c-b, and make statistic tests on the Pearson correlations.

The full Matlab codes of the statistical simulation, xyGen, for finding relationship between causality and statistic parameters are as follows (see supplementary material also):

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| clear   |
|---|
| sel=1; %sel=1: for constructing positive dependency; sel=2: for constructing negative dependency  |
| sig=0.01; %Statistic significance level for detecting Pearson correlation between Boolean correlation r and c-b   |
| xdevi=0.2; %Deviation of dependency of y on x, e.g., 0.1, 0.2, 0.3, etc.  |
| yerr=0.7; %1-yerr: stochastic error of y, determined by random error and the influence of other unknown variables,  |
| %e.g., 0.6, 0.7, 0.8, etc.  |
| m=200; %For determining the maximum size of Boolean variables x and y   |
| sim=20000; %Number of simulations (randomizations); generally, sim>=m*100   |
| res=zeros(sim,7);   |
| nn=zeros(sim,1);  |
| for i=1:sim   |
| n=floor(m*rand()+10); %The size, n, can be fixed, e.g., n=m   |
| nn(i)=n;  |
| xprob=rand()-xdevi;   |
| x=zeros(n,1);   |
| y=zeros(n,1);   |
| xbas=rand(n,1);   |
| x=xbas>xprob;   |
| if (sel==1) yx=xbas>(xprob+xdevi);  |
| elseif (sel==2) yx=xbas<(xprob-xdevi); end;   |
| <pre>yran=rand(n,1)&gt;yerr;</pre>  |
| y=yx   yran;  |
| [r,a,b,c,d]=quartilecorr(x,y);  |
| res(i,:)=[sum(x) sum(y) r a b c d];   |
| end   |
| means_of_b_and_c=mean(res(:,5:6))   |
| [h,p_value_for_difference_between_b_and_c,v]=ttest2(res(:,5),res(:,6),sig);   |
| p_value_for_difference_between_b_and_c  |
| if (h==0)   |
| sprintf(['The difference between b and c is not statistically significant at p=',num2str(sig),'\n'])  |
| else sprintf(['The difference between b and c is statistically significant (p=', num2str(p_value_for_difference_between_b_and_c),   |
| ')\n'])   |
| end   |
| r_mean=mean(res(i,3))   |
| Pearson_correlation_between_absolute_r_and_c_great_than_b=corr(abs(res(:,3)),double(res(:,6)>res(:,5)))   |
| $tvalue = abs(Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_great\_than\_b)))))$ |
| d_c_great_than_b.^2)/(n-2));  |
| alpha=(1-tcdf(tvalue,mean(nn)-2))*2;  |
| if (alpha<=sig)   |
| sprintf(['Pearson correlation between absolute r and c>b is statistically significant (p=',num2str(alpha),')\n'])   |
| else sprintf(['Pearson correlation between absolute r and c>b is not statistically significant at p=',num2str(sig),'\n'])   |
| end   |
| Pearson_correlation_between_absolute_r_and_c_minus_b=corr(abs(res(:,3)),res(:,6)-res(:,5))  |
| $tvalue = abs(Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b)./sqrt((1-Pearson\_correlation\_between\_absolute\_r\_and\_c\_minus\_b])))))$   |
| minus_b.^2)/(n-2));   |

alpha=(1-tcdf(tvalue,mean(nn)-2))\*2;

if (alpha<=sig)

 $sprintf(['Pearson correlation between absolute r and c-b is statistically significant (p=',num2str(alpha),')\n'])$ else  $sprintf(['Pearson correlation between absolute r and c-b is not statistically significant at p=',num2str(sig),'\n'])$ end

```
function [r,a,b,c,d]=quartilecorr(x,y) %x and y: two column vectors to be tested.

if (max(size(x)) \sim =max(size(y)))

error('Array sizes do not match.');

end

if ((min(size(x)) \sim =1) | (min(size(y)) \sim =1))

error('Both x and y are vectors');

end

a=sum((x==0) \& (y==0));

b=sum((x==0) \& (y==0));

c=sum((x==0) \& (y==0));

d=sum((x\sim=0) \& (y==0));

r=sin((a+d-(b+c))/(a+b+c+d)*pi/2);
```

3.2.2 Law found from statistical simulation

The results of statistical simulation indicated that for positive causality (r>0; x: independent variable, y: dependent variable), there is a significant positive Pearson correlation between absolute r and c>b (c>b: 1;  $c\leq b$ : 0), and between absolute r and c-b; for negative causality (r<0; x: independent variable, y: dependent variable), there is a significant positive Pearson correlation between absolute r and  $c\leq b$  (c>b: 0;  $c\leq b$ : 1), and between absolute r and b-c.

