

Supplementary materials

Likelihood ratios take into account the biased sampling between positives and negatives

The performance of a prediction method is usually measured by its precision, defined as:
Precision = $P_+ / (P_+ + P_-)$;

However, in most biological cases, this quantity could sometimes be misleading due to the biased sampling between positives and negatives, whereas the likelihood ratio L does not have similar issues.

For example, let us suppose that there are 10^3 positives and 10^6 negatives in total for a biological feature that we would like to predict. In many biological prediction situations, one has to sample positives and negatives separately, just like in (Jansen, et al., 2003). Let us suppose that there are two ways to sample positives and negatives:

1. We could find all 10^3 positives and 10^5 negatives and form a training set of 1.01×10^5 elements;
2. We could find all 10^3 positives and 10^4 negatives and form a training set of 1.1×10^4 elements;

Let us suppose that there is a prediction method that, after learning on the training set, can discover 1/10 of the positives (i.e. P_+), but also mistakes 1/1000 of the negatives as positives (i.e. P_-).

Using the first training set:

$$\text{Precision}_1 = (10^3 \times 10^{-1}) / (10^3 \times 10^{-1} + 10^5 \times 10^{-3}) = 50\%$$

Using the second training set:

$$\text{Precision}_2 = (10^3 \times 10^{-1}) / (10^3 \times 10^{-1} + 10^4 \times 10^{-3}) = 91\%$$

The method does not change, at all. But because of the size of the training set, especially the unbalance between positives and negatives, Precision₂ appears to be extremely good.

The likelihood ratio L naturally takes this into account:

$$L_1 = \frac{\frac{10^3 \times 10^{-1}}{10^3}}{\frac{10^5 \times 10^{-3}}{10^5}} = 100$$

$$L_2 = \frac{\frac{10^3 \times 10^{-1}}{10^3}}{\frac{10^4 \times 10^{-3}}{10^4}} = 100 = L_1$$

P-value calculated by hyper-geometric distributions

Our defective clique method is able to predict 437 new interactions, 73 of which also in overlap with the gold standard positives. In order to determine whether the overlap is statistically significant, we used a hyper-geometric distribution to model the randomization process (i.e. create random networks by edge randomization):

Suppose that the total sample space is N . In the first round, a sample of size S_1 is randomly selected without replacement from N . Then, the entire initial sample (S_1) is subsequently returned to the sample space. In the second round, another sample of size S_2 is randomly selected without replacement from N . The size of the overlap (denoted as i) between the two samples (S_1 and S_2) is a hyper-geometric random variable. The probability of observing an overlap of a given size X or greater is calculated by the formula:

$$P(i \geq X) = 1 - \sum_{i=0}^{X-1} \frac{\binom{S_1}{i} \binom{N-S_1}{S_2-i}}{\binom{N}{S_2}}$$

To calculate the statistical significance of the overlap between the gold standard positives and our predictions, we first need to determine the total sample space (N). As we discussed in the text, there are 2283 proteins in the large-scale datasets. Therefore, the sample space (N) is 2.6×10^6 ($= 2283 \times 2282 / 2$); $S_1 = 2373$ (there are 2373 gold standard positives among these 2283 proteins); $S_2 = 437$ (Total number of predictions); $X = 71$ (the overlap). The calculated P value is smaller than 10^{-10} , which is statistically significant.

P values in Figure 5B were calculated in a similar fashion.

