Appendix

A. Case study 3

Fig. 7 shows all the valid adjustment sets with their corresponding variance for the small E. Coli Case study.

arcA,crp,oxyR,rpoD,rpoS,soxS	arcA,crp,ihfB,oxyR,rpoD,rpoS,soxS	arcA,crp,lrp,oxyR,rpoD,rpoS,soxS
0.137	0.137	0.137
arcA,crp,oxyR,phoB,rpoD,rpoS,soxS	arcA,crp,ihfB,lrp,oxyR,rpoD,rpoS,soxS	arcA,crp,ihfB,oxyR,phoB,rpoD,rpoS,soxS
0.137	0.137	0.137
crp,oxyR,rpoD,rpoS,soxS	arcA,crp,oxyR,phoB,rpoD,soxS	crp,ihfB,oxyR,rpoD,rpoS,soxS
0.138	0.138	0.138
crp,lrp,oxyR,rpoD,rpoS,soxS	crp,oxyR,phoB,rpoD,rpoS,soxS	arcA,crp,ihfA,oxyR,rpoD,rpoS,soxS
0.138	0.138	0.138
crp,ihfB,lrp,oxyR,rpoD,rpoS,soxS	crp,ihfB,oxyR,phoB,rpoD,rpoS,soxS	crp,lrp,oxyR,phoB,rpoD,rpoS,soxS
0.138	0.138	0.138
arcA,crp,ihfA,ihfB,oxyR,rpoD,rpoS,soxS	arcA,crp,ihfA,lrp,oxyR,rpoD,rpoS,soxS	arcA,crp,ihfA,oxyR,phoB,rpoD,rpoS,soxS
0.138	0.138	0.138
arcA,crp,lrp,oxyR,phoB,rpoD,rpoS,soxS	crp,ihfB,lrp,oxyR,phoB,rpoD,rpoS,soxS	arcA,crp,ihfA,ihfB,lrp,oxyR,rpoD,rpoS,soxS
0.138	0.138	0.138
arcA,crp,ihfA,ihfB,oxyR,phoB,rpoD,rpoS,soxS	arcA,crp,ihfA,lrp,oxyR,phoB,rpoD,rpoS,soxS	arcA,crp,ihfB,lrp,oxyR,phoB,rpoD,rpoS,soxS
0.138	0.138	0.138
arcA,crp,ihfA,ihfB,lrp,oxyR,phoB,rpoD,rpoS,soxS	crp,oxyR,rpoD,soxS	arcA,crp,oxyR,rpoD,soxS
0.138	0.139	0.139
crp,ihfB,oxyR,rpoD,soxS	crp,lrp,oxyR,rpoD,soxS	crp,oxyR,phoB,rpoD,soxS
0.139	0.139	0.139
arcA,crp,ihfA,oxyR,rpoD,soxS	arcA,crp,ihfB,oxyR,rpoD,soxS	arcA,crp,lrp,oxyR,rpoD,soxS
0.139	0.139	0.139
crp,ihfA,oxyR,rpoD,rpoS,soxS	crp,ihfB,lrp,oxyR,rpoD,soxS	crp,ihfB,oxyR,phoB,rpoD,soxS
0.139	0.139	0.139
crp,lrp,oxyR,phoB,rpoD,soxS	arcA,crp,ihfA,lrp,oxyR,rpoD,soxS	arcA,crp,ihfA,oxyR,phoB,rpoD,soxS
0.139	0.139	0.139
arcA,crp,ihfB,lrp,oxyR,rpoD,soxS	arcA,crp,ihfB,oxyR,phoB,rpoD,soxS	arcA,crp,lrp,oxyR,phoB,rpoD,soxS
0.139	0.139	0.139
crp,ihfA,ihfB,oxyR,rpoD,rpoS,soxS	crp,ihfA,lrp,oxyR,rpoD,rpoS,soxS	crp,ihfA,oxyR,phoB,rpoD,rpoS,soxS
0.139	0.139	0.139
crp,ihfB,lrp,oxyR,phoB,rpoD,soxS	arcA,crp,ihfA,lrp,oxyR,phoB,rpoD,soxS	arcA,crp,ihfB,lrp,oxyR,phoB,rpoD,soxS
0.139	0.139	0.139
crp,ihfA,ihfB,lrp,oxyR,rpoD,rpoS,soxS	crp,ihfA,ihfB,oxyR,phoB,rpoD,rpoS,soxS	crp,ihfA,lrp,oxyR,phoB,rpoD,rpoS,soxS
0.139	0.139	0.139
crp,ihfA,ihfB,lrp,oxyR,phoB,rpoD,rpoS,soxS	crp,ihfA,oxyR,rpoD,soxS	crp,ihfA,ihfB,oxyR,rpoD,soxS
0.139	0.140	0.140
crp,ihfA,lrp,oxyR,rpoD,soxS	crp,ihfA,oxyR,phoB,rpoD,soxS	arcA,crp,ihfA,ihfB,oxyR,rpoD,soxS
0.140	0.140	0.140
crp,ihfA,ihfB,lrp,oxyR,rpoD,soxS	crp,ihfA,ihfB,oxyR,phoB,rpoD,soxS	crp,ihfA,lrp,oxyR,phoB,rpoD,soxS
0.140	0.140	0.140
arcA,crp,ihfA,ihfB,lrp,oxyR,rpoD,soxS	arcA,crp,ihfA,ihfB,oxyR,phoB,rpoD,soxS	crp,ihfA,ihfB,lrp,oxyR,phoB,rpoD,soxS
0.140	0.140	0.140
arcA,crp,ihfA,ihfB,lrp,oxyR,phoB,rpoD,soxS		
0.140		

