# Learning gene regulatory networks from gene expression measurements using non-parametric molecular kinetics (Supplementary material)

## Tables

Table 1: Areas under ROC and P-ROC curves on different IRMA data sets.

| | Switch-on | Switch-off | Galactose | Glucose |
|---|---|---|---|---|
| AUROC | 0.8382 | 0.8750 | 0.7794 | 0.8603 |
| AUPR | 0.8362 | 0.8485 | 0.7428 | 0.6575 |

Table 2: Used values of parameters $\mathbf{b}$ and $\sigma^2$ ($B = \sigma^2 I$).

| | Switch-on | Switch-off | Galactose | Glucose |
|---|---|---|---|---|
| $\sigma^2$ | 0.0108 | 0.0108 | 0.0680 | 0.0680 |
| $\mathbf{b}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ | $\mathbf{0}$ |

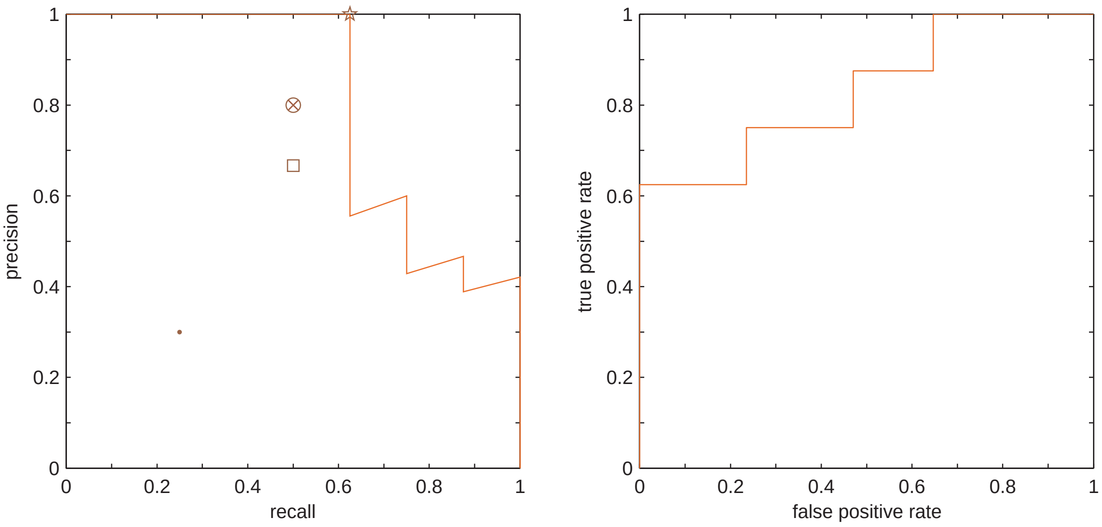
Table 3: Areas under ROC and P-ROC curves on different DREAM3 InSilicoSize100 data sets.

| | Ecoli1 | Ecoli2 | Yeast1 | Yeast2 | Yeast3 |
|---|---|---|---|---|---|
| AUROC | 0.8054 | 0.8305 | 0.7638 | 0.6538 | 0.5988 |
| AUPR | 0.3321 | 0.3720 | 0.3518 | 0.2287 | 0.1882 |

Table 4: AUROC and AUPR p-values on different DREAM3 InSilicoSize100 data sets.

| | Ecoli1 | Ecoli2 | Yeast1 | Yeast2 | Yeast3 |
|---|---|---|---|---|---|
| AUROC p-value | 1.278e-026 | 2.591e-024 | 1.615e-029 | 7.113e-022 | 6.379e-014 |
| AUPR p-value | 4.416e-072 | 1.363e-080 | 1.670e-082 | 6.236e-103 | 4.114e-085 |

