Bayesian Networks

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Dataset description

This contains data on coronary artery disease from a Danish heart clinic. The dataset contains 14 discrete variables recorded for 236 patients, 107 of whom actually had the disease. The dataset includes five background variables (sex, hypercholesterolemia, smoking, heridary disposition and workload), one recording whether or not the patient has coronary artery disease, four variables representing disease manifestation (hypertrophy, previous myocardial infarct, angina pectoris, other heartfailures), and four clinical measurements (Qwave, T-wave, Q-wave informative and T-wave informative). Angina pectoris has 3 levels and the remaining 13 variables are binary.

```
##
   cad1
##
##
   14 Variables
                        236 Observations
## Sex
##
          n missing distinct
        236
##
                    0
##
## Value
              Female
                        Male
## Frequency
                         189
                   47
## Proportion 0.199 0.801
##
## AngPec
##
             missing distinct
##
        236
##
              Atypical
## Value
                            None
                                  Typical
## Frequency
                              85
                                       121
                     30
## Proportion
                 0.127
                           0.360
                                     0.513
##
## AMI
##
          n missing distinct
##
        236
                   0
##
## Value
                Definite NotCertain
## Frequency
                       63
## Proportion
                               0.733
                    0.267
##
##
  QWave
##
            missing distinct
##
        236
                    0
## Value
                       Yes
                 No
## Frequency
                153
                        83
```

```
## Proportion 0.648 0.352
## -----
## QWavecode
 n missing distinct
##
    236
       0
##
## Value Nonusable
## Frequency 13
                223
## Proportion 0.055
                0.945
## STcode
    n missing distinct
##
##
    236 0
##
## Value Nonusable
                Usable
## Frequency 79
                157
## Proportion 0.335
                0.665
## ------
## STchange
 n missing distinct
##
    236 0
##
## Value
         No Yes
## Frequency 133 103
## Proportion 0.564 0.436
## SuffHeartF
  n missing distinct
##
    236 0
##
## Value
         No
            Yes
        167
## Frequency
## Proportion 0.708 0.292
## Hypertrophi
    n missing distinct
    236 0 2
##
##
## Value
         No Yes
        172 64
## Frequency
## Proportion 0.729 0.271
## -----
## Hyperchol
## n missing distinct
##
    236 0
##
         No
## Value
            Yes
## Frequency
        108
            128
## Proportion 0.458 0.542
## -----
## Smoker
##
    n missing distinct
    236 0 2
##
##
```

```
## Value
               No
                    Yes
## Frequency
               51
                    185
## Proportion 0.216 0.784
##
  Inherit
##
         n missing distinct
##
                 0
       236
##
## Value
               No
                    Yes
                     74
## Frequency
              162
  Proportion 0.686 0.314
##
  Heartfail
##
         n missing distinct
##
       236
                 0
##
## Value
                 Yes
              No
## Frequency
             177
  Proportion 0.75 0.25
                      _____
##
  CAD
##
         n missing distinct
##
       236
                 0
##
## Value
               No
                    Yes
## Frequency
              129
## Proportion 0.547 0.453
```

Blacklist

A better approach is to incorporate our prior knowledge of the system under study into the model selection process.

The variables are divided into four blocks, namely background variables, disease (which includes CAD and hypertrophy), disease manifestations and clinical measurements. We restrict the model selection process by blacklisting arcs that point from a later to an earlier block. We also blacklist arcs that point from being a smoker to having an hereditary disposition and from smoker, hypercholesterolemia, hereditary and workload to sex. In addition, we assume independence between different clinical tests, so that STchange and STcode cannot influence QWave and QWavecode and viceversa. Finally, we impose that the confidence on a test result (STcode and QWavecode) cannot influence whether or not a test is run (STchange, QWave).

```
##
              from
                             to
## 1
           AngPec
                            Sex
## 2
           AngPec
                    SuffHeartF
           AngPec Hypertrophi
## 3
## 4
           AngPec
                     Hyperchol
           AngPec
## 5
                         Smoker
## 6
           AngPec
                        Inherit
## 7
            AngPec
                            CAD
## 8
               IMA
                            Sex
## 9
               IMA
                    SuffHeartF
## 10
               AMI Hypertrophi
## 11
               IMA
                     Hyperchol
```

