List of Figures

2.1-a Undirected labeled 9
2.1-b Directed unlabeled 9
2.1-c Directed labeled 9
2.1 Graph Examples 9

3.1 Homeomorphic edit path from G to H 27
3.2 Node contraction on the graph H 30
3.3 GED vs HGED computation 37
3.4 Homeomorphic Graphs 37
3.5 Fraction of graphs with their size for AIDS dataset 39
3.6 GED vs. k^*-GED computation on letter graphs 39
3.7 *GED* vs. *k*GED* computation on AIDS graphs 40
3.8 *GED* vs. *k*GED* computation on AIDS graphs using beam search 40
3.9 Effect of k^*-NC and k^*-ND on the topology of Letter A 43
3.10 Effect of k^*-NC and k^*-ND on the topology of active molecules of AIDS dataset 43

4.1 Comparison of execution time for letter A dataset 51
4.2 Comparison of execution time for letter E dataset 51
4.3 Comparison of execution time for active class of AIDS dataset 52
4.4 Comparison of execution time for inactive class of AIDS dataset 52
4.5 Comparison of accuracy ratio of letter A dataset 53
4.6 Comparison of accuracy ratio of letter E dataset 53
4.7 Comparison of accuracy for active class of AIDS dataset 56
4.8 Comparison of accuracy for inactive class of AIDS dataset 56

5.1 Geometric Graphs G_1 and G_2 63
5.2 Triangle inequality: $d(a,x) \leq d(a,u) + d(u,x)$ 63
5.3 Edge Distance from G_1 to G_4 is 0 67
5.4 Geometric graphs with VD and ED both 0 68
5.5 t-tolerant geometric graph isomorphism 77
5.6 Accuracy Low 78
5.7 Accuracy Medium 78
5.8 Accuracy High 78

5.9 Accuracy 79
5.10 GDM vs GED for high distortion letter graphs 80
5.11 GDM vs GED for medium distortion letter graphs 81
5.12 GDM vs GED for low distortion letter graphs 81
5.13 Comparison of accuracy on letter dataset 82