

Contents

1	Introduction	1
1.1	Background	1
1.2	Related Work	2
1.3	Alignment-Free Methods for Homology Detection and Fold Recognition	2
1.3.1	Generative and Discriminative Learning for Alignment-Free Homology Detection and Fold Recognition	4
1.3.2	Kernel-Based Learning Methods for Alignment-Free Homology Detection	4
1.4	Alignment-Based Methods for Homology Detection and Fold Recognition	5
1.4.1	Sequence Alignment for Homology Detection and Fold Recognition	7
1.4.2	Profile-Based Alignment for Homology Detection and Fold Recognition	8
1.4.3	Scoring Function for Profile-Based Alignment and Homology Detection	9
1.4.4	Scoring Function for Sequence-Profile Alignment and Comparison	10
1.4.5	Scoring Function for Profile-Profile Alignment and Comparison	11
1.5	Contribution of This Book	12
	References	13
2	Method	17
2.1	Modeling a Protein Family Using Markov Random Fields	17
2.2	Estimating the Parameters of Markov Random Fields	18
2.3	Scoring Similarity of Two Markov Random Fields	21

2.4	Node Alignment Potential of Markov Random Fields	22
2.5	Edge Alignment Potential of Markov Random Fields	24
2.6	Scoring Similarity of One Markov Random Fields and One Template	26
2.7	Algorithms for Aligning Two Markov Random Fields.	26
	References.	29
3	Software.	31
3.1	Overview of Program	31
3.2	Software Download	31
3.3	Feature Files	32
3.4	MRFsearch Ranking File.	33
3.5	Interpreting P-Value	34
3.6	Interpreting a Pairwise Alignment.	35
	References.	36
4	Experiments and Results.	37
4.1	Training and Validation Data.	37
4.2	Test Data.	38
4.3	Reference-Dependent Alignment Recall.	39
4.4	Reference-Dependent Alignment Precision.	41
4.5	Success Rate of Homology Detection and Fold Recognition	42
4.6	Contribution of Edge Alignment Potential and Mutual Information.	44
4.7	Running Time	45
4.8	Is Our MRFalign Method Overtrained?	45
	References.	47
	Conclusion	49
	Acknowledgments	51

Protein Homology Detection Through Alignment of
Markov Random Fields

Using MRFalign

Xu, J.; Wang, S.; Ma, J.

2015, VIII, 51 p. 13 illus., 1 illus. in color., Softcover

ISBN: 978-3-319-14913-4