Abstract Submitted for the MAR06 Meeting of The American Physical Society

Ranked solutions to a class of combinatorial optimizations - with applications in mass spectrometry based peptide sequencing TIMOTHY DOERR, GELIO ALVES, YI-KUO YU, NCBI/NLM/NIH — Typical combinatorial optimizations are NP-hard; however, for a particular class of cost functions the corresponding combinatorial optimizations can be solved in polynomial time. This suggests a way to efficiently find approximate solutions - - find a transformation that makes the cost function as similar as possible to that of the solvable class. After keeping many high-ranking solutions using the approximate cost function, one may then re-assess these solutions with the full cost function to find the best approximate solution. Under this approach, it is important to be able to assess the quality of the solutions obtained, e.g., by finding the true ranking of kth best approximate solution when all possible solutions are considered exhaustively. To tackle this statistical issue, we provide a systematic method starting with a scaling function generated from the fininte number of high-ranking solutions followed by a convergent iterative mapping. This method, useful in a variant of the directed paths in random media problem proposed here, can also provide a statistical significance assessment for one of the most important proteomic tasks - - peptide sequencing using tandem mass spectrometry data.

¹This work was supported by the Intramural Research Program of the NLM at NIH/DHHS.

Gelio Alves NCBI/NLM/NIH

Date submitted: 09 Dec 2005 Electronic form version 1.4