Chapter 1

Appendix

1.1 Suicide data

```
25
                             256
          40
                83
                      123
1
     27
          49
                84
                      126
                             257
1
     27
          49
                84
                      129
                             311
5
     30
          54
                84
                      134
                             314
7
     30
          56
                90
                      144
                             322
8
     31
          56
                91
                      147
                             369
8
     31
          62
                92
                      153
                             415
13
     32
          63
                93
                      163
                             573
     34
                93
                             609
14
          65
                      167
14
     35
          65
                103
                      175
                             640
17
     36
          67
                103
                      228
                             737
18
     37
          75
                111
                      231
21
     38
          76
                112
                      235
21
     39
          79
                      242
                119
22
     39
          82
                122
                      256
```

Table 1.1: The length of treatment of control patients in suicide study. The data originates from the Mental Health Enquiry (MHE) of England of Wales and was published in 1967.

1.1.1 A better spline

In theory, we could make a set of splines ourselves, that has both of the desired properties of B-splines and M-splines. I.e. a set of piecewise polynomials, which we shall denote $Q_{i,p}$, that has both the property that

$$\sum_{i=1}^{n} Q_{i,p}(t) = 1$$

and

$$\int_0^1 Q_{i,p}(t) dt = \frac{1}{n}$$

Actually, both M- and B-splines satisfies this for p=0 as they are then both piecewise constant and non-zero on disjoint intervals. From this, one can the construct such sets of $Q_{i,p}$ in the following way. Namely, start with the piecewise constant functions, $Q_{i,0}$ depicted in Figure 1.1 as boxes in the case n=5.

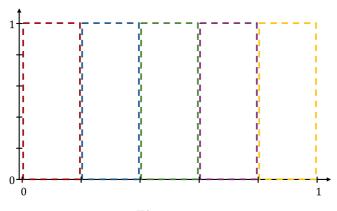


Figure 1.1

A better spline

Cut off function has derivative 0 at top and is halfway down at the sides

This example does however not work well for many bins, in particular, due to the splines not overlapping that much i.e. a poor regularization on the smoothness. However, the method used for constructing this set of splines can be extended to bleed into multiple neighboring bins just as for B- and M-splines.

1.1 Suicide data 3

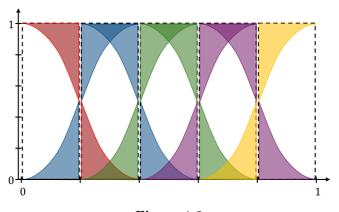


Figure 1.2

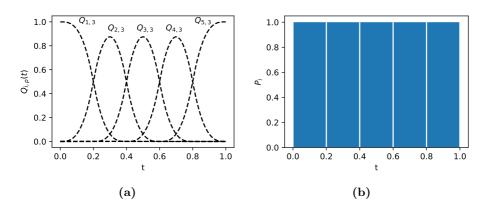


Figure 1.3: P_i is area of each rectangle i.e. 0.2.

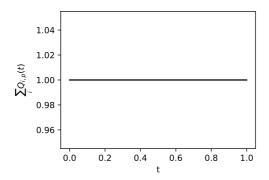


Figure 1.4

1.2 M-spline based MI estimation

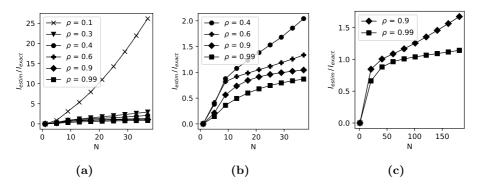


Figure 1.5

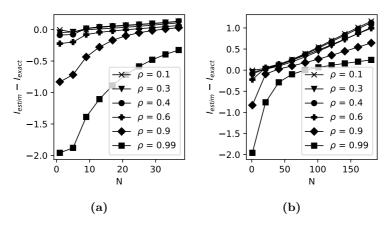


Figure 1.6

1.3 Confidence interval for absolute correlation in bivariate Gaussian

From [?], given a bivariate Gaussian, the confidence distribution of ρ given the empirical correlation r based on n observations is given by

