Demo-Bayesian Network Learning-R

April 8, 2020

1 Bayesian Network Learning

1.1 Steps

1. Load the data
2. Install and test the Bayesian Network library
3. Analyze the data before starting with Bayesian Network learning
4. Learn and apply the Bayesian Network

1.2 Load the data

Load the epedemic process data from `epidemic_process.csv`:

[1]:
```
df <- read.csv("data/epidemic_process.csv",header = FALSE)
head(df,5)
```

A data.frame: 5 × 8

	V1 <dbl>	V2 <dbl>	V3 <dbl>	V4 <dbl>	V5 <dbl>	V6 <dbl>	V7 <dbl>	V <dbl>
1	5.484789	31.727771	6.910956	1.08608836	0.3646911	-1.16771646	155.6258	0.
2	8.578305	34.552430	3.908585	1.46419574	-4.3507474	-0.66412494	120.7446	0.
3	1.525187	3.581051	7.528895	0.07795365	0.4458266	0.03096206	357.8053	0.
4	6.151596	33.205968	6.199945	1.14855785	-1.5739643	-0.61707895	133.9650	0.
5	4.443471	30.324971	8.335484	0.97068688	2.7658724	-1.67206454	162.8004	0.

[2]:
```
colnames(df)[1] <- "N_50"
colnames(df)[2] <- "N_150"
colnames(df)[3] <- "N_300"
colnames(df)[4] <- "D_50"
colnames(df)[5] <- "D_150"
colnames(df)[6] <- "D_300"
colnames(df)[7] <- "T_peak"
colnames(df)[8] <- "X_500"
head(df,5)
```

A data.frame: 5 × 8

	N_50 <dbl>	N_150 <dbl>	N_300 <dbl>	D_50 <dbl>	D_150 <dbl>	D_300 <dbl>	T_peak <dbl>	X_ <dbl>
1	5.484789	31.727771	6.910956	1.08608836	0.3646911	-1.16771646	155.6258	0.
2	8.578305	34.552430	3.908585	1.46419574	-4.3507474	-0.66412494	120.7446	0.
3	1.525187	3.581051	7.528895	0.07795365	0.4458266	0.03096206	357.8053	0.
4	6.151596	33.205968	6.199945	1.14855785	-1.5739643	-0.61707895	133.9650	0.
5	4.443471	30.324971	8.335484	0.97068688	2.7658724	-1.67206454	162.8004	0.

1.3 Install and test the Bayesian Network library

In R the package bnlearn [1] is recommended.

[3]:
```
install.packages("bnlearn")
library("bnlearn")
```

```
The downloaded binary packages are in
/var/folders/ct/4pcck8t94sdfc73rhymq4t140000gp/T//RtmpEBHx76/downloaded_packages
```

```
Attaching package: 'bnlearn'
```

```
The following object is masked from 'package:stats':

    sigma
```

We check a few steps from the bnlearn tutorial [2]. It instructs us to take the following steps:

1. learning the structure of the network, or creating one manually, gives an object of class bn that encodes a graph;
2. learning the parameters for a given structure starts from a bn object and gives an object of class bn.fit that encodes the graph and the graph and the conditional probabilities;
3. using the object of class bn.fit for inference.

Step 1: Create a Bayesian Network structure from data. It is of class bn (documentation ?"bn class").

[4]:
```
#?"bn class" #(comment/uncomment to hide/see the documentation)
```

[5]:
```
dag = hc(df)
dag
```

```
  Bayesian network learned via Score-based methods

  model:
   [N_150][D_300][T_peak|N_150][N_50|N_150:D_300:T_peak]
   [N_300|N_50:N_150:T_peak][X_500|N_150:N_300:T_peak]
   [D_150|N_150:N_300:D_300:X_500][D_50|N_50:D_150]
```

```
  nodes:                                  8
  arcs:                                   16
    undirected arcs:                      0
    directed arcs:                        16
  average markov blanket size:            5.25
  average neighbourhood size:             4.00
  average branching factor:               2.00

  learning algorithm:                     Hill-Climbing
  score:                                  BIC (Gauss.)
  penalization coefficient:               1.956012
  tests used in the learning procedure:   140
  optimized:                              TRUE
```

Step 2: Learn the conditional probabilities and create an object of class `bn.fit` (documentation `?"bn.fit class"`).

[6]:
```
#?"bn.fit class" #(comment/uncomment to hide/see the documentation)
```

[7]:
```
fitted = bn.fit(dag, data = df)
fitted
```

```
  Bayesian network parameters

  Parameters of node N_50 (Gaussian distribution)

Conditional density: N_50 | N_150 + D_300 + T_peak
Coefficients:
(Intercept)        N_150        D_300       T_peak
22.53354499  -0.13569241   2.89241010  -0.05903338
Standard deviation of the residuals: 2.052607

  Parameters of node N_150 (Gaussian distribution)

Conditional density: N_150
Coefficients:
(Intercept)
   26.08403
Standard deviation of the residuals: 9.34882

  Parameters of node N_300 (Gaussian distribution)

Conditional density: N_300 | N_50 + N_150 + T_peak
Coefficients:
(Intercept)         N_50        N_150       T_peak
40.98092906  -0.99421836  -0.52720012  -0.08138731
```

```
Standard deviation of the residuals: 0.9271315

  Parameters of node D_50 (Gaussian distribution)

Conditional density: D_50 | N_50 + D_150
Coefficients:
(Intercept)         N_50        D_150
-0.23500075   0.23925440   0.02785962
Standard deviation of the residuals: 0.1327802

  Parameters of node D_150 (Gaussian distribution)

Conditional density: D_150 | N_150 + N_300 + D_300 + X_500
Coefficients:
(Intercept)        N_150        N_300        D_300        X_500
  0.7787538    0.1502129    0.4896753   -1.5231319  -11.2175948
Standard deviation of the residuals: 1.295241

  Parameters of node D_300 (Gaussian distribution)

Conditional density: D_300
Coefficients:
(Intercept)
  -1.249822
Standard deviation of the residuals: 0.5404926

  Parameters of node T_peak (Gaussian distribution)

Conditional density: T_peak | N_150
Coefficients:
(Intercept)        N_150
 321.725655    -5.925472
Standard deviation of the residuals: 30.47764

  Parameters of node X_500 (Gaussian distribution)

Conditional density: X_500 | N_150 + N_300 + T_peak
Coefficients:
 (Intercept)         N_150         N_300        T_peak
 1.056397645   0.003065925   0.012091517  -0.002010491
Standard deviation of the residuals: 0.0292708
```

Step 3: Now we are ready to use the `bn.fit` object.

We can generate random samples:

[8]:
```
set.seed(1)
random_sample <- rbn(fitted, n = 10)
head(random_sample,5)
```

A data.frame: 5 × 8

	N_50 <dbl>	N_150 <dbl>	N_300 <dbl>	D_50 <dbl>	D_150 <dbl>	D_300 <dbl>	T_peak <dbl>	X_ <d
1	7.755674	20.22743	3.744598	1.7232889	1.4204171	-0.4327158	229.87686	0.7
2	4.869642	27.80088	6.530647	0.8433825	0.2715994	-1.0391149	180.82999	0.8
3	3.528535	18.27189	10.928453	0.7732084	2.9756058	-1.5855982	215.72864	0.8
4	8.710506	40.99803	9.744541	1.7715346	1.6704454	-2.4468511	18.16227	1.2
5	3.987244	29.16454	7.345600	0.5033554	-1.7642717	-0.6418055	167.80281	0.9

We can predict new observations:

[9]:
```
library(dplyr)
new_data <- random_sample[1,]
new_data <- select(new_data,-c(8))
new_data
predict(fitted, node = "X_500", data = new_data)
```

```
Attaching package: ‘dplyr’


The following objects are masked from ‘package:stats’:

    filter, lag


The following objects are masked from ‘package:base’:

    intersect, setdiff, setequal, union
```

A data.frame: 1 × 7

	N_50 <dbl>	N_150 <dbl>	N_300 <dbl>	D_50 <dbl>	D_150 <dbl>	D_300 <dbl>	T_peak <dbl>
1	7.755674	20.22743	3.744598	1.723289	1.420417	-0.4327158	229.8769

0.701525985455266

This is quite close to `0.7131789`.