Figure 7. **Case study 3.** Ranked adjustment sets of the small E Coli Case study with their corresponding variance.

B. Case study 4: Extended *E. coli* K-12 transcriptional network

Fig. 8 shows the weighted ADMG for the extended *E. coli* K-12 transcriptional network. Fig. 9 shows selected valid adjustment sets from the large E. Coli example with their corresponding variance.

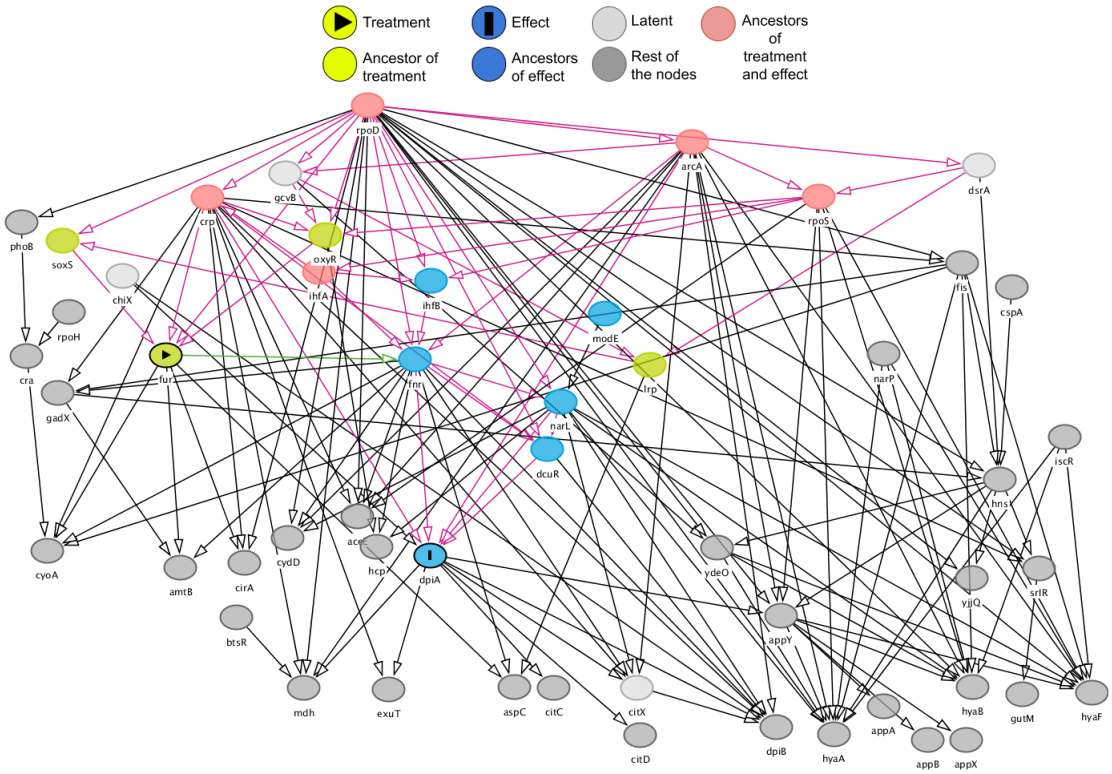

Figure 8. **Case study 4.** Weighted ADMG for the extended *E. coli* K-12 transcriptional network. The cost of each variable is set to 1.

Ranking	3	100	2000	2336
Selected adjustment sets	arcA, cra, crp, ihfB, modE, rpoD, rpoH, rpoS	arcA, crp, ihfB, lrp,rpoD,rpoH, rpoS	arcA,crp,fis, ihfB,lrp,phoB, rpoD,rpoS,soxS	crp,fis,ihfA, lrp,oxyR,phoB, rpoD,rpoS,soxS
Variance	0.158	0.159	0.162	0.164
Query estimation value	4.828497 $\approx$ 4.83	4.4.828672 $\approx$ 4.83	4.826809 $\approx$ 4.83	4.827704 $\approx$ 4.83

Figure 9. **Case study 4:** Selected rankings of the valid adjustment sets with their corresponding variance. The cost of measuring each variable is 1, hence the cost of an adjustment set is the total number of its variables. The query estimation value is $\hat{E}(dpiA|do(fur = 0))$