$$f\left(\rho \mid r,\nu\right) = \frac{\nu(\nu-1)\Gamma(\nu-1)}{\sqrt{2\pi}\Gamma(\nu+\frac{1}{2})} \frac{\left(1-r^2\right)^{\frac{\nu-1}{2}} \left(1-\rho^2\right)^{\frac{\nu-2}{2}}}{\left(1-r\rho\right)^{\frac{2\nu-1}{2}}} F\left(\frac{3}{2},-\frac{1}{2},\nu+\frac{1}{2},\frac{1+r\rho}{2}\right)$$

where F(a,b,c,z) is the Gaussian hypergeometric function and $\nu=n-1$. That is, given a sample correlation r, what is the confidence in ρ in terms of a distribution. In the following figure, a sample correlation r=0.8 and r=0 has been used with varying number of observations (degrees of freedom) in figures Figure 1.7a and Figure 1.7b respectively. A key property is that f is even

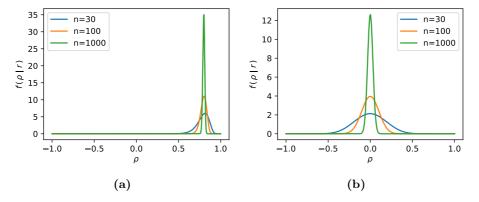


Figure 1.7: $f(\rho \mid r, \nu)$ shown for r = 0.8 and r = 0 in (a) and (b) with $n \in \{30, 100, 1000\}$. As one would expect, the power i.e. the width of the peak decreases with increasing n and for correlations closer to 0, the width is the largest.

symmetric in ρ , r. That is $f(\rho \mid r) = f(-\rho \mid -r)$. Thus, a confidence interval for ρ given r is the negative of the confidence interval given -r. In particular, if we only observe |r|, we can calculate a confidence interval for ρ up to the sign of the bounds of the interval. Furthermore, as we want a CI for $|\rho|$, it does not matter if r is negative or positive. Hence, without loss of generality, we assume that $r \geq 0$. At this point, to construct a confidence interval for $|\rho|$ we list the following desired properties. Firstly, it should be an exact confidence interval, meaning that for a given significance level α , the CI includes the true value exactly $1-\alpha$ fraction of the times. Secondly, if for a given r, it can not be rejected that ρ is 0, 0 should also be contained in the interval. Finally, if we reject

that $\rho = 0$, we shall have $\alpha/2$ probability mass above and below the bounds of the interval. The above is enough to uniquely define a confidence interval in all cases. Before continuing with how this CI is calculated, we mention that as r is an unbiased estimator of ρ , we would preferably want $|r| \in CI_{1-\alpha}(|\rho|)$ (where $CI_{1-\alpha}(|\rho|)$ denotes the $1-\alpha$ confidence interval for $|\rho|$). However, although this will in almost every scenario be the case, we can not be sure of this from the above properties and in fact examples with large α can be constructed such that |r| lies just outside the constructed CI.

First, to conform with the second desired property, if it can not be rejected that $\rho=0$ on a significance level α , we will initially compute a CI for ρ (not $|\rho|$) based on r (wlog chosen to be non-negative). This CI will just be a symmetric CI in the sense that $\alpha/2$ of the probability mass will lie below the lower bound of the CI and above the upper bound of the CI respectively. If 0 is contained in this CI, we can not reject that $\rho=0$ and vice versa on an α significance level. Thus, if 0 is contained in this initial CI for ρ , we will start the CI for $|\rho|$ at 0 and determine and upper bound b such that α probability mass is above this b. Otherwise, we shall find a and b such that $\alpha/2$ probability mass is below a and above b respectively. Choosing a and b this way also conforms with the third property. Finally, to ensure that the CI contains exactly $1-\alpha$, we define \tilde{f} as the reflected f in ρ such that

$$\tilde{f}(\rho_a \mid r_a, \nu) = f(\rho_a \mid r_a, \nu) + f(-\rho_a \mid r_a, \nu), \quad \rho_a, r \in [0, 1]$$

where ρ_a and r_a is the absolute correlation and empirical correlation respectively. With this \tilde{f} , the density at ρ_a is both the density for the negative and positive correlation ensuring that the \tilde{f} has probability mass 1. Thus, if a=0 (i.e. the CI must contain 0), we find b as the $1-\alpha$ percentile of \tilde{f} and if $a \neq 0$, we take a as the $\alpha/2$ percentile and b as the $1-\alpha/2$ percentile of \tilde{f} .

