UNIVERSITY OF ADELAIDE

DOCTORAL THESIS

Parameterized Analysis of Bio-inspired Computation and the Traveling Salesperson Problem

Author: Samadhi Nallaperuma Principle Supervisor: A/Prof. Frank Neumann

Co Supervisor: Prof. Zbigniew Michalewicz

A thesis submitted in fulfilment of the requirements for the degree of Doctor of Philosophy

in the

Optimization and Logistics School of Computer Science

March 2015

Declaration

I, Samadhi Nallaperuma certify that this work contains no material which has been accepted for the award of any other degree or diploma in my name in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text. In addition, I certify that no part of this work will, in the future, be used in a submission in my name for any other degree or diploma in any university or other tertiary institution without the prior approval of the University of Adelaide and where applicable, any partner institution responsible for the joint award of this degree.

I give consent to this copy of my thesis when deposited in the University Library, being made available for loan and photocopying, subject to the provisions of the Copyright Act 1968.

I also give permission for the digital version of my thesis to be made available on the web, via the University's digital research repository, the Library Search and also through web search engines, unless permission has been granted by the University to restrict access for a period of time.

Signed:

Date:

" Student: Dr. Einstein, Aren't these the same questions as last year's [physics] final exam ? Dr. Einstein: Yes; But this year the answers are different."

- Albert Einstein

UNIVERSITY OF ADELAIDE

Abstract

Engineering, Computer and Mathematical Sciences School of Computer Science

Doctor of Philosophy

Parameterized Analysis of Bio-inspired Computation and the Traveling Salesperson Problem

by Samadhi Nallaperuma

Bio-inspired algorithms such as evolutionary algorithms (EA) and ant colony optimization (ACO) have become very popular in recent years to solve a wide range of complex real world problems. However, the understanding about the conditions under which these algorithms perform well is still limited. Classical computational complexity analysis often taking a worst case perspective, hardly captures what is happening during the actual algorithm run and, lacks implications for guiding algorithm design. This issue is more significant on the problems such as the traveling salesperson problem (TSP) where the problem is hard in a theoretical sense and has a lot of real world applications. Thus, more practical perspectives of algorithm analysis and design are essential to bridge the gap between the theory and the practice in bio-inspired computation specially with respect to the hard problems such as the TSP. We introduce "parameterized analysis" of bio-inspired computation by linking together several emerging methods of algorithm analysis and design with the aim of explaining the relationship between various problem and algorithm parameters and their effects on the algorithm performance. Moreover, we gain novel insights into bio-inspired computation and the TSP through parameterized analysis.

Acknowledgements

I would like to present my sincere gratitude

- Firstly, to the principle supervisor Frank Neumann for the great inspiration to pursue research in bio-inspired computation and the all time guidance and support,
- To the co-supervisor Zbyzek Michalewicz for the kind advices enriched with a lifetime of research experience,
- To the co-authors of the papers Markus Wagner, Andrew Sutton, Dirk Sudholt, Mohommad Reza Bonyadi, Heike Trautmann, Bernd Bischl and Olaf Mersmann for their collaboration and feedback that yielded to successful outcomes,
- To the optimization and logistics research group, for the brainstorming sessions,
- To the anonymous reviewers of the conference and the journal papers and the examiners of this thesis for their generous efforts that shape our work and adapt to the best direction,
- To all the scientists whose work is refereed in this thesis for their great efforts made for the advances in science, that laid the foundations for this work,
- To the university of Adelaide Graduate Center for offering me a PhD scholarship and evaluating the progress through milestones that kept the PhD schedule well in shape,
- To the head of school Katrina Falkner, the postgraduate coordinator David Suter and the school manager Joane Rogers for providing an ideal environment for research,
- To the school's staff and the fellow PhD students for their encouragement by, providing feedback at the major review and offering me the "best poster award" at the Poster Day 2013,
- To the Dagstul seminar 13271 in the theory of evolutionary computation for the generous invitation that exposed me, to the cutting edge research that resulted in a strong motivation and, to be inspired by the experts,
- To the school, Google and GECCO for supporting my conference travel,
- To all my teachers from the kindergarten to the university for cherishing my intellect, passion and discipline that lead to a PhD,
- And finally to my beloved mom Sumithra, dad Wiraj, sister Oshadhi, my relatives, dear friends and my loving husband Namal for providing all kind of support and the persistent encouragement to conduct research.

