kpcalg: R Package tutorial

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1 Kernel Independence Test

Kernel PC algorithm is heavily based on the Independence Criteria. We use Hilbert-Schmidt Independence Criterion ($HSIC$) and Distance Covariance Criterion (DCC). We use these criteria to test the $H_0 : x \perp y$ (x independent of y) vs $H_1 : x \not\perp y$ (x is not independent of y). Under the null hypothesis H_0 both $HSIC$ and $DCC \approx 0$. We can find a probability of observing data as extreme as ours (the p-value) under the null hypothesis in two ways:

1. Permutation test
2. Gamma test

Permutation test permutes the y values to get $y_{(i)}$ and recalculates the $HSIC_{(i)}$ or $DCC_{(i)}$ and compares it with the original $HSIC$ or DCC respectively. Gamma test approximates the HSIC or DCC distribution under the null hypothesis H_0 by gamma function.

DCC permutation test is implemented in the package "energy".

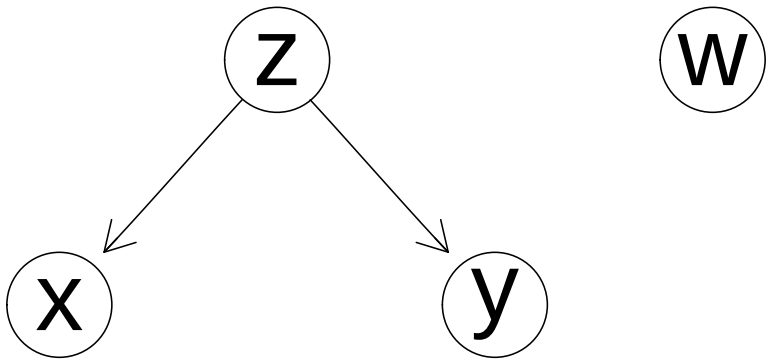
Here we present a small example of independent (x and y) and dependent (z and w) variables. We apply $HSIC$ and DCC based tests to estimate the dependency between them:

```
library(energy)
library(kpcalg)
set.seed(10)
#independence
x <- runif(300)
y <- runif(300)

hsic.gamma(x,y)$p.value

## [1] 0.4950817

hsic.perm(x,y)$p.value

## [1] 0.5148515

dcov.gamma(x,y)$p.value

## [1] 0.7095448

dcov.test(x,y,R=100)$p.value

## [1] 0.7029703

#uncorelated but not dependent
z <- 10*(runif(300)-0.5)
w <- z^2 + 10*runif(300)

cor(z,w)

## [1] -0.0837645
```

```
hsic.gamma(z,w)$p.value

## [1] 0

hsic.perm(z,w)$p.value

## [1] 0.00990099

dcov.gamma(z,w)$p.value

## [1] 0

dcov.test(z,w,R=100)$p.value

## [1] 0.00990099
```

2 Kernel Conditional Independence Test

We consider a simple model with non-linear relationships and non-gaussian noise; $x = \sin(z) + U(0,1)$ and $y = \cos(z) + U(0,1)$



First we generate data from the model above. We generate 300 sample points.

```
set.seed(10)
z <- 10*runif(300)
w <- 10*runif(300)
x <- sin(z) + runif(300)
y <- cos(z) + runif(300)
data <- cbind(x,y,z,w)
```