We can compute probabilities with queries:

[10]:
```
cpquery(fitted, event = (N_50 <= 7) & (N_150 <= 20) & (N_300 <= 10), evidence =␣
↪(T_peak >= 100))
```

0.0730853391684902

We can generate (weighted) observations from arbitrary conditional distributions.

[11]:
```
N_x <- cpdist(fitted, nodes = c("N_50", "N_150", "N_300"), evidence = (T_peak
 ↪>= 100), n = 1000)
head(N_x,5)
```

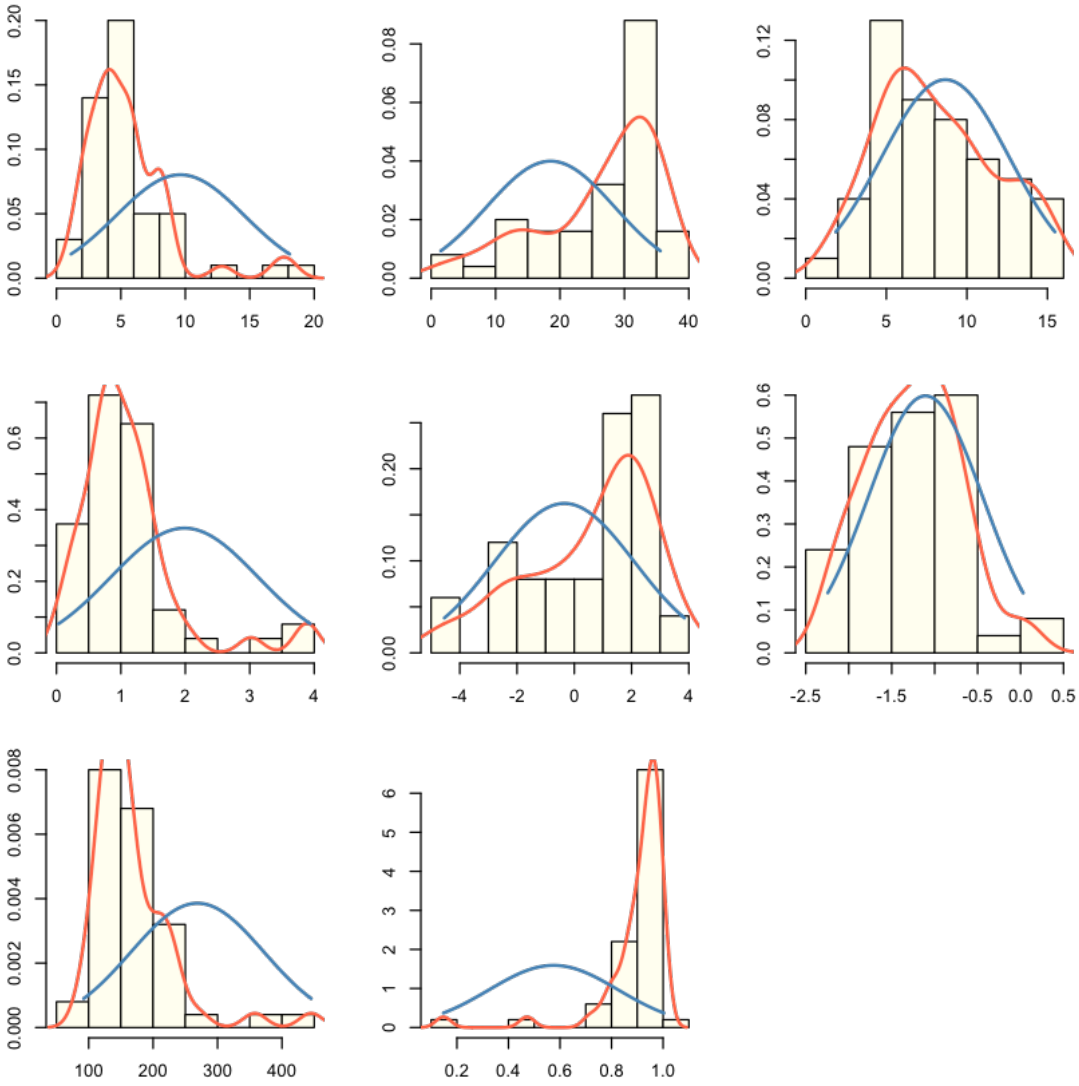
A bn.cpdist: 5 × 3

	N_50 <dbl>	N_150 <dbl>	N_300 <dbl>
1	0.2238915	24.77605	9.851049
2	10.6485287	33.44829	1.473389
3	8.3452148	31.75850	4.931674
4	7.1837007	33.26271	6.596407
5	2.9710913	29.21923	10.728515

1.4 Analyze the data before starting with Bayesian Network learning

Since we will be using Gaussian Bayesian Networks for the analysis, it also interesting to check whether the variables are normally distributed, at least marginally.

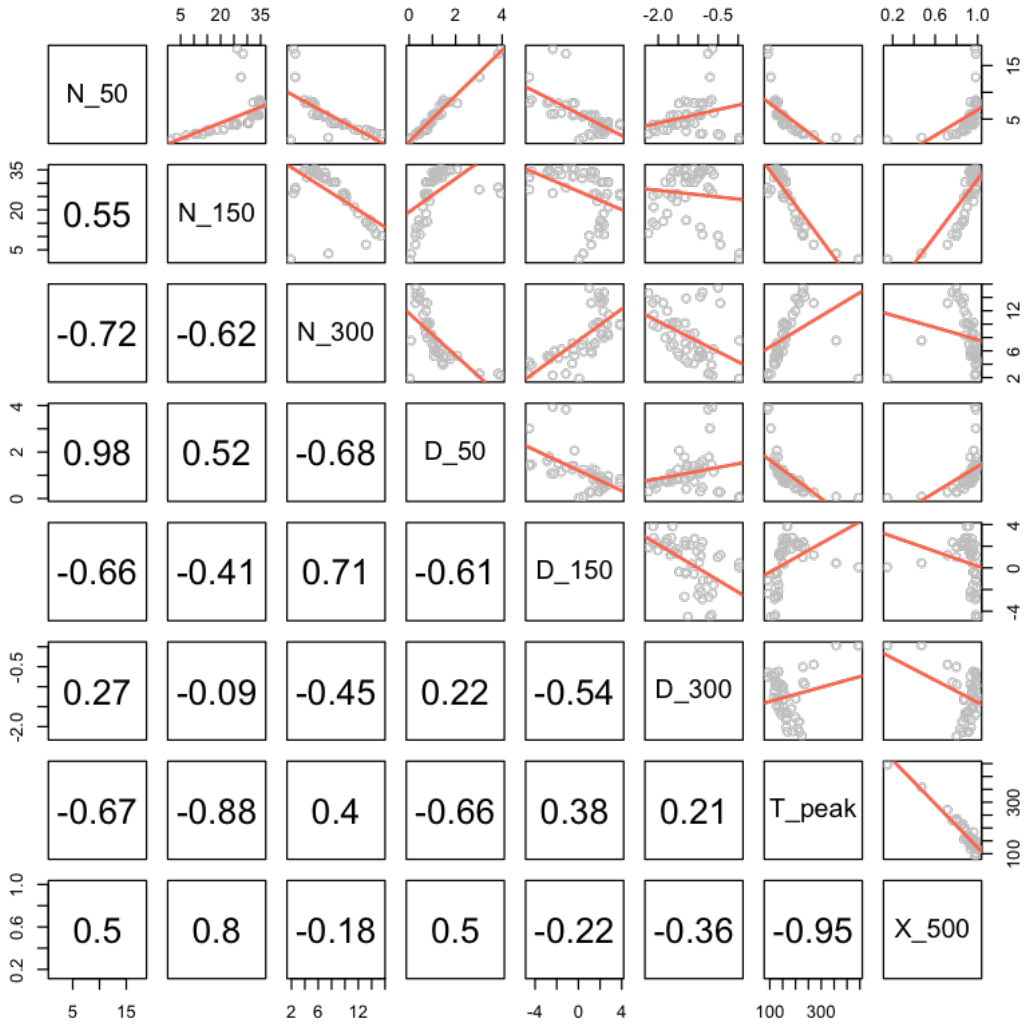
[12]:
```
par(mfrow = c(3, 3), mai=c(0.3,0.3,0.3,0.3))
for (var in c("N_50", "N_150", "N_300", "D_50", "D_150", "D_300", "T_peak",
 ↪"X_500")) {
    x = df[, var]
    hist(x, prob = TRUE, xlab = var, ylab = "", main = "", col = "ivory")
    lines(density(x), lwd = 2, col = "tomato")
    curve(dnorm(x, mean = mean(x), sd = sd(x)), from = min(x), to = max(x), add
 ↪= TRUE, lwd = 2, col = "steelblue")
}
```



Interprete the results! Your answer goes here.