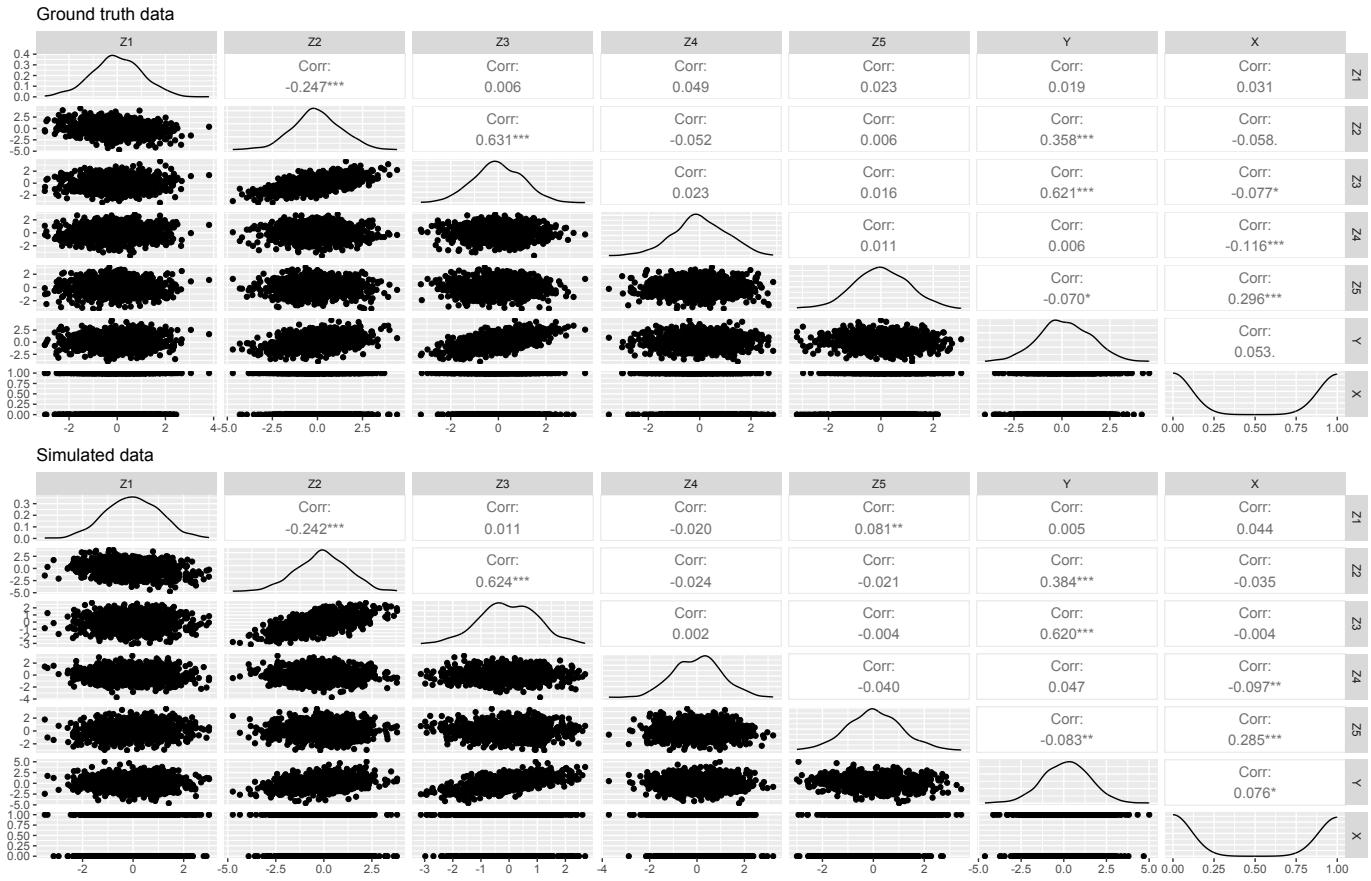

Figure 10. **Case study 1:** Above: Pairwise scatterplots and marginal density of experimental data. Below: Pairwise scatter plots and marginal density of simulated data

C. Marginal and pairwise scatter plot of Case studies

C.1. Case study 1