Now we test $H_0 : x \perp y|z$ (x independent of y given z) vs $H_1 : x \not\perp y|z$ (x is not independent of y given z). H_0 is true, so we should get high p-values:

```
library(pcalg)
library(kpcalg)
#conditionally independent
test1a <- kernelCItest(x=1,y=2,S=c(3),suffStat = list(data=data,ic.method="dcc.gamma"))
test2a <- kernelCItest(x=1,y=2,S=c(3),suffStat = list(data=data,ic.method="dcc.perm"))
test3a <- kernelCItest(x=1,y=2,S=c(3),suffStat = list(data=data,ic.method="hsic.gamma"))
test4a <- kernelCItest(x=1,y=2,S=c(3),suffStat = list(data=data,ic.method="hsic.perm"))
test5a <- kernelCItest(x=1,y=2,S=c(3),suffStat = list(data=data,ic.method="hsic.clust"))
test6a <- gaussCItest( x=1,y=2,S=c(3),suffStat = list(C=cor(data),n=4))

cat("DCC (gamma test): \t\t\t",test1a,
    "\nDCC (permutation test): \t\t",test2a,
```

```
    "\nHSIC-residuals (gamma test): \t\t",test3a,
    "\nHSIC-residuals (permutation test): \t",test4a,
    "\nHSIC-cluster: \t\t\t\t",test5a,
    "\nFisher's Z test: \t\t\t",test6a)

## DCC (gamma test):   0.6455592
## DCC (permutation test):   0.5643564
## HSIC-residuals (gamma test):   0.4868527
## HSIC-residuals (permutation test):   0.4257426
## HSIC-cluster:   0.4158416
## Fisher's Z test:   1
```

All five tests find independence.

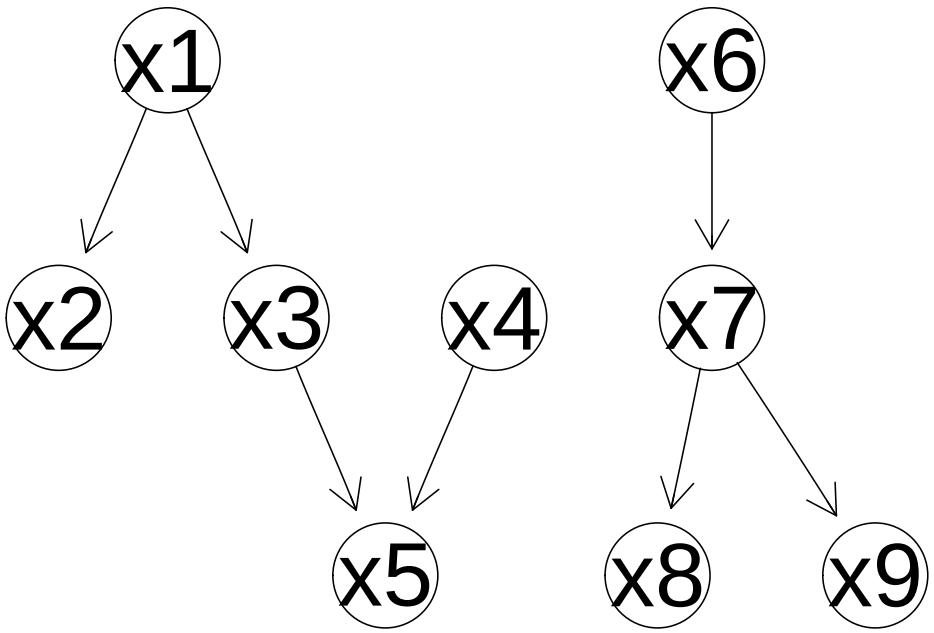
Now we test $H_0 : x \perp y|w$ (x independent of y given w) vs $H_1 : x \not\perp y|w$ (x is not independent of y given w). H_0 is not true, so we should get very low p-values:

```
#dependent
test1b <- kernelCItest(x=1,y=2,S=c(4),suffStat = list(data=data,ic.method="dcc.gamma"))
test2b <- kernelCItest(x=1,y=2,S=c(4),suffStat = list(data=data,ic.method="dcc.perm"))
test3b <- kernelCItest(x=1,y=2,S=c(4),suffStat = list(data=data,ic.method="hsic.gamma"))
test4b <- kernelCItest(x=1,y=2,S=c(4),suffStat = list(data=data,ic.method="hsic.perm"))
test5b <- kernelCItest(x=1,y=2,S=c(4),suffStat = list(data=data,ic.method="hsic.clust"))
test6b <- gaussCItest( x=1,y=2,S=c(4),suffStat = list(C=cor(data),n=4))

cat("DCC (gamma test): \t\t\t",test1b,
    "\nDCC (permutation test): \t\t",test2b,
    "\nHSIC-residuals (gamma test): \t\t",test3b,
    "\nHSIC-residuals (permutation test): \t",test4b,
    "\nHSIC-cluster: \t\t\t\t",test5b,
    "\nFisher's Z test: \t\t\t",test6b)

## DCC (gamma test):   0.03469079
## DCC (permutation test):   0.04950495
## HSIC-residuals (gamma test):   0.000292712
## HSIC-residuals (permutation test):   0.00990099
## HSIC-cluster:   0.00990099
## Fisher's Z test:   1
```