Are the variables linked by linear relationships?

[13]:
```
pairs(df[, names(df)],
      upper.panel = function(x, y, ...) {
          points(x = x, y = y, col = "grey")
          abline(coef(lm(y ~ x)), col = "tomato", lwd = 2)
      },
      lower.panel = function(x, y, ...) {
          par(usr = c(0, 1, 0, 1))
          text(x = 0.5, y = 0.5, round(cor(x, y), 2), cex = 2)
      }
     )
```

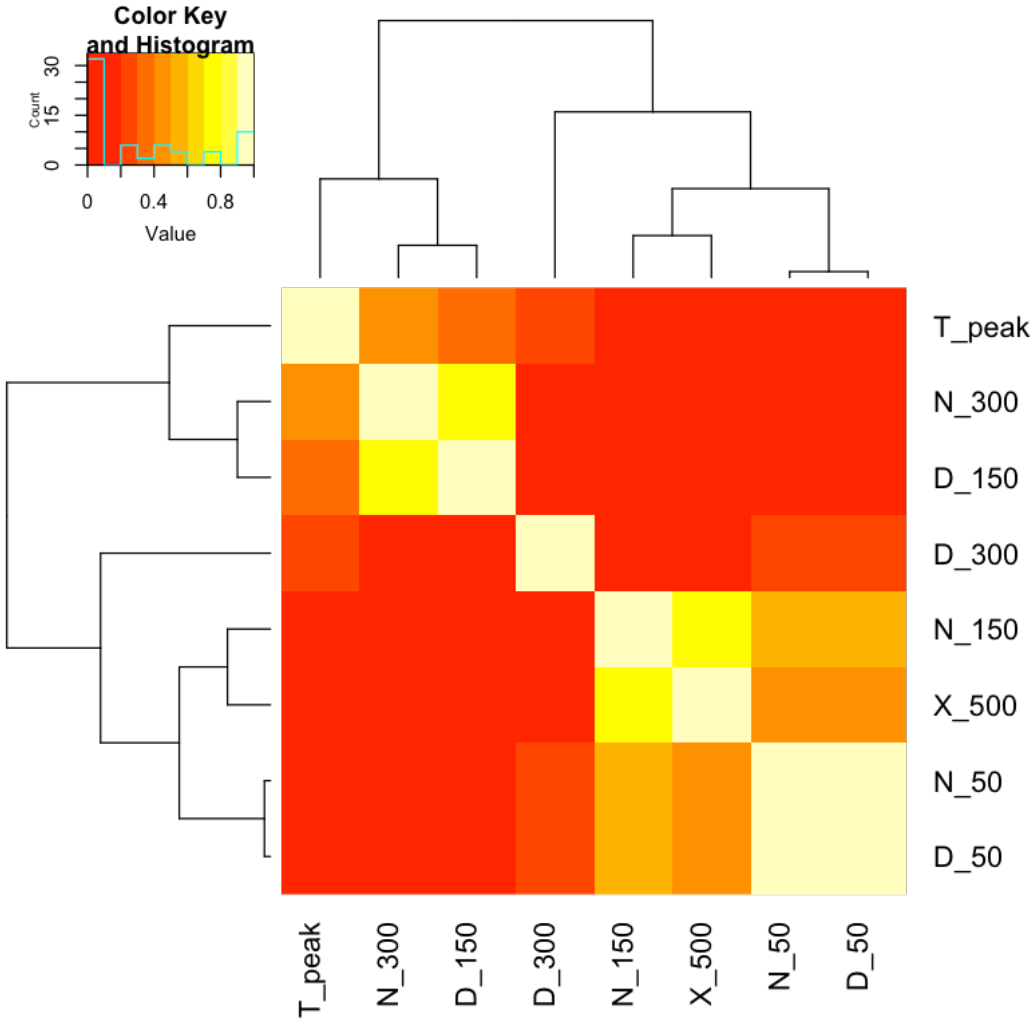


Actually, we've checked their correlation already. But watch out for outliers and leverage points! Double check the pairwise correlation in detail if interesting! Interprete the results! Your answer goes here.

Finally, we can take a look at whether the variables cluster by correlation, since variables that cluster together are more likely to be linked in the Bayesian Network.

[14]:
```
install.packages("gplots")
library("gplots")
rho = cor(df)
palette.breaks = seq(0, 1, 0.1)
par(oma = c(2, 2, 2, 1))
heatmap.2(rho, scale = "none", trace = "none", revC = TRUE, breaks = palette.
 ↪breaks)
```

```
The downloaded binary packages are in
/var/folders/ct/4pcck8t94sdfc73rhymq4t140000gp/T//RtmpEBHx76/downloaded_packages

Attaching package: 'gplots'


The following object is masked from 'package:stats':

    lowess
```



Lighter colors correspond to higher correlation. We can see two clusters in the heatmap: the first comprises $T_{peak}, N_{300}, D_{150}$, the second one $N_{50}, N_{150}, X_{500}, D_{150}$.

For the next steps, we install a graph (visualization) library.

