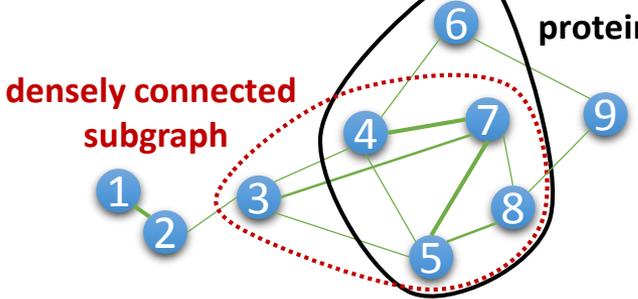


T-14 Predicting Protein Complexes by Sampling More Accurately and Efficiently

Chasanah Kusumastuti Widita, 丸山 修 (九州大学)

PPSampler2 is a protein complex prediction tool based on the Metropolis-Hastings algorithm.

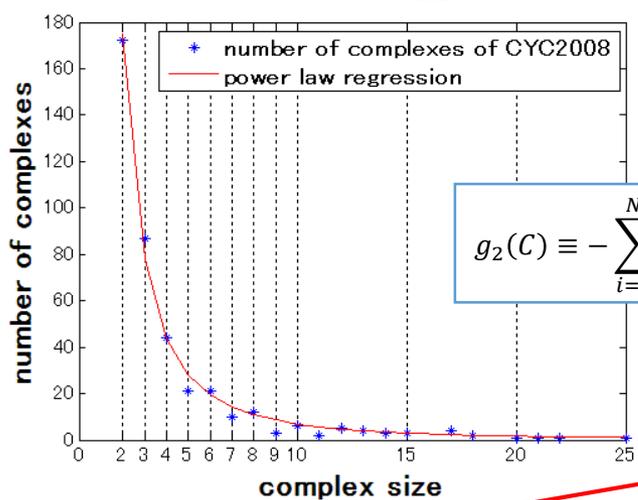
PPI network:



$$g_1(C) \equiv \sum_{d \in C} g_1(d)$$

$$g_1(d) = \begin{cases} 0 & \text{if } |d| = 1 \\ -\infty & \text{else if } |d| > N \text{ or } \\ & \exists u \in d, \forall v (\neq u) \in d, \\ & w(\{u, u\}) = 0 \\ \sum_{u, v (\neq u) \in d} \frac{w(u, v)}{\sqrt{|d|}} & \text{otherwise} \end{cases}$$

optimization (minimization) term



$$g_2(C) \equiv -\sum_{i=2}^N \frac{(\psi_C(i) - \psi(i))^2}{2\sigma_{2,i}^2}$$

regularization terms

$$g_3(C) \equiv -\frac{(s(C) - \lambda)^2}{2\sigma_3^2}$$

$s(C)$: number of proteins within the clusters of size 2 or more in C .
 λ : predefined target value of $s(C)$.

$$f(C) = -(g_1(C) + g_2(C) + g_3(C))$$

$$P(C) \propto \exp\left(-\frac{f(C)}{T}\right)$$