Calculation of functional enrichment

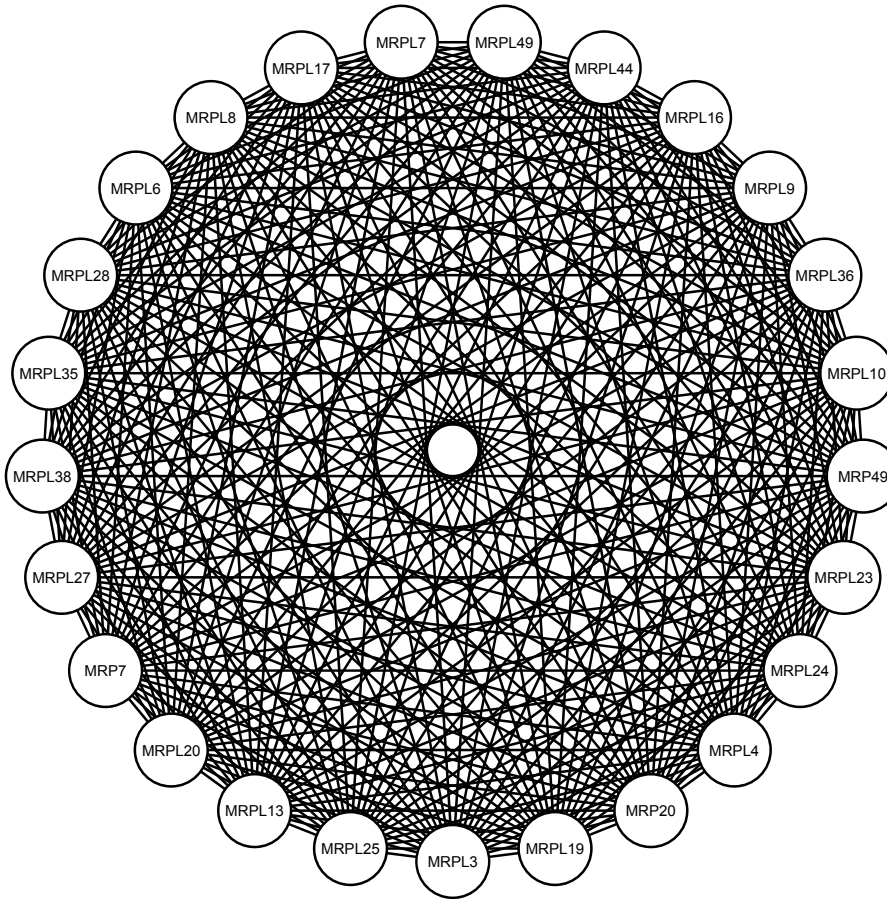
We used the MIPS functional classification to calculate the functional enrichment of our predictions. First, two genes are determined as having similar functions if the first two parts of their MIPS classifications are the same. There are about 1.8×10^7 protein pairs in yeast genome, 858557 of which have similar functions according to this criterion. The expected frequency for two randomly-picked proteins to have similar functions is therefore 4.8%. Second, we calculated the observed frequency for protein pairs that are predicted to interact to have similar functions. The functional enrichment is the ratio of the observed frequency over the expected one. Because the common assumption is that interacting pairs tend to have similar functions, the functional enrichment can be used as an indicator of how well our prediction method performs: the higher the functional enrichment, the better the performance of our method.

Supplementary Figure 1. Network view of the four maximal cliques in the complete gold standard set as in Figure 3A.

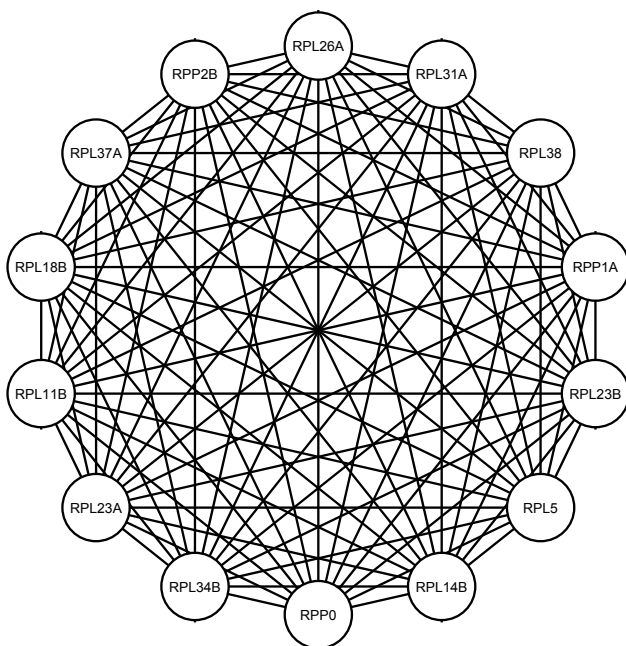
References:

Jansen, R., Yu, H., Greenbaum, D., Kluger, Y., Krogan, N.J., Chung, S., Emili, A., Snyder, M., Greenblatt, J.F. and Gerstein, M. (2003) A Bayesian networks approach for predicting protein-protein interactions from genomic data, *Science*, **302**, 449-453.