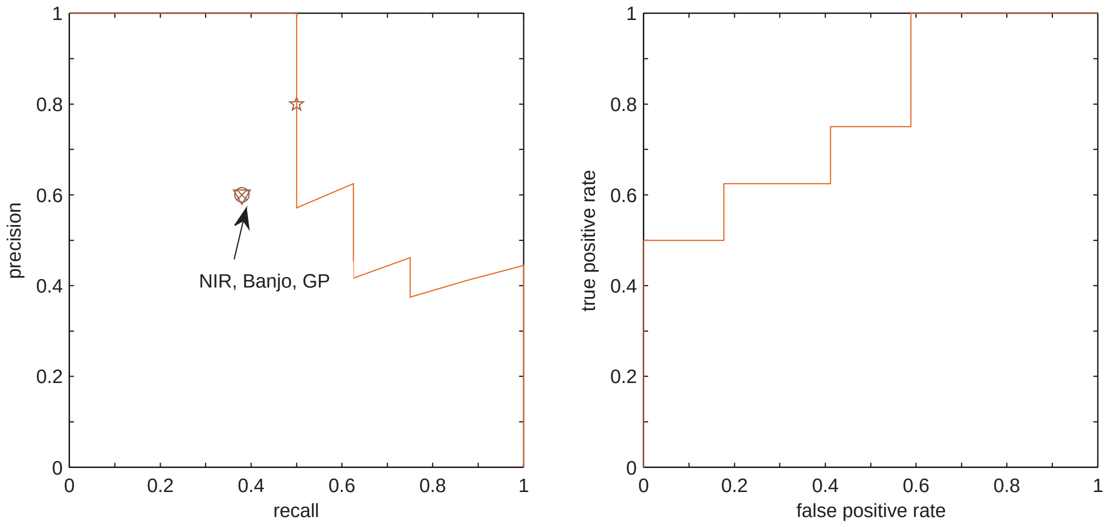
# Figures



(a) P-ROC curve

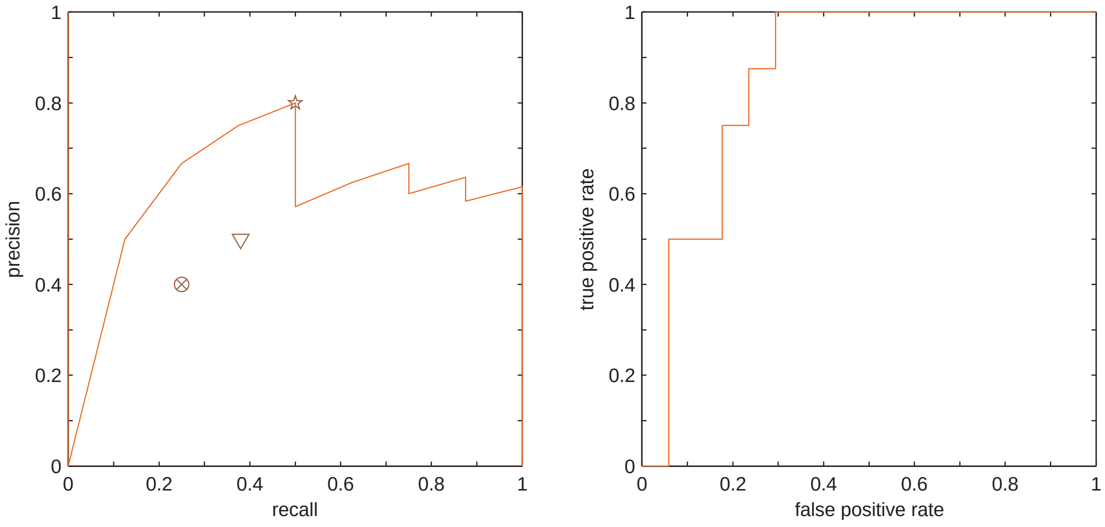
(b) ROC curve

Figure 1: Inference results on the switch-on data set. Obtained P-ROC curve is shown in Figure 1(a) and ROC curve is shown in Figure 1(b). The cross in circle marks the results obtained with TSNI method, the triangle marks the results obtained with Banjo and the star marks our results if we take 5 most probable interactions into consideration.



(a) P-ROC (b) ROC

Figure 2: Inference results on the galactose data set. Obtained P-ROC curve is in Figure (a) and ROC curve is in Figure (b). The cross in circle marks the results obtained with NIR method, the triangle marks the results obtained with Banjo and the star marks our results if we take 5 most probable interactions into consideration.



(a) P-ROC (b) ROC

Figure 3: Inference results on the glucose data set. Obtained P-ROC curve is in Figure (a) and ROC curve is in Figure (b). The cross in circle marks the results obtained with NIR method, the triangle marks the results obtained with Banjo and the star marks our results if we take 5 most probable interactions into consideration.