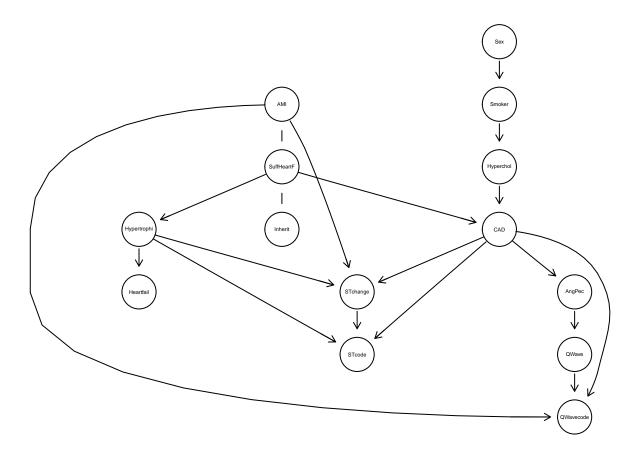
##	12	AMI	Smoker
##	13	AMI	Inherit
##	14	IMA	CAD
##	15	QWave	Sex
##	16	QWave	${\tt AngPec}$
##	17	QWave	AMI
##	18	QWave	STcode
##	19	QWave	STchange
##	20	QWave	SuffHeartF
##	21	QWave	Hypertrophi
##	22	QWave	Hyperchol
##	23	QWave	Smoker
##	24	QWave	Inherit
##	25	QWave	Heartfail
##	26	QWave	CAD
##	27	QWavecode	Sex
##	28	QWavecode	${\tt AngPec}$
##	29	QWavecode	IMA
##	30	QWavecode	QWave
##	31	QWavecode	STcode
##	32	QWavecode	STchange
##	33	QWavecode	SuffHeartF
##	34	QWavecode	Hypertrophi
##	35	QWavecode	Hyperchol
##	36	QWavecode	Smoker
##	37	QWavecode	Inherit
##	38	QWavecode	Heartfail
##	39	QWavecode	CAD
##	40	STcode	Sex
##	41	STcode	${\tt AngPec}$
##	42	STcode	AMI
##	43	STcode	QWave
##	44	STcode	QWavecode
##	45	STcode	STchange
##	46	STcode	SuffHeartF
##	47	STcode	Hypertrophi
##	48	STcode	Hyperchol
##	49	STcode	Smoker
##	50	STcode	Inherit
##	51	STcode	Heartfail
##	52	STcode	CAD
##	53	STchange	Sex
##	54	STchange	AngPec
##	55	STchange	AMI
##	56	STchange	QWave
##	57	STchange	QWavecode
##	58	STchange	SuffHeartF
##	59	STchange	Hypertrophi
##	60	STchange	Hyperchol
##	61	STchange	Smoker
##	62	STchange	Inherit
##	63	STchange	Heartfail
##	64	STchange	CAD
##	65	SuffHeartF	Sex
ırπ	50	Darringar of	Dev

```
## 66 Hypertrophi
                           Sex
## 67 Hypertrophi
                   SuffHeartF
## 68 Hypertrophi
                     Hyperchol
## 69 Hypertrophi
                        Smoker
## 70 Hypertrophi
                       Inherit
## 71
        Hyperchol
                           Sex
## 72
           Smoker
                           Sex
## 73
           Smoker
                       Inherit
## 74
          Inherit
                           Sex
## 75
        Heartfail
                           Sex
## 76
        Heartfail SuffHeartF
        Heartfail Hypertrophi
## 77
## 78
        Heartfail
                     Hyperchol
## 79
        Heartfail
                        Smoker
## 80
        Heartfail
                       Inherit
## 81
        Heartfail
                           CAD
## 82
              CAD
                           Sex
## 83
              CAD
                    SuffHeartF
## 84
              CAD
                     Hyperchol
## 85
              CAD
                        Smoker
## 86
              CAD
                       Inherit
```

Learn network structure

True CPDAG

We assume that the true CPDAG is the one described in Hojsgaard and Thiesson (1993). The true CPDAG has 19 arcs of which 2 undirected.

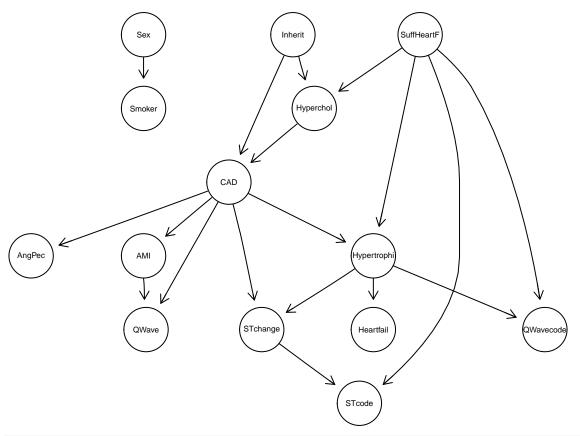


Score based algorithms

Hill climbing algorithm

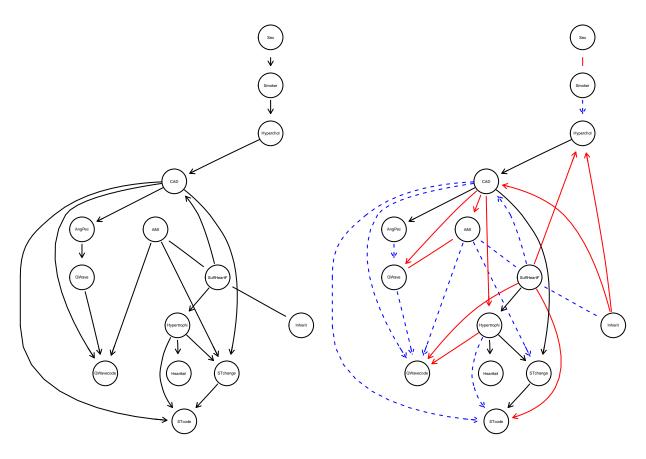
The hill climbing algorithm produces a network with 19 directed arcs.