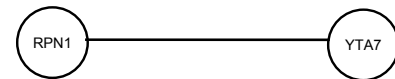
A. Clique G_1



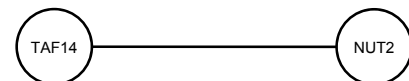
B. Clique G_2



C. Clique G_3



D. Clique G_4



Supplementary Table 1. Predicted interactions that are not in the MIPS complex catalog and do not have the same function based on MIPS functional classifications

Interactions	Interactions	Interactions	Interactions	Interactions					
Q0032	YNL182C	YBR287W	YPL235W	YDR211W	YNL265C	YGL237C	YIL053W	YKL166C	YML001W
Q0050	YER142C	YBR288C	YPL016W	YDR212W	YER173W	YGL237C	YIL070C	YKL166C	YNL093W
Q0092	YOR026W	YBR289W	YFL049W	YDR212W	YGL116W	YGL237C	YJL138C	YKL166C	YNL227C
REP1	YBL056W	YBR289W	YKR001C	YDR212W	YGL137W	YGL237C	YJR132W	YKL172W	YKR081C
REP1	YBR217W	YBR289W	YNL207W	YDR212W	YGL190C	YGL237C	YKL214C	YKL172W	YMR049C
REP1	YDR523C	YCL010C	YGL112C	YDR212W	YGL208W	YGL237C	YKR028W	YKL172W	YNL175C
YAL002W	YKR026C	YCL010C	YGR252W	YDR212W	YJL106W	YGL237C	YLR423C	YKL172W	YNL230C
YAL003W	YML064C	YCL011C	YDL084W	YDR212W	YKL095W	YGL237C	YNL063W	YKL173W	YLR117C
YAL005C	YOR151C	YCL011C	YDL213C	YDR212W	YKR036C	YGL237C	YNR031C	YKL173W	YMR213W
YAL005C	YPR010C	YCL011C	YHR167W	YDR212W	YLL011W	YGL237C	YOL139C	YKL173W	YNL147W
YAL007C	YAR002C	YCL011C	YLR432W	YDR212W	YLR196W	YGL237C	YOR272W	YKL173W	YOR159C
YAL007C	YDR087C	YCL011C	YML062C	YDR212W	YNL317W	YGL237C	YPL166W	YKL173W	YPR178W
YAL007C	YDR101C	YCL011C	YNL139C	YDR212W	YNL323W	YGL237C	YPR016C	YKL173W	YPR182W
YAL007C	YDR127W	YCL011C	YNL253W	YDR212W	YOR212W	YGL237C	YPR069C	YKL176C	YOR080W
YAL007C	YER110C	YCL014W	YER082C	YDR212W	YOR230W	YGL237C	YPR085C	YKL189W	YMR058W
YAL007C	YGL200C	YCL014W	YGR220C	YDR214W	YDR523C	YGL241W	YKR048C	YKL189W	YMR303C
YAL007C	YLR342W	YCL014W	YHR197W	YDR214W	YER173W	YGL241W	YLL050C	YKL193C	YML049C
YAL007C	YML012W	YCL017C	YPL135W	YDR214W	YHR030C	YGL244W	YHR009C	YKL193C	YPL036W
YAL007C	YMR290C	YCL024W	YKR048C	YDR214W	YIL038C	YGL244W	YOL145C	YKL193C	YPL179W
YAL007C	YPL211W	YCL028W	YDR128W	YDR214W	YOL094C	YGL244W	YOR123C	YKL204W	YOL139C
YAL009W	YDL040C	YCL028W	YDR260C	YDR214W	YOL139C	YGL245W	YGR040W	YKL205W	YLR291C
YAL009W	YDR211W	YCL028W	YDR499W	YDR214W	YOR212W	YGL245W	YHR107C	YKL206C	YPL051W
YAL009W	YJL176C	YCL028W	YEL021W	YDR214W	YPR110C	YGL245W	YKL081W	YKL210W	YLR096W
YAL009W	YLR342W	YCL028W	YER125W	YDR216W	YER177W	YGL245W	YML064C	YKL210W	YOR184W
YAL010C	YJL066C	YCL028W	YIL066C	YDR219C	YDR328C	YGL245W	YMR049C	YKL213C	YOR116C