As expected the HSIC and DCC based independence tests reject H_0, while the Fisher's Z test does not.

3 Kernel PC algorithm

This establishes the effectiveness of the kernel and distance based independence tests for testing conditional dependence in data with non-linear relationships and non-gaussian noise. Now we will test the Kernel PC algorithm on a toy network on 9 nodes.



First we generate data from this DAG. We again generate 300 data points.

```
set.seed(4)
n <- 300
data <- NULL
x1 <- 2*(runif(n)-0.5)
x2 <- x1 + runif(n)-0.5
x3 <- x1^2 + 0.6*runif(n)
x4 <- rnorm(n)
x5 <- x3 + x4^2 + 2*runif(n)
x6 <- 10*(runif(n)-0.5)
x7 <- x6^2 + 5*runif(n)
x8 <- 2*x7^2 + 1.5*rnorm(n)
x9 <- x7 + 4*runif(n)
data <- cbind(x1,x2,x3,x4,x5,x6,x7,x8,x9)
```

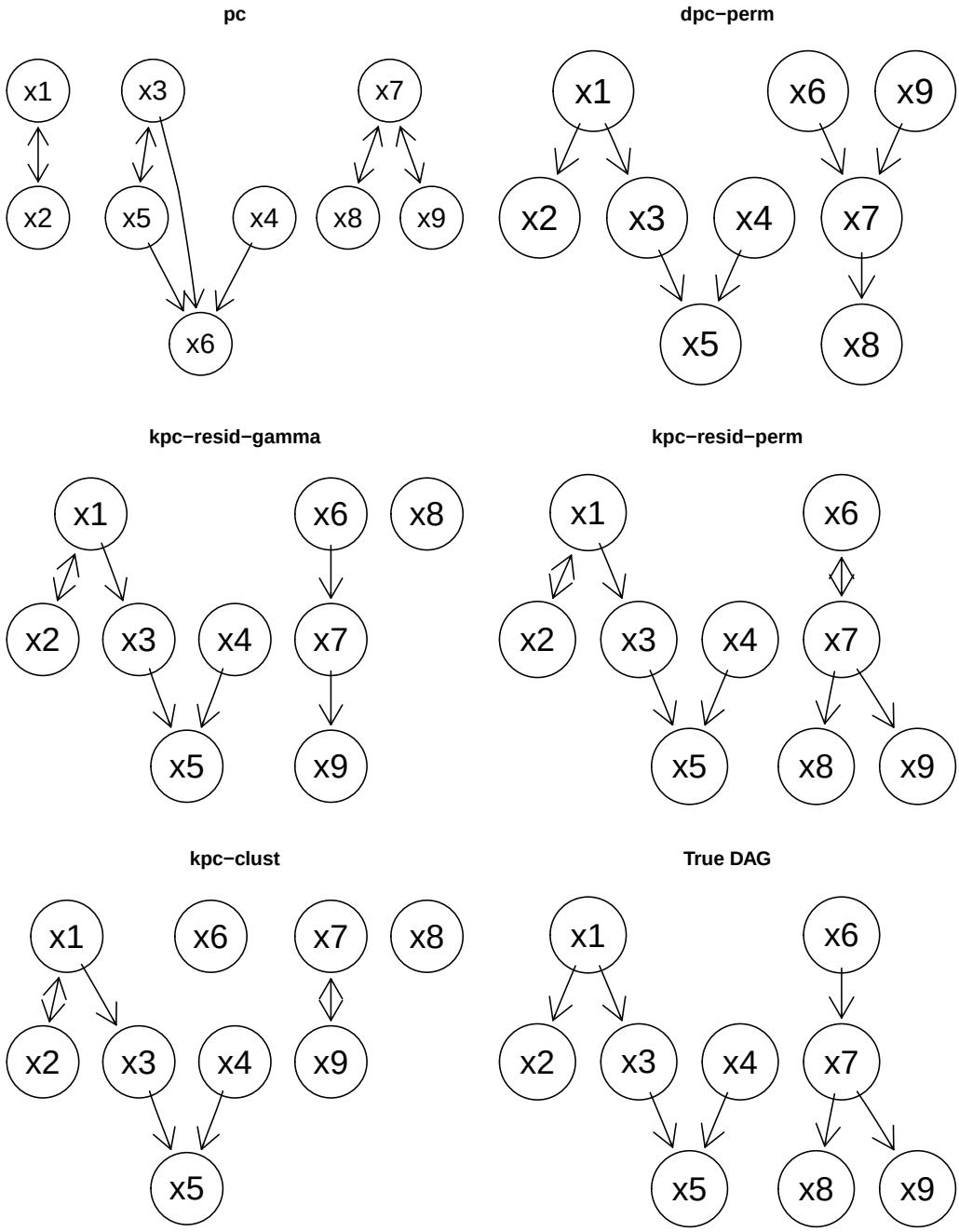
Now we apply PC, Kernel PC residuals (with gamma and permutation independence tests), Kernel PC cluster and Distance PC algorithms to infer the underlying network.

```
library(pcalg)
library(kpcalg)
pc <- pc(suffStat = list(C = cor(data), n = 9),
           indepTest = gaussCItest,
           alpha = 0.9,
           labels = colnames(data),
           u2pd = "relaxed",
           skel.method = "stable",
           verbose = F)
kpc1 <- kpc(suffStat = list(data=data, ic.method="dcc.perm"),
           indepTest = kernelCItest,
           alpha = 0.1,
           labels = colnames(data),
           u2pd = "relaxed",
           skel.method = "stable",