## 3.3 Statistical simulation for causality inference based on observed Boolean data

According to the law above, a significant *r* and c > b (r > 0; *x*: independent variable, *y*: dependent variable) or c < b (r > 0; *y*: independent variable, *x*: dependent variable) can be used as the criteria for possible causality of Boolean variables.

First, assume that the Boolean correlation between the two Boolean variables is statistically significant. Following the principle of randomization tests (Manly, 1997; Solow, 1993; Zhang, 2007, 2010, 2011a; Zhang and Schoenly, 1999), I try to use statistical simulation to find the causality based on observed Boolean data. In each randomization process, two re-arranged Boolean variables, xx and yy, are generated based on the observed data, x and y. The elements with shared 0 and 1 in original observed data are reserved in re-arranged x and y. And other elements are proportionally randomized re-arranged as follows:

 $v_1 = c/(b+c)$   $v_2 = b/(b+c)$  z = rand(n)  $xy = x \lor y$   $xx = (x \land y) \lor (xy \land (z > 1 - v_1))$   $yy = (x \land y) \lor (xy \land (z \le v_2))$ 

Then calculate and record *b* and *c*. Repeat the procedure many times, finally calculate the proportions (i.e., calculated *p* values,  $p_1, p_2$ ) of c > b and  $c \le b$ .

For r>0, if c>b and  $p_2 < p$ , where p is the given significance level, then x is the independent variable and y is the dependent variable; or else if c<b and  $p_1<p$ , then y is the independent variable and x is the dependent variable. For r<0, if c<b and  $p_1<p$ , then x is the independent variable and y is the dependent variable; or else if c>b and  $p_2<p$ , then y is the independent variable.

The full Matlab codes, causalInferBool, of the statistical simulation for causality inference based on observed Boolean data are as follows (see supplementary material also):

clear

```
xyd=input('Input the Excel file name of raw data (e.g., xyd.xls: xyd=(dij)n\times 2, dij=0 or 1, i=1,2,...,n; j=1,2. In the file, column 1 is for variable 1 and column 2 is for variable 2): ','s');
```

sel=input('Choose a correlation measure (1: point correlation; 2: quartile correlation; 3: cosine correlation; 4: cosine+ correlation; 5: Jaccard correlation): ');

```
p=input('Input the statistical significance level p for correlation inference (e.g., 0.001): ');
```

sig=input('Input the statistical significance level p for causality inference (e.g., 0.05, 0.1, 0.2, etc.): ');

```
sim=input('Input the number of simulations (e.g., 10000): ');
```

xyd=xlsread(xyd);

n=size(xyd,1);

x=xyd(:,1);

y=xyd(:,2);

switch (sel)

case 1

[r,a,b,c,d]=pointcorr(x,y); str='point correlation';

```
case 2
```

[r,a,b,c,d]=quartilecorr(x,y); str='quartile correlation';

```
case 3
```

[r,a,b,c,d]=cosinecorr(x,y); str='cosine correlation';

```
case 4
```

```
[r,a,b,c]=cosinepluscorr(x,y); str='cosine+ correlation';
```

case 5

[r,b,c,d]=jaccard(x,y); str='Jaccard correlation';

```
end
```

```
if (isnan(r) | (r==Inf) | (r==-Inf))
```

sprintf(['The ',str,' measure is not valid. Try to use another correlation measure.\n'])

```
pause();
```

end

- nx=sum(x);
- ny=sum(y);

```
ww=0;
```

ss=0;

for s=1:sim

xx=zeros(n,1);

yy=zeros(n,1);

idx=randperm(n);

```
idy=randperm(n);
for i=1:nx
xx(idx(i))=1;
end
for i=1:ny
yy(idy(i))=1;
end
switch (sel)
     case 1
          [rs,as,bs,cs,ds]=pointcorr(xx,yy);
     case 2
          [rs,as,bs,cs,ds]=quartilecorr(xx,yy);
     case 3
          [rs,as,bs,cs,ds]=cosinecorr(xx,yy);
     case 4
          [rs,as,bs,cs]=cosinepluscorr(xx,yy);
     case 5
          [rs,bs,cs,ds]=jaccard(xx,yy);
end
if (isnan(rs) | (rs==Inf) | (rs==-Inf)) continue; end
ss=ss+1;
if (((r>0) \& (rs>r)) | ((r<0) \& (rs<r))) ww=ww+1; end
end
id=0;
if ((ww/ss)<p)
sprintf(['There is a significant ',str,' (r=',num2str(r),') between two variables (p=',num2str(ww/ss),')\n'])
id=1;
else sprintf(['There is not significant ',str,' (r=',num2str(r),') between two variables (p=',num2str(ww/ss),')\n'])
sprintf(['So, causality may not exist between two variables based on ',str,'\n'])
end
v1=c/(b+c);
v2=b/(b+c);
for s=1:sim
z=rand(n,1);
xy=x | y;
xx=(x & y) | (xy & (z>1-v1));
yy=(x & y) | (xy & (z<=v2));
bs=sum((xx==0) & (yy~=0));
cs=sum((xx~=0) & (yy==0));
bc(s,:)=[bs cs];
end
p1=sum(bc(:,2)>bc(:,1))/sim;
p2=sum(bc(:,2)<=bc(:,1))/sim;
if (r>0)
if ((c>b) & (id==1) & (p2<sig))
```