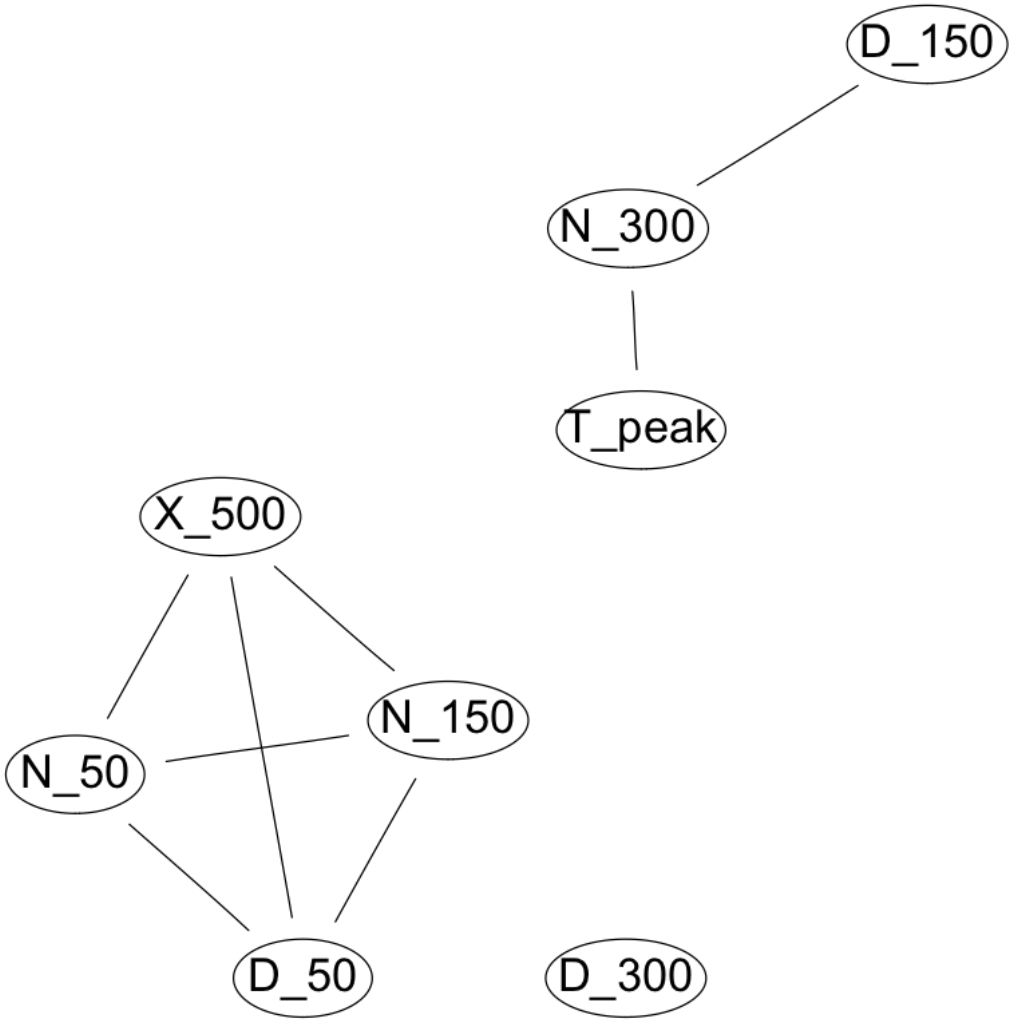
[15]:
```
if (!requireNamespace("BiocManager", quietly = TRUE))
  install.packages("BiocManager")
BiocManager::install()
BiocManager::install(c("graph", "Rgraphviz"))
```

```
Bioconductor version 3.10 (BiocManager 1.30.10), R 3.6.2 (2019-12-12)

Old packages: 'DT', 'MASS', 'Rcpp', 'backports', 'boot', 'broom', 'callr',
  'class', 'cli', 'covr', 'crosstalk', 'devtools', 'digest', 'dplyr',
  'forcats', 'foreign', 'fs', 'ggplot2', 'ggrepel', 'gh', 'glue', 'gtools',
  'jsonlite', 'knitr', 'lattice', 'lifecycle', 'lubridate', 'mime', 'modelr',
  'nlme', 'nnet', 'plyr', 'prettyunits', 'processx', 'ps', 'remotes', 'repr',
  'rlang', 'rmarkdown', 'roxygen2', 'rstudioapi', 'shiny', 'stringi',
  'survival', 'testthat', 'tibble', 'tidyr', 'tidyselect', 'tinytex', 'uuid',
  'vctrs', 'xml2', 'yaml'

Bioconductor version 3.10 (BiocManager 1.30.10), R 3.6.2 (2019-12-12)

Installing package(s) 'graph', 'Rgraphviz'



The downloaded binary packages are in
/var/folders/ct/4pcck8t94sdfc73rhymq4t140000gp/T//RtmpEBHx76/downloaded_packages
Old packages: 'DT', 'MASS', 'Rcpp', 'backports', 'boot', 'broom', 'callr',
  'class', 'cli', 'covr', 'crosstalk', 'devtools', 'digest', 'dplyr',
  'forcats', 'foreign', 'fs', 'ggplot2', 'ggrepel', 'gh', 'glue', 'gtools',
  'jsonlite', 'knitr', 'lattice', 'lifecycle', 'lubridate', 'mime', 'modelr',
  'nlme', 'nnet', 'plyr', 'prettyunits', 'processx', 'ps', 'remotes', 'repr',
  'rlang', 'rmarkdown', 'roxygen2', 'rstudioapi', 'shiny', 'stringi',
  'survival', 'testthat', 'tibble', 'tidyr', 'tidyselect', 'tinytex', 'uuid',
  'vctrs', 'xml2', 'yaml'
```

We plot the connected components of the following graph: the nodes are the variables, there is an edge between any two node iff the corresponding variables are correlated with $\rho > 0.4$ (moderately or strongly correlated).

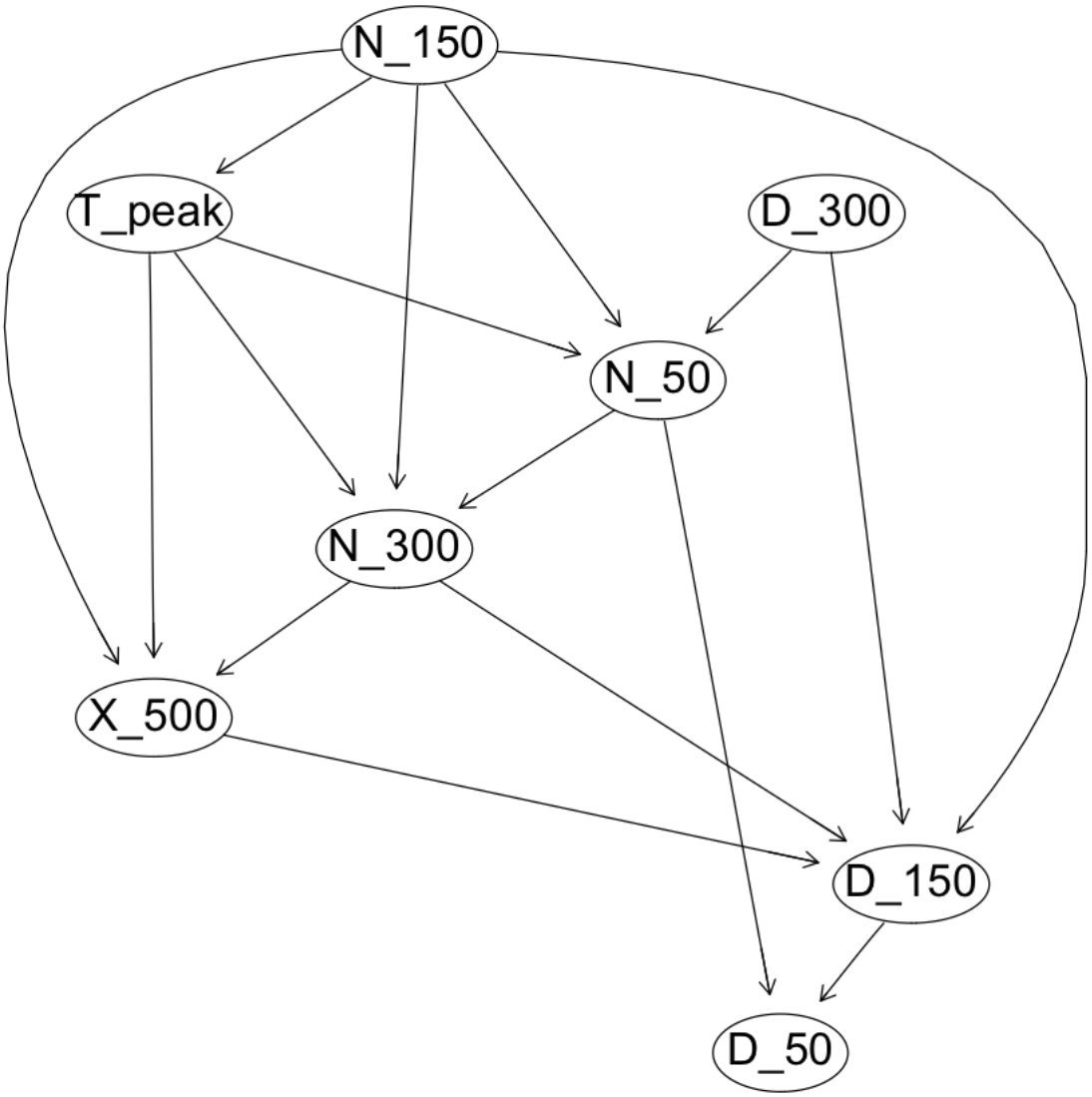
[16]:
```
#colnames(rho)
ug = empty.graph(colnames(rho))
amat(ug) = (rho > 0.4) + 0L - diag(1L, nrow(rho))
graphviz.plot(ug, layout = "fdp", shape = "ellipse")
```

```
Loading required namespace: Rgraphviz
```