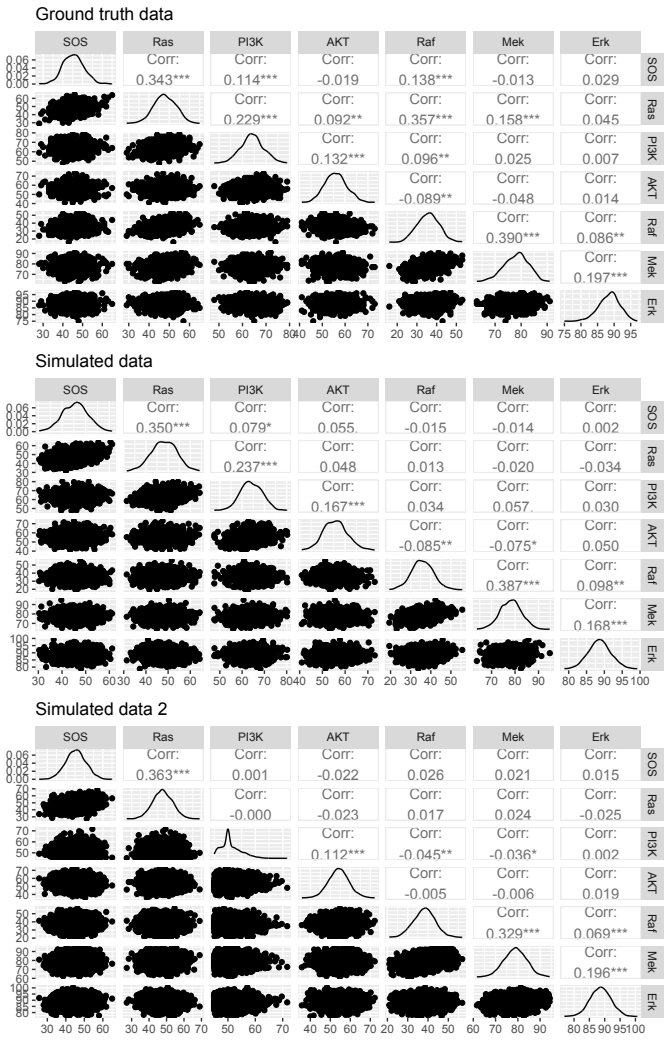

Figure 11. **Case study 2:** Above: Pairwise scatterplots and marginal density of experimental data. Middle: Pairwise scatter plots and marginal density of simulated data 1 (BN). Below: Pairwise scatter plots and marginal density of simulated data 2 (Hill)

