

A Review of Recent Developments in Protein Sequence Alignment

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Objectives

- Review of Literature (so no independent evaluation/benchmarking)
- Summarize use of MSA for Protein Sequence Alignment
- Application of MSA algorithms/methods
- Implementation of MSA algorithms/methods
- Improvements/enhancements included in implementation

Why do we care?

- Protein alignment informs structural analysis
- Evolutionary conservation
- Large peptide sequence reads (millions – even trillions in size)
- How do we address increasing size of datasets?
- Constraints of current hardware
- Limitations of current software
- Availability of publicly accessible peptide/nucleotide databases

Bioinformatics Background

- Sequence alphabet: 21 amino acids
- Alphabet above used to form string representation of peptides
- Pairwise alignments
- (Dis)similarity scores
- Profile HMM
- MAFFT
- T-coffee

What will be summarized

- Input
- Methodology
 - MSA Algorithms
- Enhancements
 - Domain-specific knowledge
 - Protein/genomic external databases
- Output
 - Results
 - Accuracy (according to authors; will not be evaluating this myself)
 - Running time (also according to authors)

Software to be explored

ConSurf 2016 MAFFT

PROSOMALS3D (2014)

PSI/T-Coffee (2016)

Primary References

- [1]H. Ashkenazy et al., “ConSurf 2016: an improved methodology to estimate and visualize evolutionary conservation in macromolecules,” *Nucleic Acids Res*, vol. 44, no. W1, pp. W344–W350, Jul. 2016.
- [2]J. Pei and N. Grishin, “PROMALS3D: Multiple Protein Sequence Alignment Enhanced with Evolutionary and Three-Dimensional Structural Information,” in *Multiple Sequence Alignment Methods*, D. J. Russell, Ed. Humana Press, 2014, pp. 263–271.
- [3]E. W. Floden, P. D. Tommaso, M. Chatzou, C. Magis, C. Notredame, and J.-M. Chang, “PSI/TM-Coffee: a web server for fast and accurate multiple sequence alignments of regular and transmembrane proteins using homology extension on reduced databases,” *Nucleic Acids Res*, vol. 44, no. W1, pp. W339–W343, Jul. 2016.