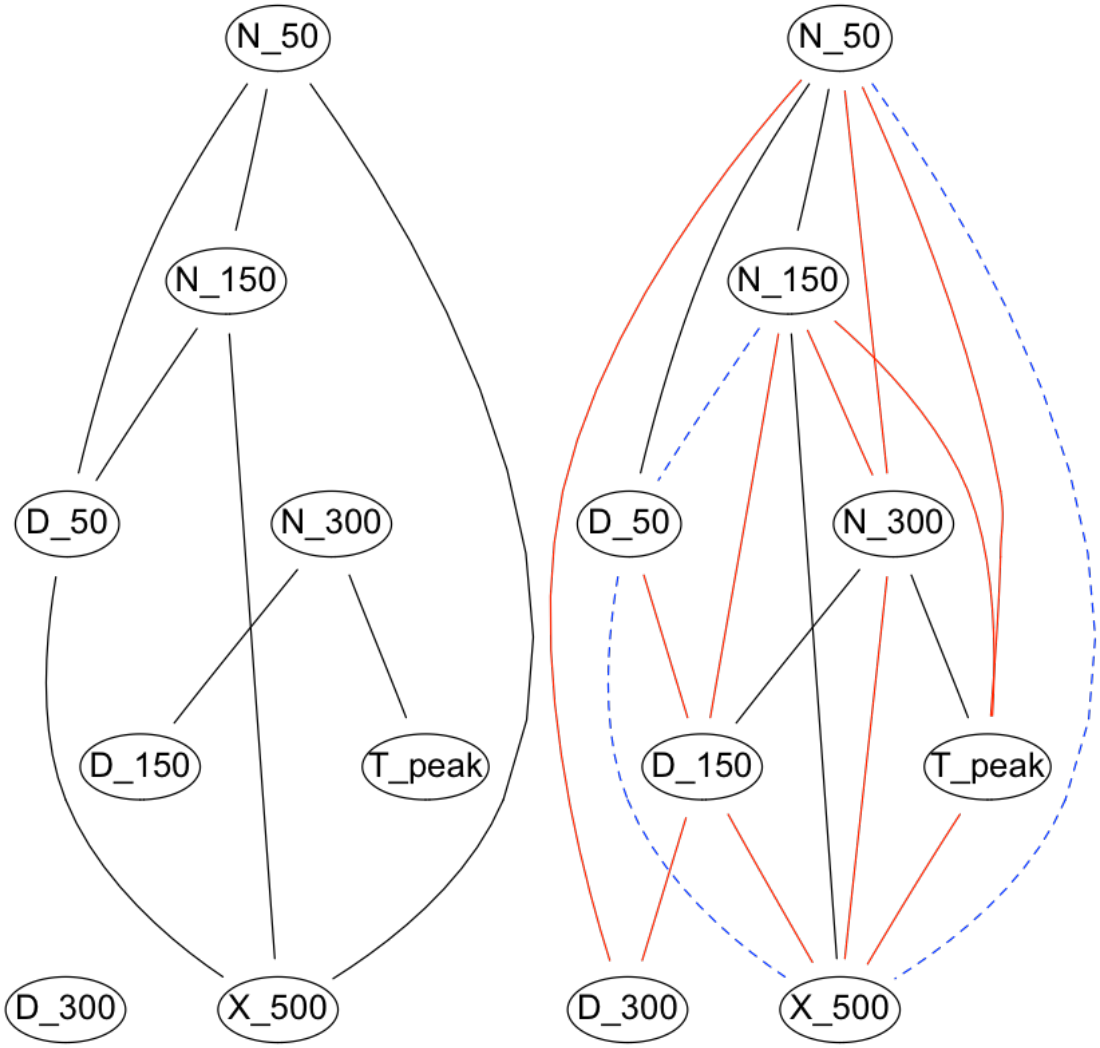
Recall the learned Bayesian Network structure.

[17]:
```
graphviz.plot(dag, shape = "ellipse")
```



We can compare the learned structure with the clustered graph. Therefore, we transform the learned Bayesian Network into an undirected graph and compare it with the correlation graph.

[31]:
```
ug2 = empty.graph(colnames(rho))
for (edge in 1:nrow(dag$arcs)){
    f = dag$arcs[edge, 1]
    t = dag$arcs[edge, 2]
    ug2$arcs <- rbind(ug2$arcs, c(f,t))
    ug2$arcs <- rbind(ug2$arcs, c(t,f))
}
par(mfrow = c(1, 2))
graphviz.compare(ug, ug2, shape = "ellipse")
```



1.5 Learn and apply the Bayesian Network

Step 1: learning the structure of the network.

Before we relearn the Baysian Network structure, we blacklist a few edges that are of little help in prediction.

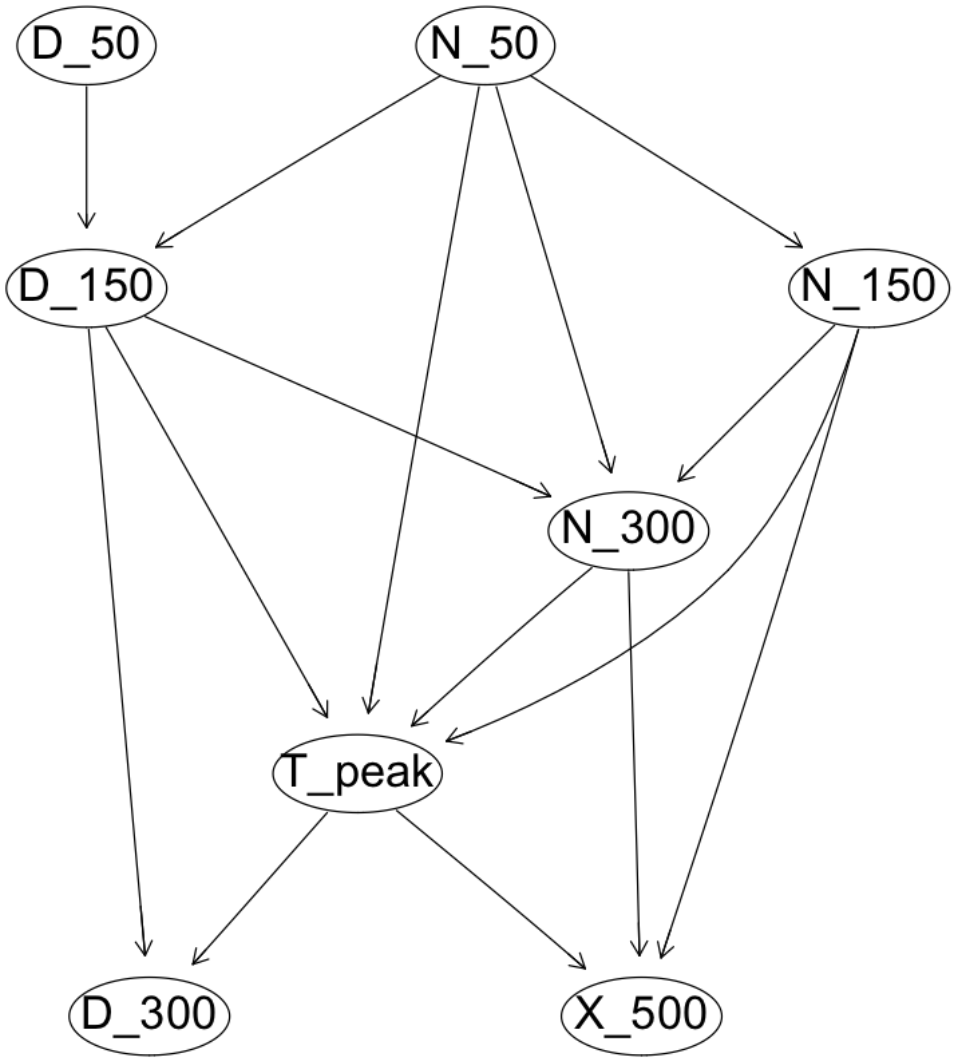
[19]:
```
bl = tiers2blacklist(list(c("N_50", "N_150", "N_300", "D_50", "D_150", "D_300",␣
 ↪"T_peak"), "X_500"))
bl = rbind(bl, c("N_300", "N_50"), c("N_300", "D_50"), c("N_300", "N_150"),␣
 ↪c("N_300", "D_150"), c("N_300", "D_300"))
bl = rbind(bl, c("D_300", "N_50"), c("D_300", "D_50"), c("D_300", "N_150"),␣
 ↪c("D_300", "D_150"), c("D_300", "N_300"))
```

```
bl = rbind(bl, c("N_150", "N_50"), c("N_150", "D_50"), c("N_150", "D_150"))
bl = rbind(bl, c("D_150", "N_50"), c("D_150", "D_50"), c("D_150", "N_150"))
bl = rbind(bl, c("N_50", "D_50"), c("D_50", "N_50"))
bl = rbind(bl, c("T_peak", "D_50"), c("T_peak", "N_50"))
bl
```

A matrix: 27 × 2 of type chr

from	to
X_500	N_50
X_500	N_150
X_500	N_300
X_500	D_50
X_500	D_150
X_500	D_300
X_500	T_peak
N_300	N_50
N_300	D_50
N_300	N_150
N_300	D_150
N_300	D_300
D_300	N_50
D_300	D_50
D_300	N_150
D_300	D_150
D_300	N_300
N_150	N_50
N_150	D_50
N_150	D_150
D_150	N_50
D_150	D_50
D_150	N_150
N_50	D_50
D_50	N_50
T_peak	D_50
T_peak	N_50

[20]:
```
dag2 = hc(df, blacklist = bl)
graphviz.plot(dag2, shape = "ellipse")
```



However, the quality of `dag2` crucially depends on whether variables are normally distributed and on whether the relationships that link them are linear; from the exploratory analysis it is not clear that is the case for all of them. We also have no idea about which arcs represent strong relationships, meaning that they are resistant to perturbations of the data. We can address both issues using `boot.strength()` to:

1. resample the data using bootstrap;
2. learn a separate network from each bootstrap sample;
3. check how often each possible arc appears in the networks;
4. construct a consensus network with the arcs that appear more often.