bn_hc <- hc(cad1, blacklist=blackL)</pre>



unlist(bnlearn::compare(true_dag, cpdag(bn_hc)))

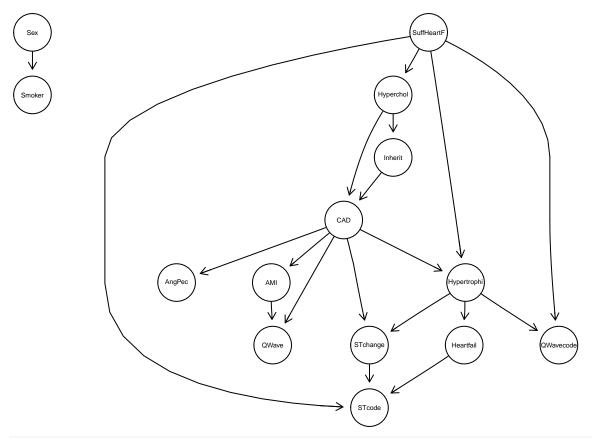
tp fp fn ## 7 11 12



Hill climbing algorithm with random restarts

The algorithm produces a network with 21 directed arcs.

hc_restart = hc(cad1, score = "bde", iss = 1, restart = 10, perturb = 5, blacklist=blackL)

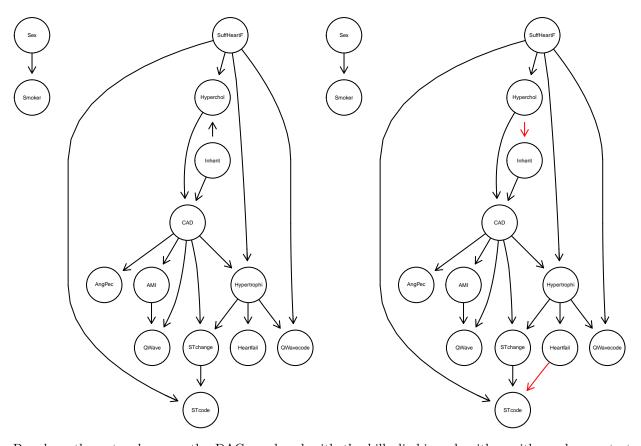


compare score based algorithms

all.equal(bn_hc, hc_restart)

[1] "Different number of directed/undirected arcs"
unlist(bnlearn::compare(bn_hc, hc_restart))

tp fp fn ## 17 2 1

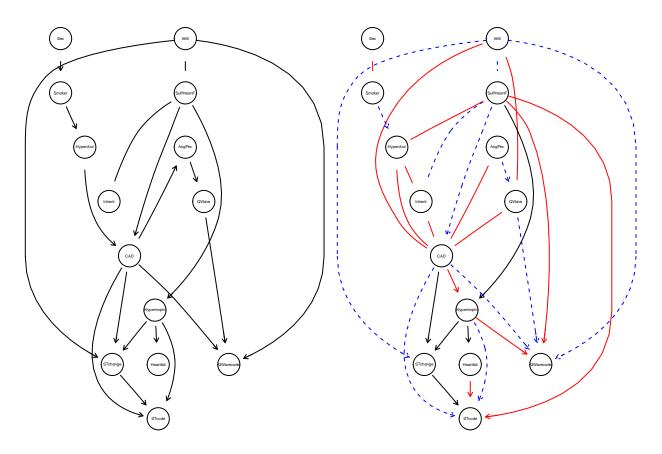


Based on the network score, the DAG produced with the hill climbing algorithm with random restarts provides a slightly worse fit to the data.

```
## [1] -1801.804 -1806.889

# compare with true dag
unlist( bnlearn::compare(true_dag, cpdag(hc_restart)) )

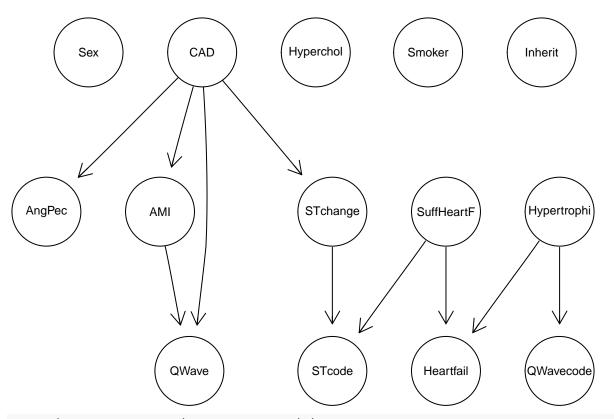
## tp fp fn
## 5 14 14
```



Constraint based algorithms

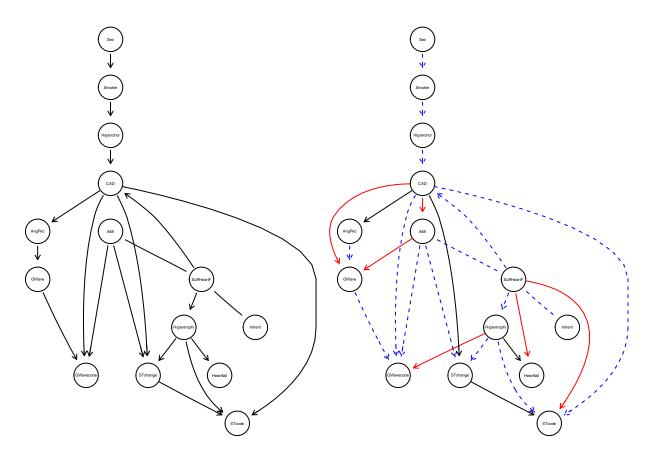
Semi-Interleaved Hiton-PC

The algorihm produces a network with $10~{\rm arcs},\,1$ of which undirected.