           verbose = F)
```

```
kpc2 <- kpc(suffStat = list(data=data, ic.method="hsic.gamma"),
            indepTest = kernelCItest,
            alpha = 0.1,
            labels = colnames(data),
            u2pd = "relaxed",
            skel.method = "stable",
            verbose = F)
kpc3 <- kpc(suffStat = list(data=data, ic.method="hsic.perm"),
            indepTest = kernelCItest,
            alpha = 0.1,
            labels = colnames(data),
            u2pd = "relaxed",
            skel.method = "stable",
            verbose = F)
kpc4 <- kpc(suffStat = list(data=data, ic.method="hsic.clust"),
            indepTest = kernelCItest,
            alpha = 0.1,
            labels = colnames(data),
            u2pd = "relaxed",
            skel.method = "stable",
            verbose = F)
```

We plot all five outputs as well as the true underlying graph structure:

```
par(mfrow=c(3,2))
plot(pc@graph,attrs=list(node=list(fontsize=5)),main="pc")
plot(kpc1@graph,attrs=list(node=list(fontsize=5)),main="dpc-perm")
plot(kpc2@graph,attrs=list(node=list(fontsize=5)),main="kpc-resid-gamma")
plot(kpc3@graph,attrs=list(node=list(fontsize=5)),main="kpc-resid-perm")
plot(kpc4@graph,attrs=list(node=list(fontsize=5)),main="kpc-clust")
plot(as(true,"graphNEL"),attrs=list(node=list(fontsize=5)),main="True DAG")
```



We observe that all independence based PC versions significantly outperform the original PC algorithm.