[21]:
```
str.df = boot.strength(df, R = 200, algorithm = "hc", algorithm.args =␣
 ↪list(blacklist = bl))
head(str.df)
```

A bn.strength: 6 × 4

	from <chr>	to <chr>	strength <dbl>	direction <dbl>
1	N_50	N_150	0.87	1
2	N_50	N_300	0.78	1
3	N_50	D_50	0.00	0
4	N_50	D_150	0.98	1
5	N_50	D_300	0.28	1
6	N_50	T_peak	0.67	1

The return value of `boot.strength()` includes, for each pair of nodes, the strength of the arc that connects them (say, how often we observe `N_50` → `N_150`, answer quite often) and the strength of its direction (say, how often we observe `N_50` → `N_150` when we observe an arc at all between `N_50` and `N_150`, answer always).

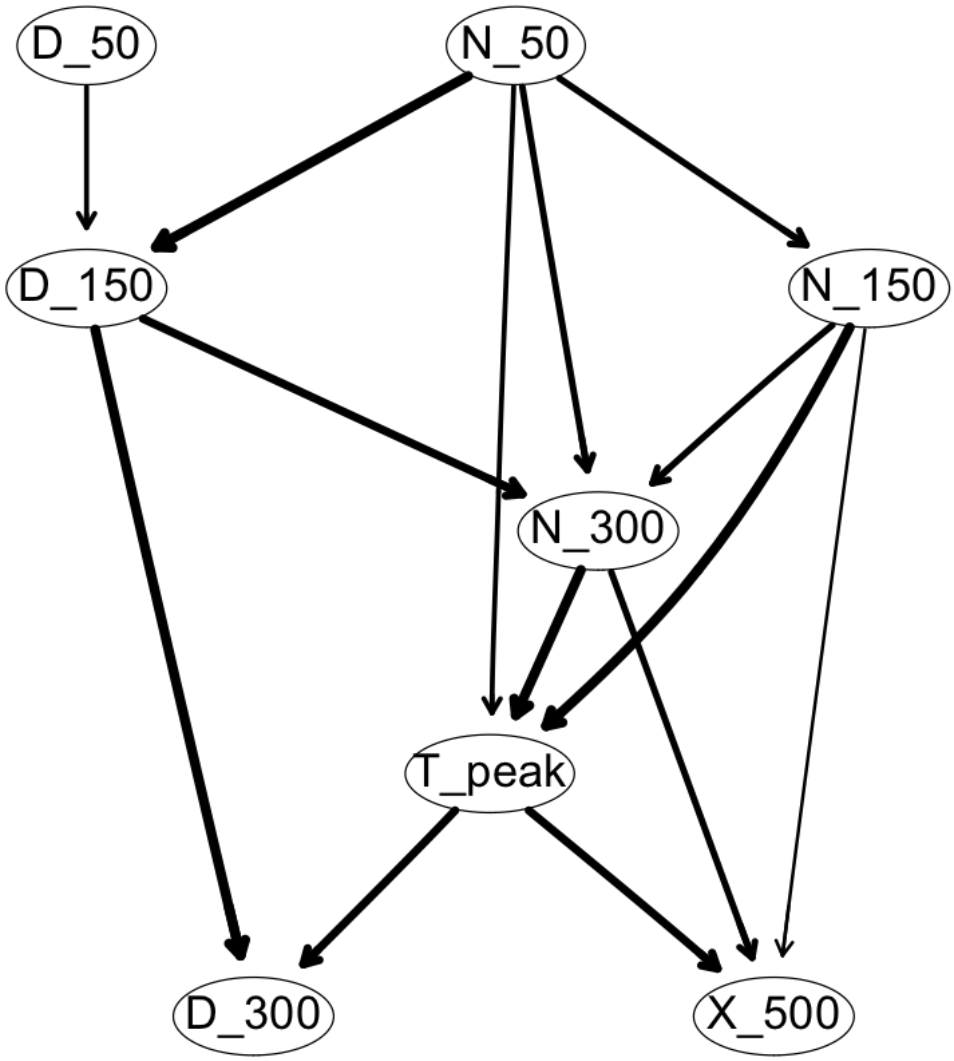
`boot.strength()` also computes the threshold that will be used to decide whether an arc is strong enough to be included in the consensus network.

[22]:
```
attr(str.df, "threshold")
```

0.4

So, `averaged.network()` takes all the arcs with a strength of at least `0.4` and returns an averaged consensus network, unless a different threshold is specified. This this a plot of the network:

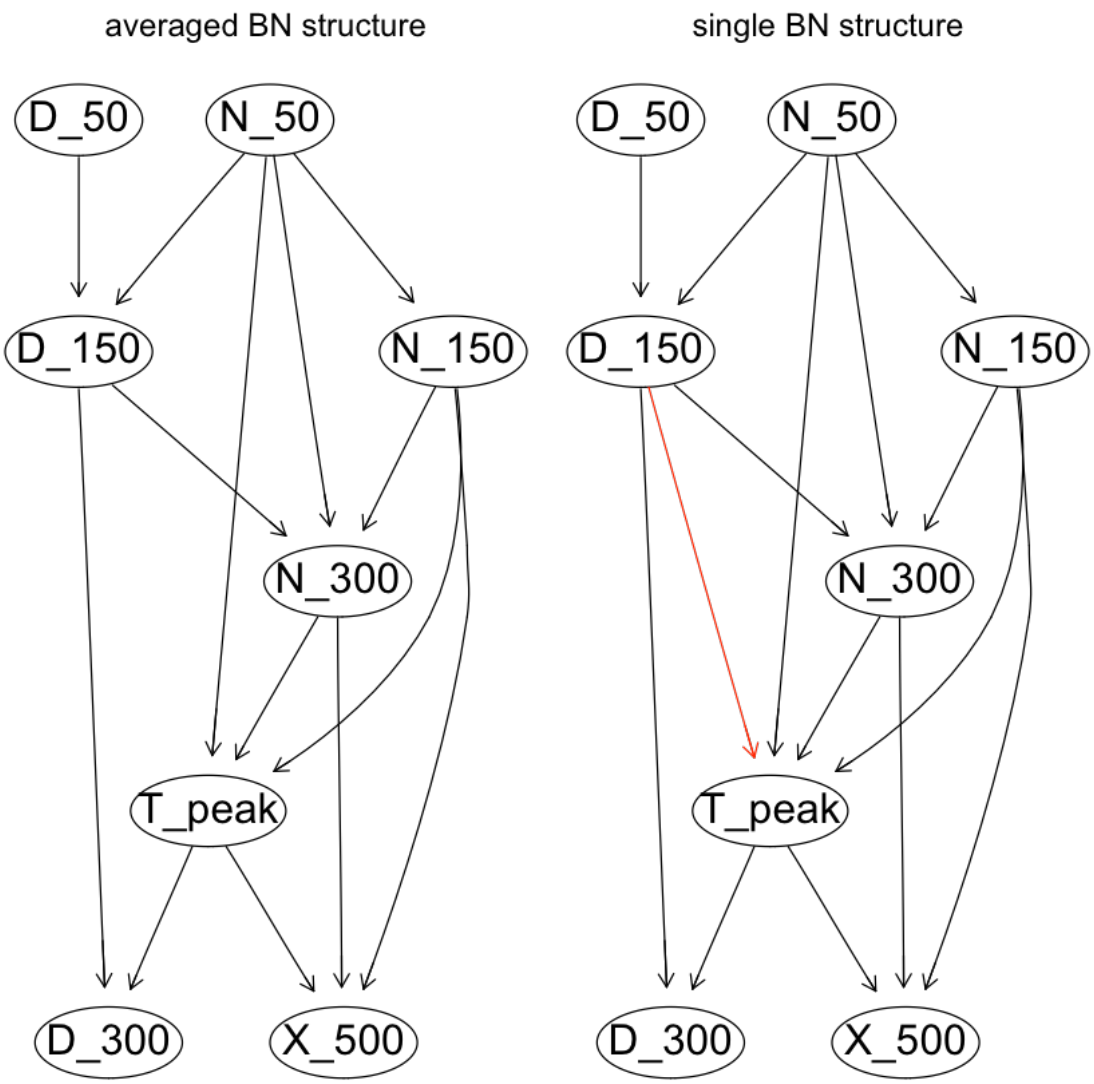
[23]:
```
avg.df = averaged.network(str.df)
strength.plot(avg.df, str.df, shape = "ellipse")
```



