On protocols and measures for the validation of supervised methods for the inference of biological networks

SUPPLEMENTARY INFORMATION

Section 3.4

Adapting PR curve to another ratio $P/N$

It is possible to adapt a given PR curve to another ratio between positives and negatives than the one adopted to generate it (Hue et al., 2010). Let us assume a PR curve estimated from $P_1$ positives and $N_1$ positives and let us estimate from this curve a new curve corresponding to $P_2 = P_1$ positives and $N_2 \neq N_1$ negatives respectively drawn from the same distribution as the original $P_1$ positives and $N_1$ negatives. For a given confidence threshold, the recall (i.e., the proportion of positives greater than the threshold) is unchanged since $P_1 = P_2$. Denoting by $TP_1$ and $TP_2$ (resp. $FP_1$ and $FP_2$) the number of positives (resp. negatives) with a score greater than the threshold in both cases, we have $precision_1 = \frac{TP_1}{TP_1 + FP_1}$ and $precision_2 = \frac{TP_2}{TP_2 + FP_2}$. Given that $TP_1 = TP_2$ and $FP_2 = \frac{N_2}{N_1} FP_1$ in average, it is easy to show that $precision_1$ and $precision_2$ are related as follows:

$$precision_2 = \frac{precision_1}{precision_1 + \frac{N_2}{N_1}(1 - precision_1)}.$$  

Using this formula, one can thus approximate the PR curve for an arbitrary ratio between positives and negatives from the knowledge of at least one PR curve (corresponding to an arbitrary ratio). Note that this PR curve can also be derived from a ROC curve and the knowledge of the actual ratio $\frac{P}{N}$ using the fact that, for any confidence threshold, we have:

$$precision = \frac{TPR}{TPR + FPR \frac{N}{P}},$$

and that both $TPR$ and $FPR$ are known from the ROC curve.

Section 5.2

Effect of false negatives on evaluation

To estimate the effect of false negatives on the PR and ROC curves, we suppose that the ranking of the examples in a test fold is fixed and then compute the change in PR and ROC curve when a
Inequality (4) is valid as soon as the ranking is better than random. Indeed, it can be shown by some straightforward manipulations that inequality (4) is equivalent to the following inequality:

\[
\frac{TP}{FP} > \frac{P}{N},
\]

which is verified for any classifier that is better than random (i.e., a classifier that puts more positives above the confidence threshold than expected at random).