YAL010C	YPL235W	YCL028W	YLR403W	YDR219C	YHR122W	YGL245W	YMR059W	YKL213C	YOR341W
YAL012W	YBR055C	YCL028W	YML058W	YDR224C	YDR365C	YGL245W	YOL094C	YKL213C	YPR010C
YAL012W	YMR300C	YCL028W	YNL106C	YDR224C	YER082C	YGL245W	YOR014W	YKL214C	YMR125W
YAL012W	YPL149W	YCL028W	YNL290W	YDR224C	YIL066C	YGL245W	YPR110C	YKL215C	YLL026W
YAL013W	YNL330C	YCL028W	YOL094C	YDR224C	YKL103C	YGL246C	YOR048C	YKL216W	YKR055W
YAL015C	YDL029W	YCL028W	YOR212W	YDR224C	YLR074C	YGL251C	YNL127W	YKL218C	YPR110C
YAL015C	YDL059C	YCL028W	YPL140C	YDR224C	YOL054W	YGL252C	YNL132W	YKR001C	YLR176C
YAL015C	YDR214W	YCL029C	YKL103C	YDR225W	YGL241W	YGL256W	YJR035W	YKR001C	YNL330C
YAL015C	YEL060C	YCL030C	YDL160C	YDR225W	YGR103W	YGL256W	YKL108W	YKR001C	YPL082C
YAL015C	YJR068W	YCL030C	YGR052W	YDR225W	YLR074C	YGR016W	YMR104C	YKR002W	YNL317W
YAL015C	YMR012W	YCL030C	YLR044C	YDR225W	YLR222C	YGR017W	YIL131C	YKR024C	YLR233C
YAL015C	YMR058W	YCL030C	YML124C	YDR225W	YLR247C	YGR033C	YOL100W	YKR024C	YNL175C
YAL015C	YMR146C	YCL031C	YGR090W	YDR225W	YNL308C	YGR040W	YGR155W	YKR025W	YNR003C
YAL015C	YNL037C	YCL035C	YMR059W	YDR225W	YOL054W	YGR040W	YHR033W	YKR025W	YOR116C
YAL015C	YPR110C	YCL037C	YDL208W	YDR226W	YFR028C	YGR040W	YHR200W	YKR025W	YPR110C
YAL016W	YDR482C	YCL037C	YGL120C	YDR226W	YML064C	YGR040W	YIL142W	YKR026C	YKR046C
YAL016W	YGR161C	YCL037C	YGR162W	YDR226W	YPL031C	YGR040W	YJR072C	YKR026C	YMR145C
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YAL017W	YDR190C	YCL039W	YGL227W	YDR238C	YHR169W	YGR040W	YOL078W	YKR028W	YPL204W

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YBR089C	YFR013W	YDL190C	YMR276W	YER138C	YPR110C	YIL038C	YLR044C	YNR046W	YNR050C
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YBR094W	YOR061W	YDL192W	YPR110C	YER142C	YLR432W	YIL055C	YPL115C	YOL005C	YPR093C
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YBR247C	YLR186W	YDR155C	YJL020C	YGL137W	YKR067W	YKL010C	YKL189W	YDL213C	YBR142W
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YBR247C	YPR144C	YDR155C	YOR290C	YGL137W	YOR362C	YKL021C	YPR016C	YNL002C	YPL093W
YBR249C	YPL150W	YDR155C	YOR319W	YGL137W	YPR108W	YKL029C	YPR054W	YNL002C	YER006W
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YBR251W	YDR036C	YDR158W	YLR314C	YGL137W	YPR124W	YKL056C	YMR059W	YPL093W	YNR053C
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YBR251W	YGR162W	YDR170C	YHR020W	YGL158W	YLR113W	YKL059C	YOR344C	YBL004W	YNL132W
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