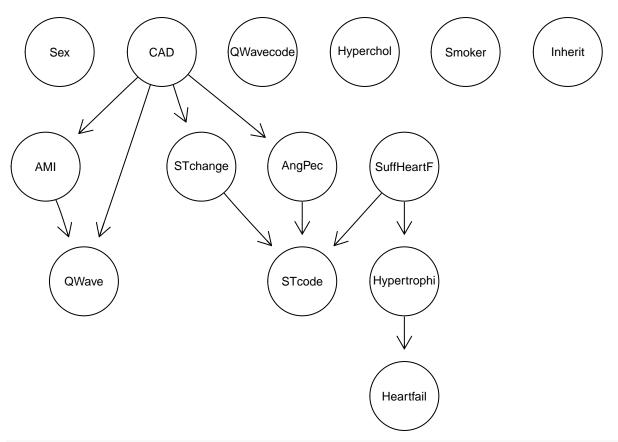
unlist(bnlearn::compare(true_dag, bn_hit))

tp fp fn ## 4 6 15



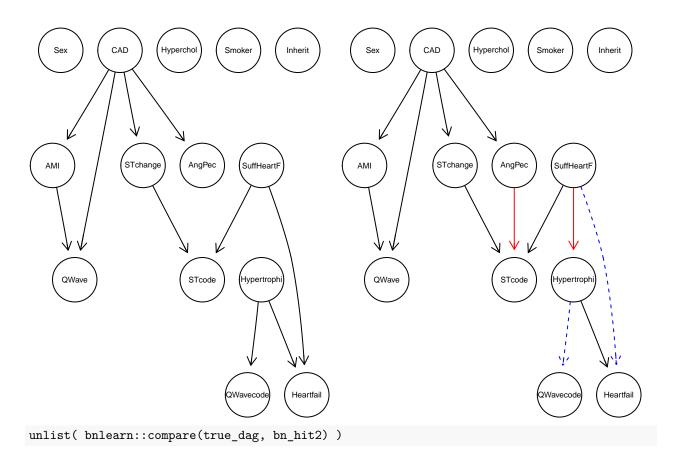
Hiton-PC with permutation tests

The network learned has the same number of directed and undirected arcs as the previous one but a different arc set (2 false positives and 1 false negative).

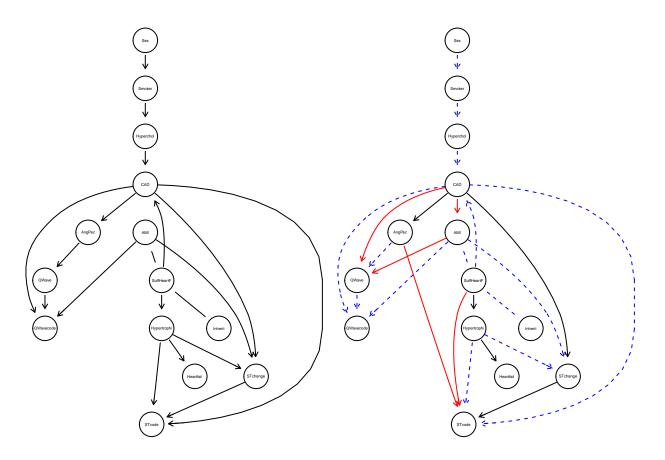


unlist(bnlearn::compare(bn_hit, bn_hit2))