As an example, suppose $r_a=0.06$ with 1000 observations. Then a 95% CI for $|\rho|$ is [0,0.11164] whereas if on had observed $r_a=0.07$ the CI would be [0.01071,0.1314]. These CI could then be used to test the absolute correlation of a bivariate Gaussian i.e. for $r_a=0.07$ based on 1000 observations would be rejected as stemming from a Gaussian with absolute correlation 0.01 on a 5% significance level.

1.4 Gaussian chain deconvolution

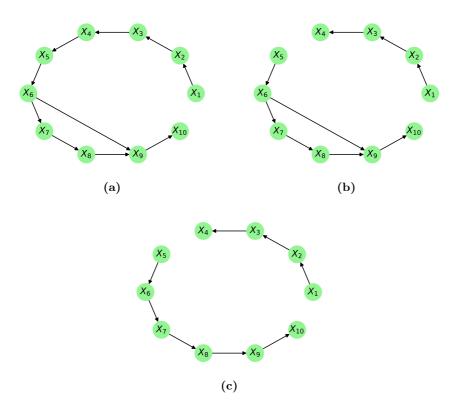


Figure 1.8: Triangular, mutual information, cutoff $2\cdot 10^{-10},\ 2.1\cdot 10^{-2}$ and $4.51\cdot 10^{-2}.$

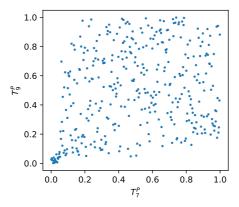


Figure 1.9

1.5 Gaussian network deconvolution

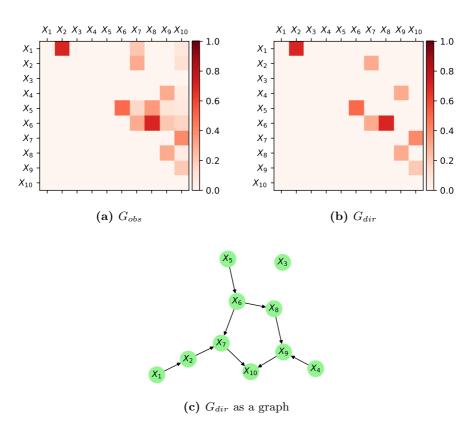


Figure 1.10: For the linear network defined in ??, using a triangular G_{obs} (a) with the true topological structure we are able to perfectly rediscover the causal structure as seen in (b) and (c).

1.6 Pharmaceutical process deconvolution

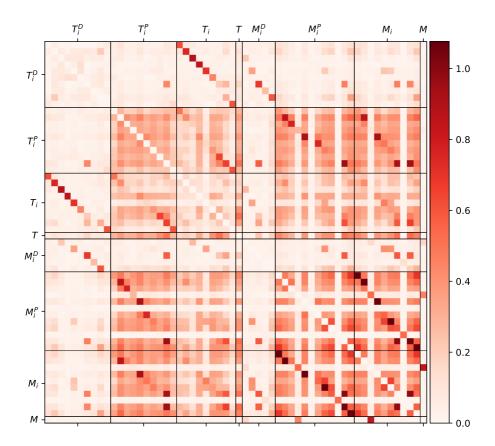


Figure 1.11: G_{obs} from pharmaceutical production data. Strong dependencies between variables and the related accumulated variables are observed.

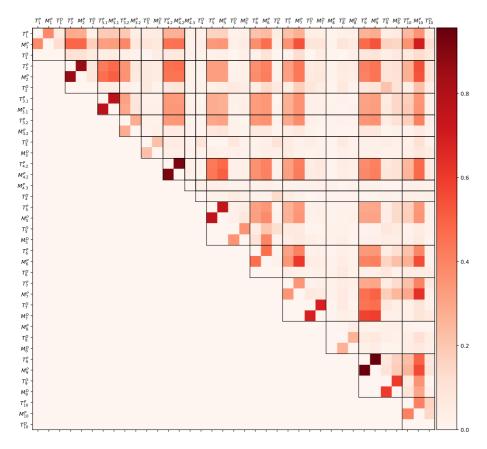


Figure 1.12: G_{obs} for both durations, delays and level changes for the simulated data from [?]. Labels related to the same process are divided by lines vertically and horizontally to easier observe what is related to what.