Now we can compare the averaged network `avg.df` with the network we originally learned in from all the data `dag`.

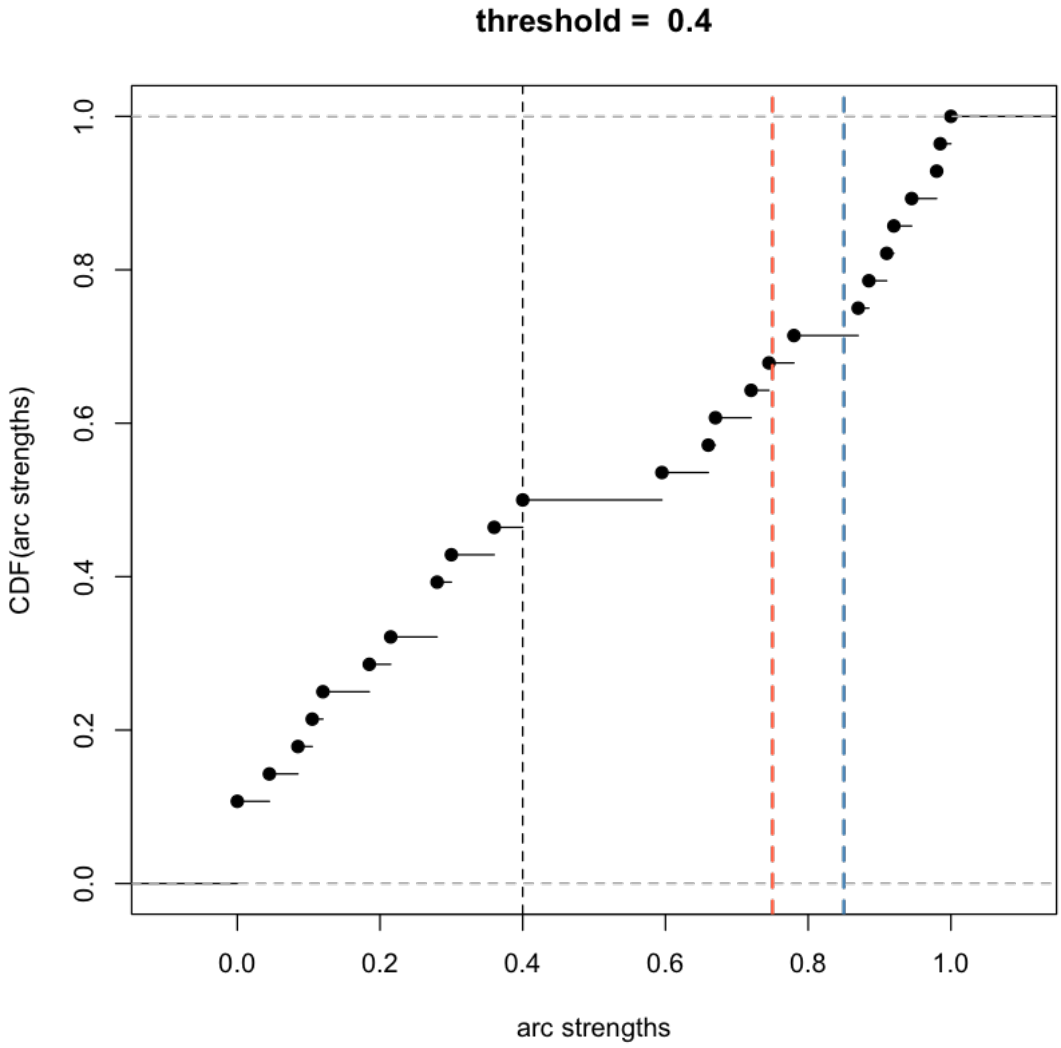
The most qualitative way is to plot the two networks side by side, with the nodes in the same positions, and highlight the arcs that appear in one network and not in the other, or that appear with different directions.

[24]:
```
par(mfrow = c(1, 2))
graphviz.compare(avg.df, dag2, shape = "ellipse", main = c("averaged BN␣
 ↪structure", "single BN structure"))
```



It is also a good idea to look at the threshold with respect to the distribution of the arc strengths:

[25]:
```
plot(str.df)
abline(v = 0.75, col = "tomato", lty = 2, lwd = 2)
abline(v = 0.85, col = "steelblue", lty = 2, lwd = 2)
```



Step 2: learning the conditional probabilities.

Having learned the structure, we can now learn the parameters. Since we are working with continuous variables, we choose to model them with a Gaussian Bayesian Network (`GBN`). Hence if we fit the parameters of the network using their maximum likelihood estimate we have that each local distribution is a classic linear regression.

[26]:
```
fitted.df = bn.fit(avg.df, df)
fitted.df
```

```
  Bayesian network parameters

  Parameters of node N_50 (Gaussian distribution)
```

```
Conditional density: N_50
Coefficients:
(Intercept)
     5.5108
Standard deviation of the residuals: 3.396421

  Parameters of node N_150 (Gaussian distribution)

Conditional density: N_150 | N_50
Coefficients:
(Intercept)         N_50
  17.805796     1.502184
Standard deviation of the residuals: 7.915052

  Parameters of node N_300 (Gaussian distribution)

Conditional density: N_300 | N_50 + N_150 + D_150
Coefficients:
(Intercept)         N_50        N_150        D_150
 12.6020150   -0.3106794   -0.1179827    0.6565141
Standard deviation of the residuals: 2.133747

  Parameters of node D_50 (Gaussian distribution)

Conditional density: D_50
Coefficients:
(Intercept)
   1.097608
Standard deviation of the residuals: 0.7842617

  Parameters of node D_150 (Gaussian distribution)

Conditional density: D_150 | N_50 + D_50
Coefficients:
(Intercept)         N_50         D_50
   3.481340    -1.326189     3.948643
Standard deviation of the residuals: 1.580773

  Parameters of node D_300 (Gaussian distribution)

Conditional density: D_300 | D_150 + T_peak
Coefficients:
 (Intercept)         D_150        T_peak
-1.854396754  -0.179020040   0.004159623
Standard deviation of the residuals: 0.392633

  Parameters of node T_peak (Gaussian distribution)
```