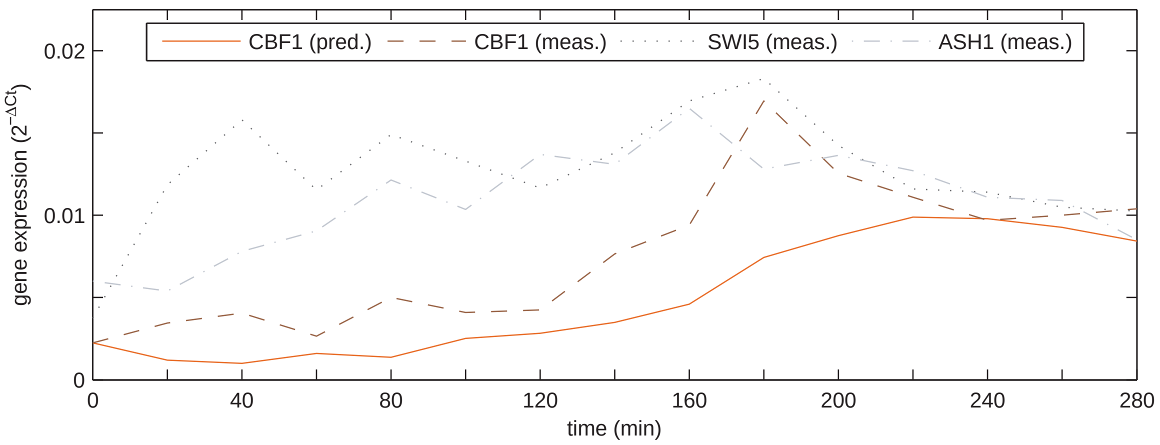
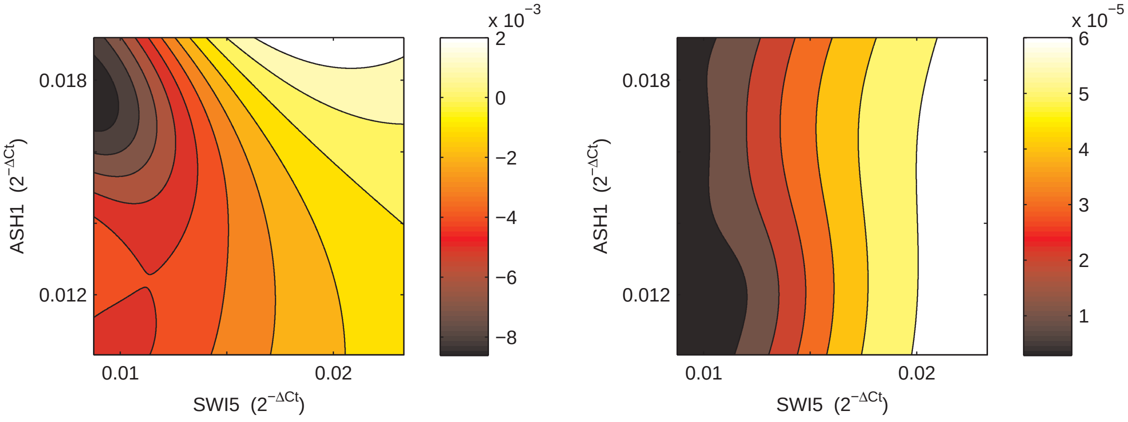


Figure 4: Predicted expression profile of gene CBF1 on the switch-on data set. Gene CBF1 has SWI5 and ASH1 as regulatory genes.



(a) Estimated regulatory function

(b) Variance of the estimate

Figure 5: Estimated regulatory function of CBF1 as a function of SWI5 and ASH1 evaluated on the test set (switch-on) is shown in Figure 5(a) and the variance of the estimate in Figure 5(b).