tp fp fn ## 8 2 2

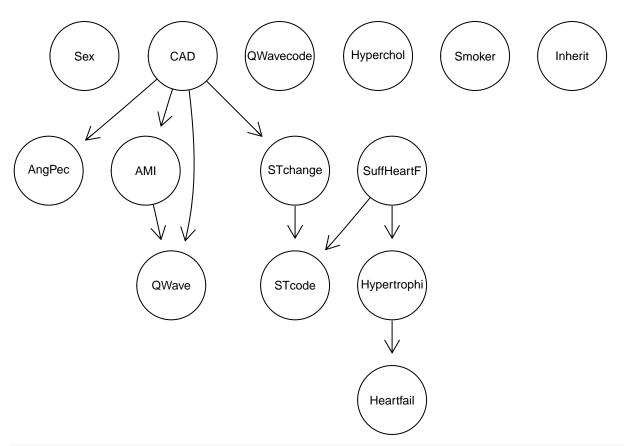


tp fp fn ## 5 5 14



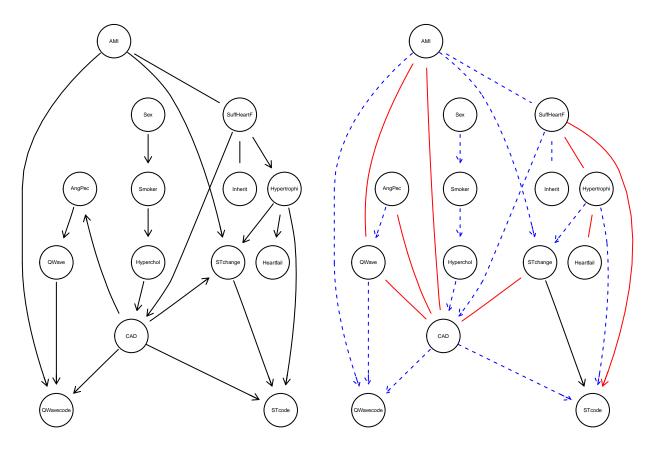
Hybrid algorithms

bn_rsmax <- rsmax2(cad1, restrict="mmpc", maximize="hc", blacklist = blackL)</pre>



unlist(bnlearn::compare(true_dag, cpdag(bn_rsmax)))

tp fp fn ## 1 8 18



Model averaging

Frequentist approach

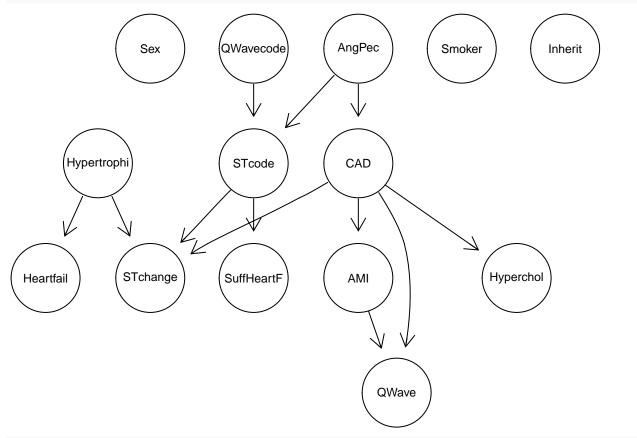
We average multiple networks to improve the structure learned. Bootstrap resampling is applied to the dataset to learn a set of 500 CPDAGS with the hill climbing algorithm. Arcs are considered significant if they appear in at least 85% of the networks, and in the direction that appears most frequently.

```
##
              from
                            to strength direction
## 18
            AngPec
                        STcode
                                   0.904 0.7577434
            {\tt AngPec}
                                   1.000 0.8380000
## 26
                           CAD
                                   0.952 0.7121849
## 29
                IMA
                         QWave
## 57
         QWavecode
                        STcode
                                   0.986 0.7474645
## 71
            STcode
                      STchange
                                   1.000 0.8870000
            STcode SuffHeartF
                                   1.000 0.8770000
## 72
## 111 Hypertrophi
                      STchange
                                   0.858 0.7703963
## 116 Hypertrophi
                                   1.000 0.7590000
                     Heartfail
## 172
                CAD
                           IMA
                                   0.982 0.5458248
## 173
                CAD
                         QWave
                                   0.990 0.7020202
## 176
                CAD
                      STchange
                                   0.938 0.6023454
## 179
               CAD
                     Hyperchol
                                   0.946 0.9809725
```

Since all the values in the direction column are well above 0.5, we can infer that the direction of the arcs is well established and that they are not score equivalent. Lowering the threshold from 85% to 50% does not

change the results of the analysis, which seems to indicate that in this case the results are not sensitive to its value.

avg.boot <- averaged.network(boot, threshold = 0.85)</pre>



unlist(bnlearn::compare(true_dag, cpdag(avg.boot)))

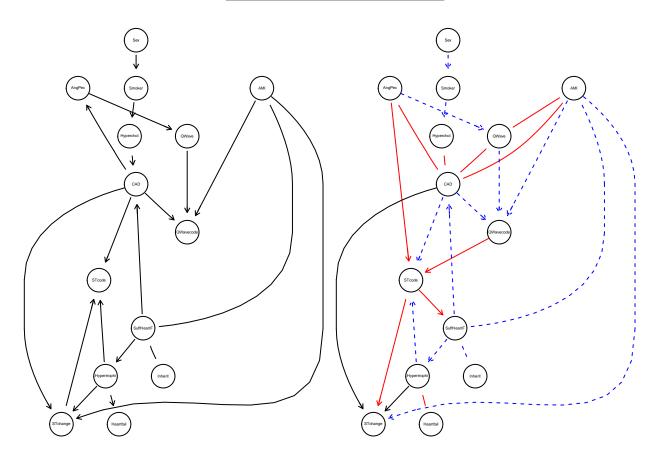
tp fp fn ## 2 10 17

Table 1: Compare CPDAGS

	tp	fp	fn
HC restarts	5	14	14
HC	7	11	12
Hiton	4	6	15
Hiton permutations	5	5	14
Hybrid	1	8	18
Averaging	2	10	17

Table 2: Compare skeletons

	tp	fp	fn
HC restarts	8	11	11
HC	8	10	11
Hiton	4	6	15
Hiton permutations	5	5	14
Hybrid	5	4	14
Averaging	6	6	13



Model comparison

There are 5 archs that appear both in the true DAG and in the DAG learned by the Hill Climbing algorithm and 14 arcs that appear in the current DAG but not in the true DAG and viceversa.