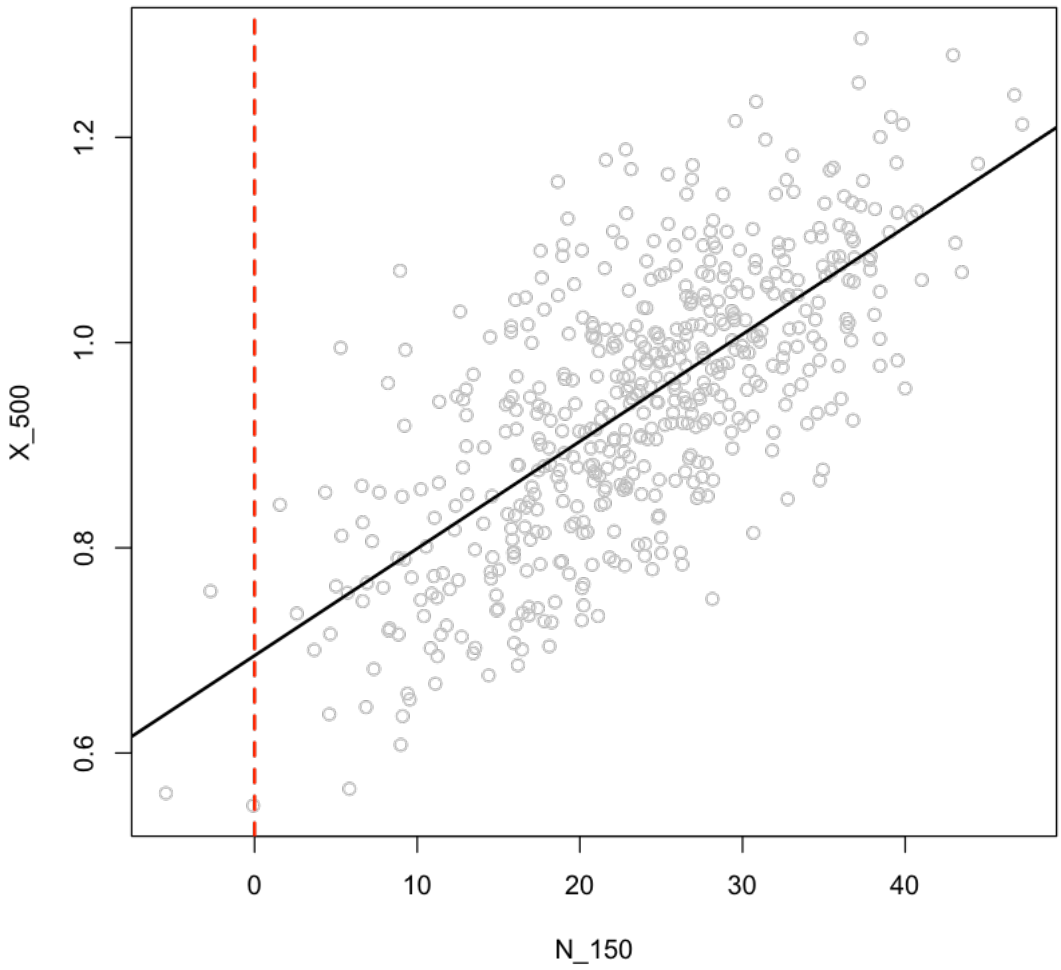
```
Conditional density: T_peak | N_50 + N_150 + N_300
Coefficients:
(Intercept)         N_50        N_150        N_300
 476.766539   -11.160817    -6.244805   -10.460750
Standard deviation of the residuals: 10.51101

  Parameters of node X_500 (Gaussian distribution)

Conditional density: X_500 | N_150 + N_300 + T_peak
Coefficients:
 (Intercept)         N_150         N_300        T_peak
 1.056397645   0.003065925   0.012091517  -0.002010491
Standard deviation of the residuals: 0.0292708
```

We could validate the network by checking again st "expert" knowlege.

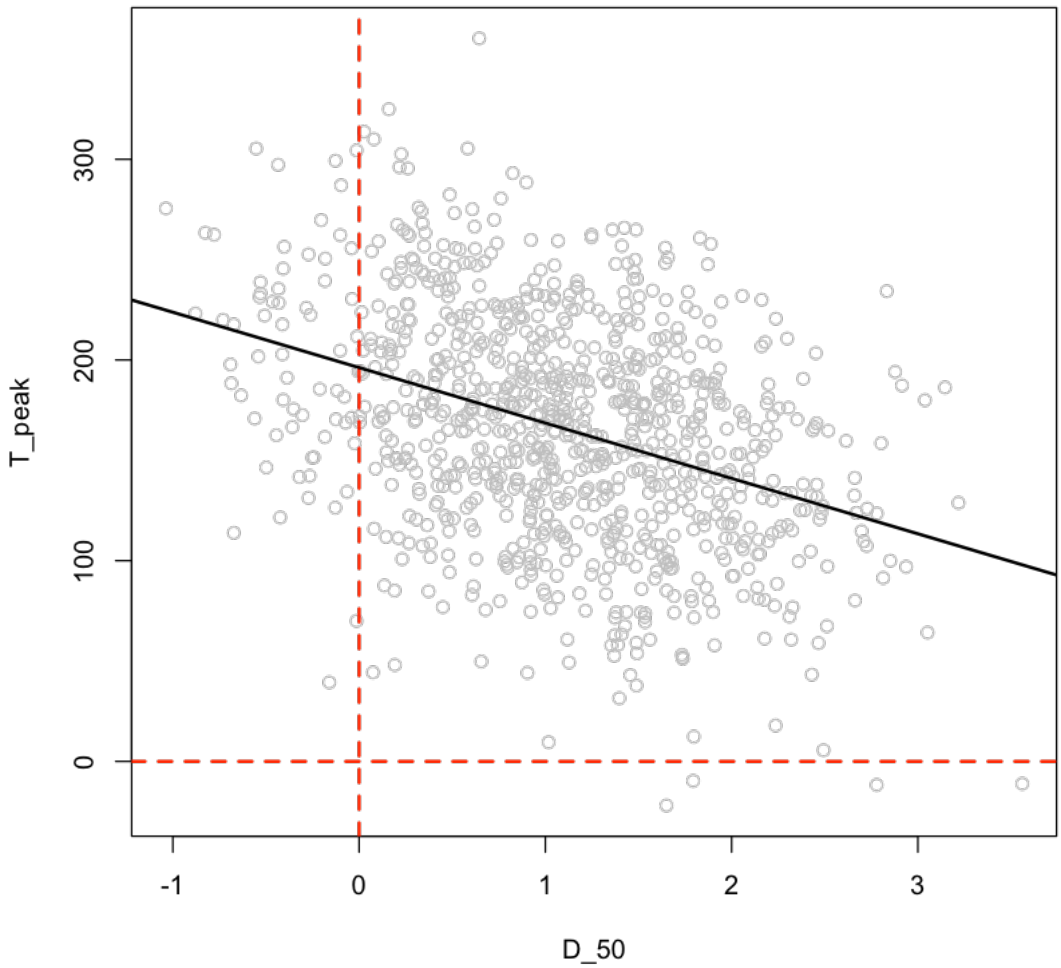
1. "*Low/high N_{150} values should be a predictor of low/high casulties X_{500}*"
2. "*Low/high D_{50} values should be a predictor of late/early infection peaks T_{peak}*"

Both is confirmed.

[27]:
```
sim = cpdist(fitted.df, nodes = c("N_150", "X_500"), n = 1000, evidence =␣
 ↪(D_150 > 0))
plot(sim, col = "grey")
abline(v = 0, col = 2, lty = 2, lwd = 2)
abline(h = 0, col = 2, lty = 2, lwd = 2)
abline(coef(lm(X_500 ~ N_150, data = sim)), lwd = 2)
```



[28]:
```
sim = cpdist(fitted.df, nodes = c("D_50", "T_peak"), n = 1000, evidence = (N_50␣
↪> 0))
plot(sim, col = "grey")
abline(v = 0, col = 2, lty = 2, lwd = 2)
abline(h = 0, col = 2, lty = 2, lwd = 2)
abline(coef(lm(T_peak ~ D_50, data = sim)), lwd = 2)
```



Step 3: Using the network.

We can predicting casulties based on observation.

[29]:
```
new_data
predict(fitted.df, node = "X_500", data = new_data)
```

A data.frame: 1 × 7

	N_50 <dbl>	N_150 <dbl>	N_300 <dbl>	D_50 <dbl>	D_150 <dbl>	D_300 <dbl>	T_peak <dbl>
1	7.755674	20.22743	3.744598	1.723289	1.420417	-0.4327158	229.8769

0.701525985455266

This is still quite close to the `0.7131789` predicted earlier.

We can compute probabilities with queries:

[30]:
```
cpquery(fitted.df, event = (N_50 <= 7) & (N_150 <= 20) & (N_300 <= 10),␣
↪evidence = (T_peak >= 100))
```

0.0686953901777644

This is a bit less than `0.0730` predicted earlier.

1.6 References

1. https://www.bnlearn.com/
2. https://www.bnlearn.com/examples/useR19-tutorial/