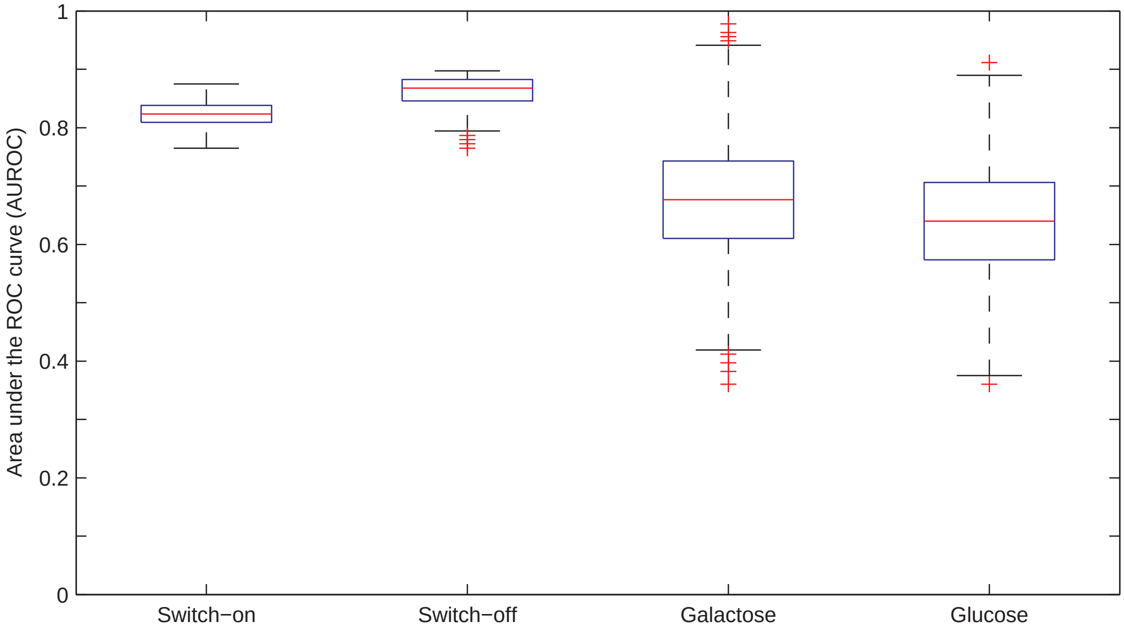
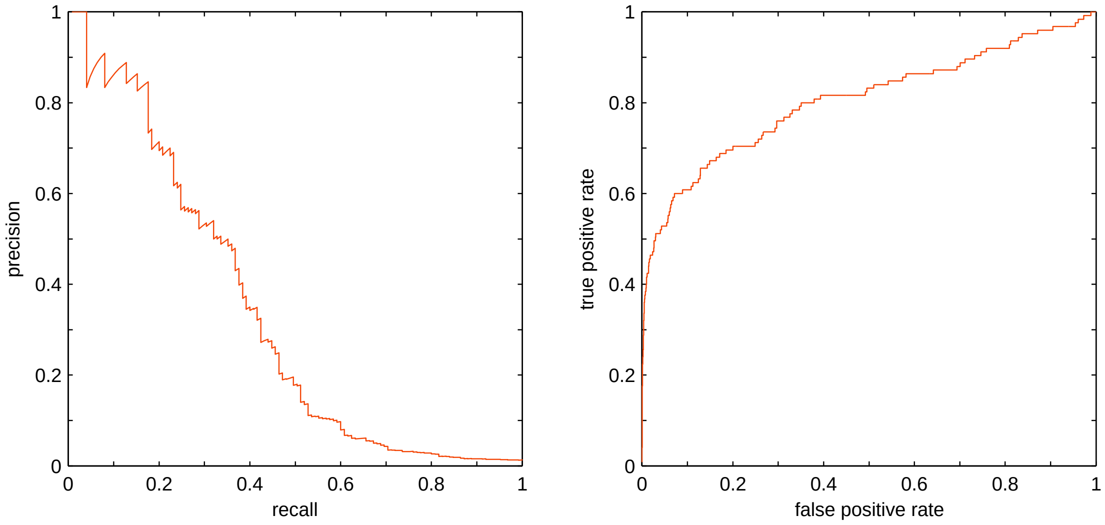