Table 3: Hamming distance

	Hamming distance	SHD
HC restarts	22	26
HC	21	23
Hiton	21	24
Hiton permutations	19	21
Hybrid	18	20
Averaging	19	22

The skeleton of the network learned by the HC algorithm differs from the skeleton of the true DAG by 21 arcs, while its CPDAG differs from the true CPDAG by 23 arcs.

Parameter estimate

We choose to use the Bayesian network produced by the hill climbing algorithm for the purpose of statistical inference. The graph is chosen because it has the largest number of true positive arcs with respect to the true CPDAG among the estimated graphs. The networks produced by the constraint based algorithms and by the hybrid algorithms are not considered eligible for selection because the node CAD has no parents, making it impossible to inquire about the underlying causes of the disease.

The joint probability distribution of the model obtained with the hill climbing algorithm factorizes according to:

P(Sex, AngPec, AMI, QWave, QWavecode, STcode, STchange, SuffHeartF, Hypertrophi, Hyperchol, Smoker, Inherit,

$$\label{eq:heartfail} \begin{split} & \operatorname{Heartfail}, \operatorname{CAD}) = \operatorname{P(Sex)P(Inherit)P(SuffHeartF)P(Smoker|Sex)P(AMI|CAD)P(CAD|\ Inherit,\ Hyperchol)} \\ & \operatorname{P(Hyperchol|Inherit,\ SuffHeartF)\ P(QWave|AMI,\ CAD)\ P(STchange|\ CAD,\ Hypertrophi)\ P(AngPec|CAD)} \\ & \operatorname{P(Hypertrophi|\ CAD,\ SuffHeartF)\ P(Heartfail|Hypertrophi)\ P(QWavecode|Hypertrophi,\ SuffHeartF)} \\ & \operatorname{P(STcode|STchange,\ SuffHeartF)} \end{split}$$

The MLE and the Bayes estimator yield similar results for the model coefficients.

```
fit_mle = bn.fit(bn_hc, cad1, method ="mle")
coef(fit_mle$CAD)
```

```
, , Inherit = No
##
##
        Hyperchol
## CAD
                          Yes
                No
     No 0.8214286 0.4487179
##
##
     Yes 0.1785714 0.5512821
##
##
     , Inherit = Yes
##
##
        Hyperchol
## CAD
                          Yes
##
     No 0.5000000 0.2600000
     Yes 0.5000000 0.7400000
fit_bay = bn.fit(bn_hc, cad1, method = "bayes", iss = 10)
coef(fit bay$CAD)
```

```
## , , Inherit = No
##
##
        Hyperchol
## CAD
                         Yes
                No
    No 0.8121387 0.4503106
##
##
     Yes 0.1878613 0.5496894
   , , Inherit = Yes
##
##
##
        Hyperchol
## CAD
                No
                         Yes
##
     No 0.5000000 0.2714286
     Yes 0.5000000 0.7285714
```

Inference

Exact inference

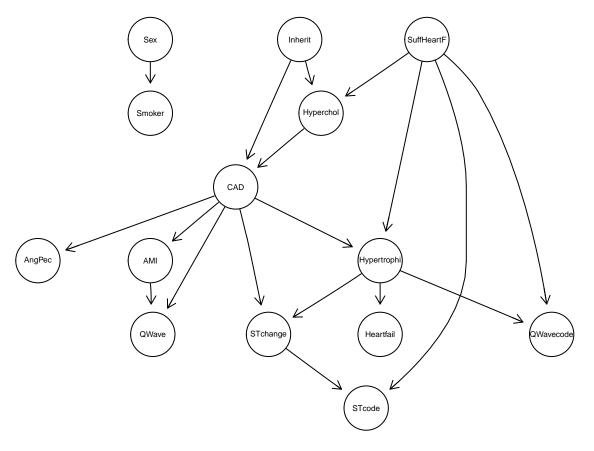


Figure 1: Bayesian network

```
querygrain(junction, nodes = "CAD")

## $CAD

## CAD

## No Yes

## 0.5464106 0.4535894
```

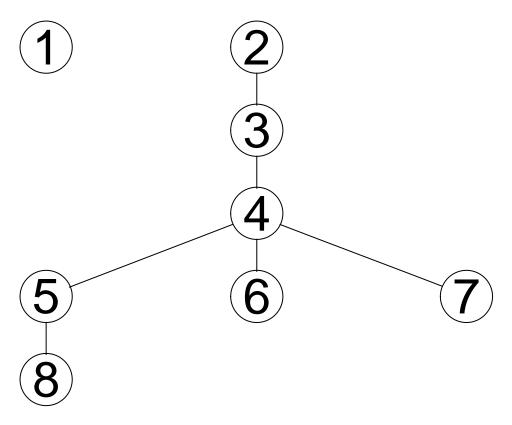


Figure 2: Junction tree

Since smoker is not directly connected to CAD in the graph, we find that P(CAD|Smoker = Yes) = P(CAD).

```
gr1.ev1 <- setFinding(junction,nodes=c("Smoker"),states=list(c("Yes")))
querygrain(gr1.ev1,nodes=c("CAD"),type = "marginal")

## $CAD
## CAD
## No Yes
## 0.5464106 0.4535894

In fact, the two nodes are d-separated in the original graph.
bnlearn::dsep(bn_hc, x = "CAD", y = "Smoker")</pre>
```