C.2. Case study 2

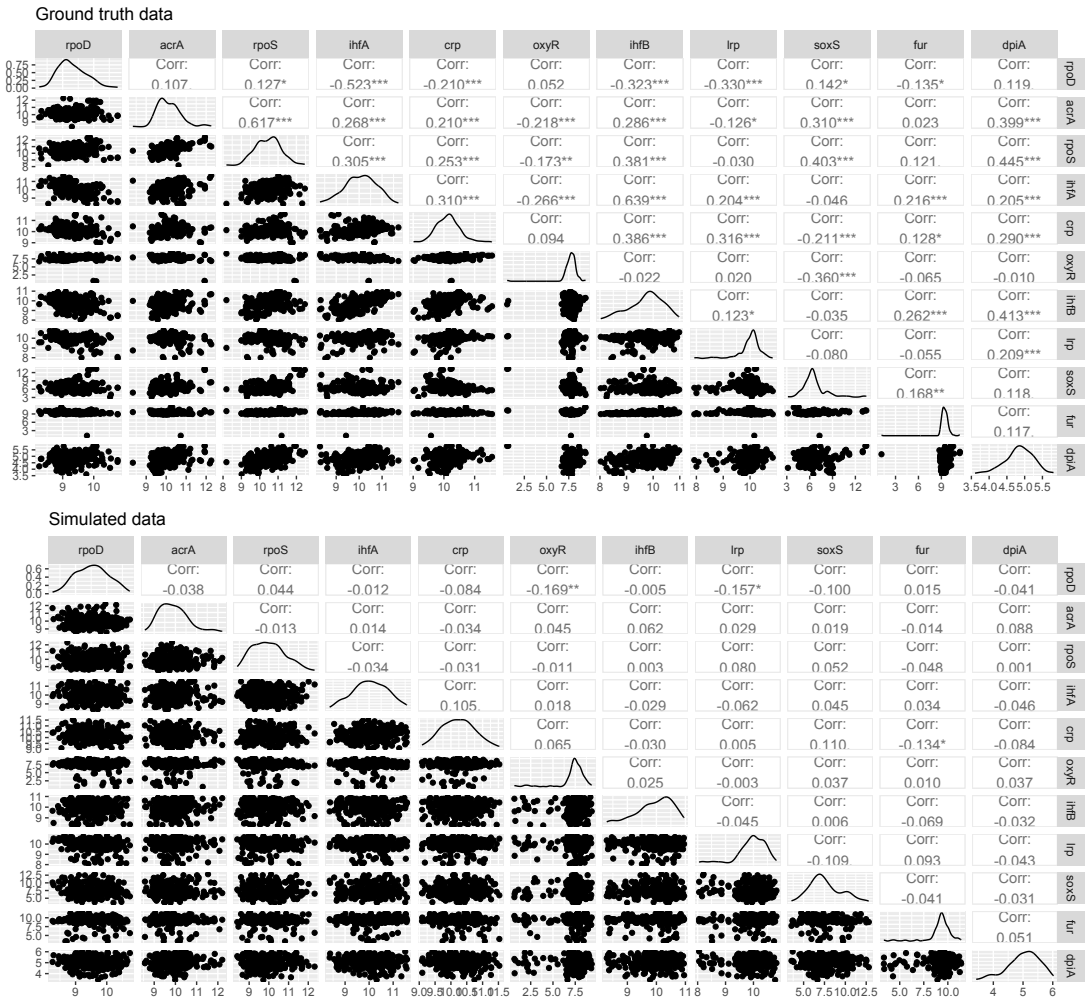

Figure 12. **Case study 3:** Above: Pairwise scatterplots and marginal density of experimental data. Below: Pairwise scatter plots and marginal density of simulated data (GAN).

C.3. Case study 3

C.4. Case study 4

The pairwise scatterplots and marginal densities are similar to Case study 3 because they are from the same real data set and the simulated data is learned with the same strategy as in Case study 3. The figure is omitted due to its size.