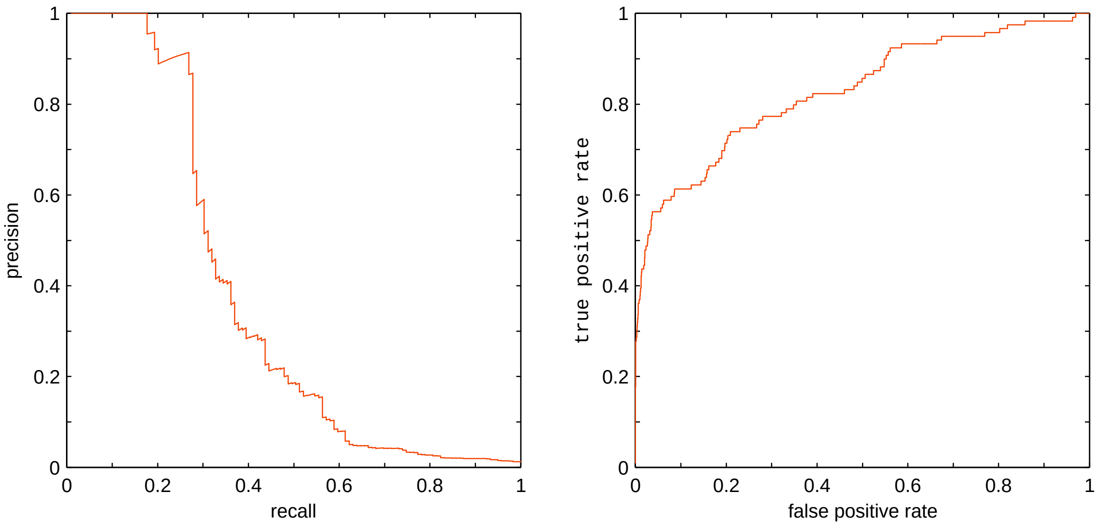
Figure 6: Sensitivity analysis of $B = \sigma^2 I$ by changing the $\sigma$ value and by recomputing all the GRN structure inference steps. 1000 different parameter values were taken from the interval determined by increasing and decreasing the original parameter value by a factor of two.



(a) P-ROC

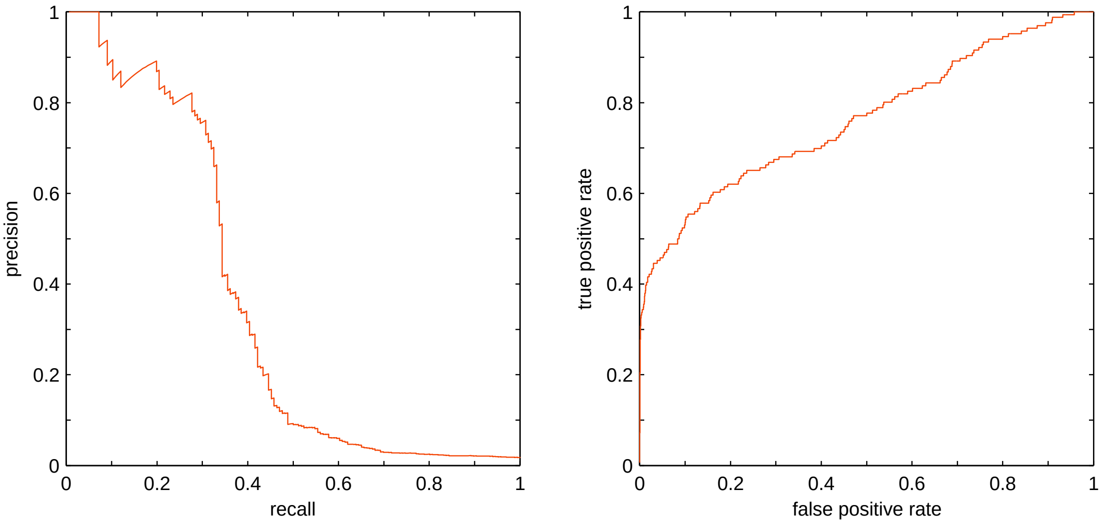
(b) ROC

Figure 7: Inference results on the ecoli1 data set. Obtained P-ROC curve is in Figure (a) and ROC curve is in Figure (b).