[1] TRUE

0.3377717 0.6622283

The probability of observing CAD = Yes is higher for the evidence Inherit = Yes (about 66%) since the two nodes are connected by an arc.

```
gr1.ev1 <- setFinding(junction,nodes=c("Inherit"),states=list(c("Yes")))
querygrain(gr1.ev1,nodes=c("CAD"),type = "marginal")

## $CAD
## CAD
## No Yes</pre>
```

If both Inherit and Hypercol are present, the probability of CAD is about 74%

```
gr1.ev2 <- setFinding(junction, nodes=c("Inherit", "Hyperchol"),states=list(c("Yes"), c( "Yes" )))</pre>
querygrain(gr1.ev2,nodes=c("CAD"),type = "marginal")
## $CAD
## CAD
##
   No Yes
## 0.26 0.74
Adding SuffHeart to the evidence does not change the probability distribution of CAD
gr1.ev3 <- setFinding(junction, nodes=c("Inherit", "Hyperchol", "SuffHeartF"), states=list(c("Yes"), c(
querygrain(gr1.ev3,nodes=c("CAD"),type = "marginal")
## $CAD
## CAD
##
    No Yes
## 0.26 0.74
gr1.ev4 <- setFinding(junction, nodes=c( "SuffHeartF"),states=list(c("Yes")))</pre>
querygrain(gr1.ev4,nodes=c("CAD"),type = "marginal")
## $CAD
## CAD
##
                    Yes
          Nο
## 0.4931176 0.5068824
However, the two nodes are not d-separated in the original graph, since there is a path going from SuffHeartF
bnlearn::dsep(bn_hc, x = "SuffHeartF", y = "CAD")
## [1] FALSE
bnlearn::path(bn_hc, from = "SuffHeartF", to = "CAD")
## [1] TRUE
SuffHeartF and CAD are not conditionally independent even if we condition on Hyperchol, since there exist
other paths between the nodes.
bnlearn::dsep(bn_hc, x = "SuffHeartF", y = "CAD", z = "Hyperchol")
## [1] FALSE
The presence of CAD makes AngPec and QWave more likely and Hypertrophi less likely
gr1.ev5 <- setFinding(junction, nodes=c( "CAD"), states=list(c("Yes")))</pre>
querygrain(gr1.ev5, nodes=c("AngPec", "Hypertrophi", "QWave"), type = "marginal")
## $QWave
## QWave
                    Yes
##
          No
## 0.4205607 0.5794393
##
## $AngPec
## AngPec
     Atypical
                     None
                              Typical
## 0.05607477 0.12149533 0.82242991
##
## $Hypertrophi
```

```
## Hypertrophi
## No Yes
## 0.8589799 0.1410201
```

Next, we investigate the joint distribution of CAD and Hyperchol given that the patient has an hereditary predisposition.

```
gr1.ev6 <- setFinding(junction, nodes=c( "Inherit"), states=list(c("Yes")))
querygrain(gr1.ev6, nodes=c("CAD", "Hyperchol"), type = "joint")

## Hyperchol</pre>
```

```
## CAD No Yes
## No 0.1620244 0.1757473
## Yes 0.1620244 0.5002039
```

Finally, we compute the probability of CAD conditional on the evidence and the values of Hyperchol $P(CAD|Inherit=Yes, Hypercol=h), h \in \{Yes, No\}.$

```
querygrain(gr1.ev6, nodes = c("CAD", "Hyperchol"), type = "conditional")

## Hyperchol
## CAD No Yes
## No 0.5 0.26
## Yes 0.5 0.74
```

Approximate inference

Logic sampling

By generating 10^6 observations from the fitted Bayesian network we find that P(CAD = Yes|Inherit = Yes) = 0.65 and P(CAD = Yes|Hyperchol = Yes,Inherit = Yes) = 0.73, in line with the previous findings obtained via exact inference. In both queries, P(E) is large enough for the logic sampling algorithm to estimate the probability with sufficient precision, which is confirmed by the fact that the likelihood weighting approach yields similar results.

```
cpquery(fit_bay, event=(CAD=="Yes"),
evidence = (Inherit=="Yes"), method="ls", n=10^6)

## [1] 0.6521307

cpquery(fit_bay, event=(CAD=="Yes"),
evidence = (Inherit=="Yes") & (Hyperchol == "Yes"), method="ls", n=10^6)

## [1] 0.7267448

cpquery(fit_bay, event=(CAD=="Yes"),
evidence = list(Inherit ="Yes", Hyperchol = "Yes"), method="lw")

## [1] 0.7299573
```