sprintf(['The variable for column 1 is the independent variable, and the variable for column 2 is the dependent variable  $(p=',num2str(p2),')\n'])$ elseif ((c<b) & (id==1) & (p1<sig)) sprintf(['The variable for column 2 is the independent variable, and the variable for column 1 is the dependent variable  $(p=',num2str(p1),')\n'])$ else sprintf(['However, causality may not exist between two variables (p=',num2str(sig),')\n']) end elseif (r<0) if ((c<b) & (id==1) & (p1<sig)) sprintf(['The variable for column 1 is the independent variable, and the variable for column 2 is the dependent variable  $(p=',num2str(p1),')\n'])$ elseif ((c>b) & (id==1) & (p2<sig)) sprintf(['The variable for column 2 is the independent variable, and the variable for column 1 is the dependent variable  $(p=',num2str(p2),')\n'])$ else sprintf(['However, causality may not exist between two variables (p=',num2str(sig),')\n']) end end function [r,a,b,c,d]=pointcorr(x,y) %x and y: two column vectors to be tested. if (max(size(x))~=max(size(y))) error('Array sizes do not match.'); end if  $((\min(size(x)) \sim 1) | (\min(size(y)) \sim 1))$ error('Both x and y are vectors'); end a=sum((x==0) & (y==0));  $b=sum((x==0) \& (y \ge 0));$ c=sum((x~=0) & (y==0));  $d=sum((x \ge 0) \& (y \ge 0));$ r = (a\*d-b\*c)/sqrt((a+b)\*(c+d)\*(a+c)\*(b+d));function [r,a,b,c,d]=quartilecorr(x,y) %x and y: two column vectors to be tested. if (max(size(x))~=max(size(y))) error('Array sizes do not match.'); end if  $((\min(size(x)) \sim 1) | (\min(size(y)) \sim 1))$ error('Both x and y are vectors'); end a=sum((x==0) & (y==0)); b=sum((x==0) & (y~=0));  $c=sum((x \ge 0) \& (y = = 0));$ d=sum((x~=0) & (y~=0));

```
r=sin((a+d-(b+c))/(a+b+c+d)*pi/2);
```

```
function [r,a,b,c,d]=cosinecorr(x,y)
                                                       %x and y: two column vectors to be tested.
if (max(size(x))~=max(size(y)))
 error('Array sizes do not match.');
end
if ((\min(size(x)) \sim = 1) | (\min(size(y)) \sim = 1))
 error('Both x and y are vectors');
end
a=sum((x==0) & (y==0));
b=sum((x==0) \& (y \ge 0));
c=sum((x~=0) & (y==0));
d=sum((x~=0) & (y~=0));
r=sqrt(a^2*d^2/((a+b)*(a+c)*(b+d)*(c+d)));
function [r,a,b,c]=cosinepluscorr(x,y)
                                                         %x and y: two column vectors to be tested.
if (max(size(x))~=max(size(y)))
 error('Array sizes do not match.');
end
if ((min(size(x))~=1) | (min(size(y))~=1))
 error('Both x and y are vectors');
end
a=sum((x==0) & (y==0));
b=sum((x==0) & (y~=0));
c=sum((x~=0) & (y==0));
r=sqrt(a^2/((a+b)^*(a+c)));
function [r,b,c,d] = jaccard(x,y)
%x and y: two column vectors to be tested.
if (max(size(x))~=max(size(y)))
 error('Array sizes do not match.');
end
if ((\min(size(x)) \sim 1) | (\min(size(y)) \sim 1))
 error('Both x and y are vectors');
end
b=sum((x==0) \& (y \ge 0));
c=sum((x \sim = 0) \& (y = = 0));
d=sum((x~=0) & (y~=0));
r =(d-(c+b))/(d+c+b);
```

A set of theoretical data were used to validate the method and the goodness of the method was confirmed.

# **4** Discussion

To increase the reliability of causality inference, the size of Boolean data should be large enough. For a large data, the present method can be used on randomly segmented data blocks (i.e., bootstrap method) in order to draw more reliable conclusion from multiple results. The present method has been tested and validated with

theoretical data. However, future applications and futher validations are expected and possible improvements on the method may be expected.

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