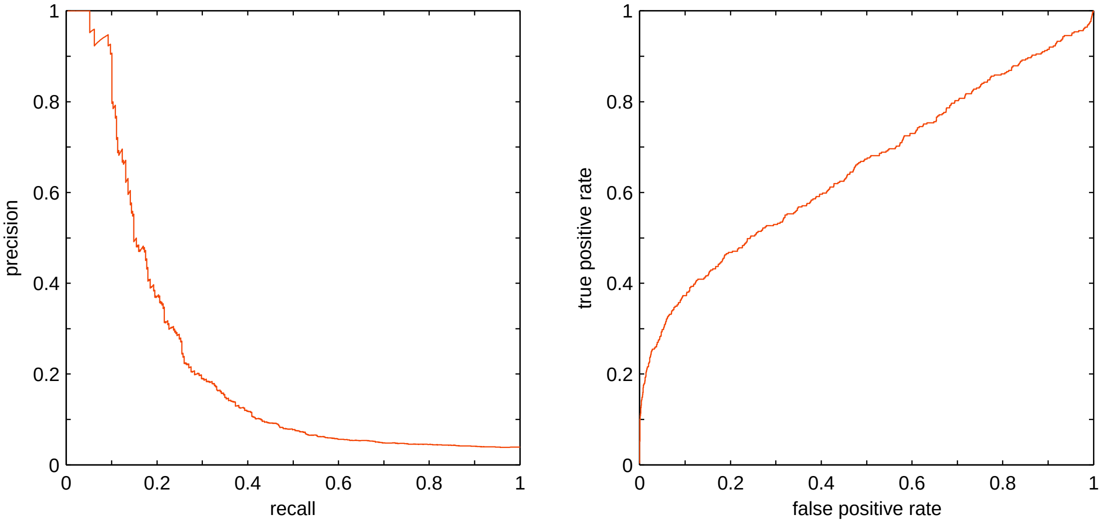
(a) P-ROC (b) ROC

Figure 8: Inference results on the ecoli2 data set. Obtained P-ROC curve is in Figure (a) and ROC curve is in Figure (b).



(a) P-ROC (b) ROC

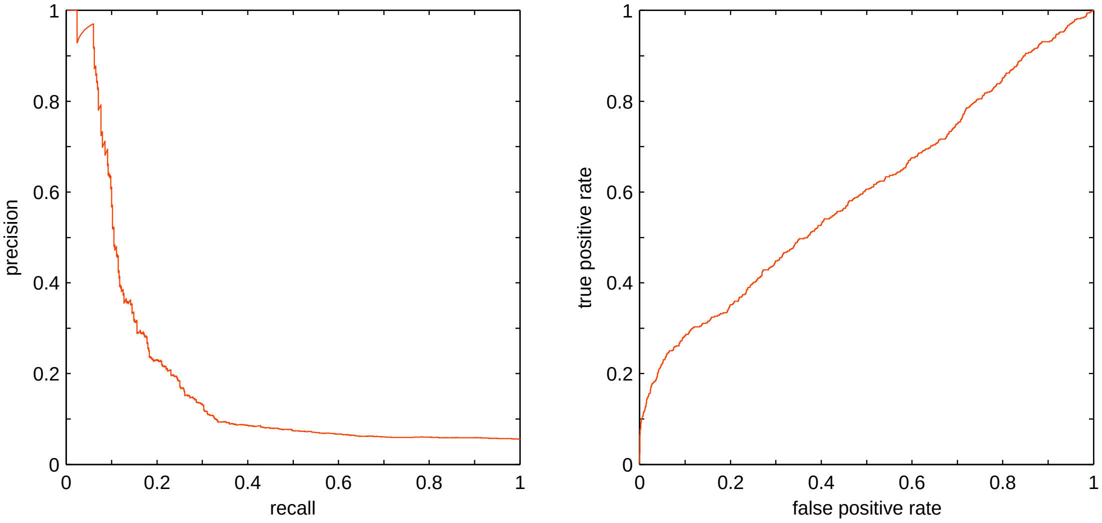
Figure 9: Inference results on the yeast1 data set. Obtained P-ROC curve is in Figure (a) and ROC curve is in Figure (b).



(a) P-ROC

(b) ROC

Figure 10: Inference results on the yeast2 data set. Obtained P-ROC curve is in Figure (a) and ROC curve is in Figure (b).



(a) P-ROC

(b) ROC

Figure 11: Inference results on the yeast3 data set. Obtained P-ROC curve is in Figure (a) and ROC curve is in Figure (b).