Classification

Naive Bayes Classifier

The naive Bayes classifier predicts the correct class about 85% of the time, whereas the original Bayesian network predicts the correct class only 67% of the time. Generating a random sample, as we did in this example, is optional since the database is large enough for the classifier to yield robust estimates even if applied to the original data.

```
set.seed(123)
survey <- bnlearn::rbn(fit_bay,1000)</pre>
nbcl <- naive.bayes (survey, training="CAD")</pre>
graphviz.plot(nbcl,layout="fdp")
                                                 Heartfail
                             AMI
                                                                     QWave
       QWavecode
                                                                                  Inherit
                                              CAD
  Smoker
                        SuffHeartF
                                                                                STchange
                                                  Hyperchol
         STcode
                                                                          Sex
                              AngPec
                                                   Hypertrophi
nbcl.trained <- bn.fit(nbcl,survey)</pre>
coef(nbcl.trained$CAD)
      No
            Yes
## 0.548 0.452
coef(nbcl.trained$Hypertrophi)
##
               CAD
## Hypertrophi
                        No
                                  Yes
##
            No 0.6478102 0.8539823
##
            Yes 0.3521898 0.1460177
set.seed(123)
cv.nb <- bn.cv(nbcl, data=survey, runs=10,</pre>
method="k-fold",folds=10)
cv.nb
##
##
     k-fold cross-validation for Bayesian networks
```

##

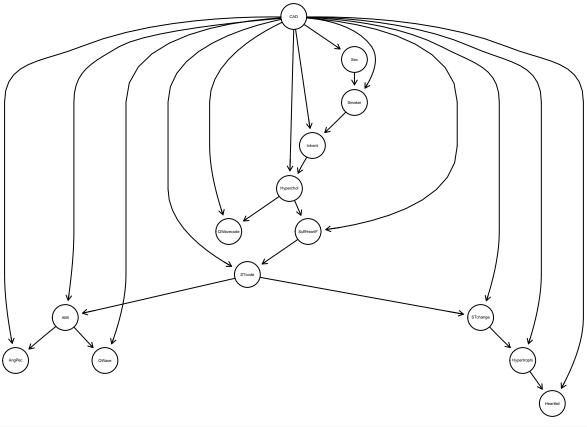
```
##
     target network structure:
##
      [Naive Bayes Classifier]
     number of folds:
##
                                             10
##
     loss function:
                                             Classification Error (Posterior, exact)
##
     training node:
##
    number of runs:
                                             10
     average loss over the runs:
                                             0.1465
     standard deviation of the loss:
                                             0.001900292
set.seed(123)
cv.orig <- bn.cv(bn_hc, data = survey, runs=10, method ="k-fold", folds=10,
                 loss="pred", loss.args = list(target="CAD"))
cv.orig
##
##
     k-fold cross-validation for Bayesian networks
##
##
     target network structure:
##
      [Sex] [SuffHeartF] [Inherit] [Hyperchol|SuffHeartF:Inherit] [Smoker|Sex]
##
      [CAD|Hyperchol:Inherit] [AngPec|CAD] [AMI|CAD] [Hypertrophi|SuffHeartF:CAD]
      [QWave|AMI:CAD] [QWavecode|SuffHeartF:Hypertrophi] [STchange|Hypertrophi:CAD]
##
##
      [Heartfail|Hypertrophi][STcode|STchange:SuffHeartF]
##
     number of folds:
     loss function:
                                             Classification Error
##
                                             CAD
     training node:
##
##
    number of runs:
                                             10
##
     average loss over the runs:
                                             0.334
##
     standard deviation of the loss:
                                             0.004242641
```

Tree-Augumented Naive Bayes Classifier

The TAN classifier has a slightly higher predictive accuracy than the Naive Bayes classifier (86%).

```
set.seed(123)

tan.cl <- tree.bayes(survey, training="CAD")
graphviz.plot(tan.cl)</pre>
```



```
tancl.trained <- bn.fit(tan.cl,survey)</pre>
coef(tancl.trained$CAD)
           Yes
##
      No
## 0.548 0.452
tancl.trained <- bn.fit(tan.cl,survey)</pre>
coef(tancl.trained$Hypertrophi)
   , , STchange = No
##
##
              CAD
## Hypertrophi
                                  Yes
                        No
           No 0.76354680 0.68604651
           Yes 0.23645320 0.31395349
##
   , , STchange = Yes
##
##
              CAD
##
## Hypertrophi
                                  Yes
                        No
           No 0.31690141 0.95714286
##
##
           Yes 0.68309859 0.04285714
set.seed(123)
cv.tan <- bn.cv("tree.bayes",data=survey,</pre>
                 method="k-fold",folds=10,algorithm.args = list(training ="CAD"))
cv.tan
```

```
##
##
     k-fold cross-validation for Bayesian networks
##
##
     target learning algorithm:
                                             TAN Bayes Classifier
     number of folds:
##
     loss function:
##
                                             Classification Error (Posterior, exact)
##
     training node:
##
     number of runs:
                                             10
##
     average loss over the runs:
                                             0.1213
     standard deviation of the loss:
                                             0.003093003
```

By generating 1000 samples from the bayesian network we obtain a distribution with very low variance.

plot(cv.orig,cv.nb,cv.tan, xlab=c("SURVEY","NBC","TAN"))

