

Contents

1	Introduction	1
2	Mathematical Preliminaries	17
2.1	Graph Theory	18
2.2	Linear Algebra	20
2.3	Polyhedral Theory	21
2.4	Linear Programming	22
2.5	Integral Polytopes	24
2.6	Polyhedral Combinatorics	25
2.7	Independence Systems	26
2.8	Stringology	28
3	Detecting Similarity – Alignments	29
3.1	Conventional Alignments	30
3.1.1	Pairwise Alignments	30
3.1.2	Multiple Alignments	35
3.2	Structural Alignment	38
4	Detecting Similarity – Traces	45
4.1	Conventional Traces	46
4.1.1	Pairwise Traces	46
4.1.2	Multiple Traces	51
4.2	Structural Traces	54
4.3	Gapped Traces	56

CONTENTS

5	The GMT and SMT Problem	59
5.1	Problem Definition	60
5.2	Dynamic Programming based Algorithms	61
5.2.1	The MT Algorithm	61
5.2.2	The SMT Algorithm	64
6	The Combinatorial Optimization Approach	67
6.1	The Generic Branch-and-Cut Algorithm	68
6.1.1	A Cutting Plane Approach	68
6.1.2	Branch-and-Bound	72
6.1.3	Branch-and-Cut	73
6.2	The GMT Problem	77
6.2.1	A Characterization of the GMT Problem as ILP	77
6.2.2	The Structure of the GMT Polytope	78
6.2.3	Bounds for the GMT Problem	88
6.2.4	Computational Results for the GMT Problem	91
6.3	The SMT Problem	102
6.3.1	A Characterization of the SMT Problem as ILP	102
6.3.2	The Structure of the SMT Polytope	104
6.3.3	Bounds for the SMT Problem	111
6.3.4	Computational Results for the SMT Problem	115
7	Discussion	137
8	Deutsche Zusammenfassung	141
9	Glossary	151
	Bibliography	155
	Curriculum Vitae	161
	Index	164