Contents

Declaration	i
Abstract	iii
Acknowledgements	iv
Contents	v
List of Figures	viii
List of Tables	x
Abbreviations	xii

1	Intr	oductio	on and a second s	1
2	The Traveling Salesperson Problem			4
	2.1	Introd	uction	4
	2.2	The M	letric Traveling Salesperson Problem	5
	2.3	Exact	Algorithms	6
	2.4	Appro	eximation Algorithms	7
	2.5	Heuri	stics	8
	2.6	Rando	mized Local Search and the Simple Evolutionary Algorithm	9
		2.6.1	Permutation Operators	10
	2.7	Ant C	olony Optimization	13
	2.8	Conclu	usions	14
3	Met	hods of	f Algorithm Analysis of Bio-inspired Computing	15
	3.1	Introd	uction	15
	3.2	Classi	cal Computational Complexity Analysis of Bio-inspired Computation	15
		3.2.1	Stochastic Processes, Markov Chains and the First Hitting Time	16
		3.2.2	Deviation Bounds	18
		3.2.3	Artificial Fitness Levels	19
		3.2.4	Drift Analysis	19
		3.2.5	Limitations and Drawbacks	20
	3.3	Param	eterized Analysis	21
		3.3.1	Smoothed Complexity	21

		3.3.2 Expected Fitness Gain and Fixed Budget Analysis	22
		3.3.3 Feature Based Analysis of Problem Hardness	23
		3.3.4 Parameterized Complexity	25
	3.4	Conclusions	26
	_		
4	Exp	cted Fitness Gain Analysis of Local Search and Simple Evolutionary Algorithms	27
	4.1	Introduction	27
	4.2	Preliminaries	28
		4.2.1 Minimum Improvement of a 2-Opt Step	29
	4.3	Analysis for Manhattan Instances	31
		4.3.1 Analysis of a Single 2-Opt Step	31
		4.3.2 Analysis of Linked Steps for RLS	32
		4.3.3 Analysis of Linked Steps for (1+1) EA	35
	4.4	Analysis for Euclidean Instances	38
		4.4.1 Analysis of a Single 2-Opt Step	38
		4.4.2 Analysis of Linked Steps for RLS	40
		4.4.3 Analysis of Linked Steps for (1+1) EA	41
	4.5	The Solution Quality over the Algorithm Run	42
	4.6	Conclusions	43
_	-		
5	Exp	cted Fitness Gain Analysis of Population based Evolutionary Algorithms	45
	5.1		45
	5.2		46
	5.3	Fitness Gain based on Single Step Improvements	47
	5.4	Fitness Gain based on Linked Steps	48
	5.5	The Solution Quality over the Algorithm Run	50
	5.6		51
6	Feat	re based Comparison of Problem Hardness for Local search and Approximation	
Ŭ	Alg	rithms	52
	6.1	Introduction	52
	6.2	Preliminaries	53
	0.2	6.2.1 Investigated Features	55
	63	Analysis of the Christofides Algorithm	56
	0.0	6.3.1 Feature Variation for the Instances with Intermediate Difficulty	58
	64	Performance Comparison of RIS and the Approximation Algorithms	65
	6.5	Conclusions	68
	0.5		00
7	Effe	ts of the Problem Features and Algorithm Parameters on Problem Hardness for	
	Ant	Colony Optimization	69
	7.1	Introduction	69
	7.2	Background	71
		7.2.1 Performance Analysis of Ant Colony Optimization	71
		7.2.2 Easy and Hard Instance Generation	72
	7.3	Features of the Hard and Easy Instances for α and β	72
		7.3.1 Experimental Setup	72
		7.3.2 Feature Analysis	73
		7.3.3 Feature Variation for the Instances with Intermediate Difficulty	74
		7.3.4 Comparison of the Parameter Settings	76

	7.4	Extending the Analysis for ρ and n	79
	7.5	Parameter Prediction	82
		7.5.1 The First Prediction Model	82
		7.5.2 More Effective Prediction Models	84
	7.6	Conclusions	89
8	Para	ameterized Complexity Analysis of Evolutionary Algorithms	91
	8.1	Introduction	91
	8.2	Preliminaries	92
		8.2.1 Parameterized Complexity Analysis	93
	8.3	Fixed-Parameter Evolutionary Algorithms	94
		8.3.1 A Population-based Approach	94
		8.3.2 Searching for Permutations of Inner Points	99
		8.3.3 Experiments	102
		8.3.3.1 Parameterized Instances	103
		8.3.3.2 Results	103
	8.4	Conclusions	108
9	Para	ameterized Complexity Analysis of Ant Colony Optimization	110
	9.1	Introduction	110
	9.2	New Construction Procedures	111
	9.3	New ACO Algorithms	115
		9.3.1 Local Search	116
	9.4	Experimental Investigations	117
		9.4.1 Parameterized Instances	119
		9.4.2 Solution Quality Results	119
	9.5	Conclusions	124
10	Con	clusions	126

Bibliography

128

List of Figures

2.1	The effect of the inversion σ_{ij}^{I} operation on a Hamiltonian cycle. Inverting a subsequence in the permutation representation corresponds to a 2-Opt (or 2-change) move in which a pair of edges in the current Hamiltonian cycle are replaced by a pair of edges not in the current cycle	11
2.2	The effect of the jump operation σ_{ij}^{J} on a Hamiltonian cycle.	11
2.3	The effect of the exchange operation σ_{ij}^{E} on a Hamiltonian cycle	12
6.1	Boxplots of the mean (top) and standard deviations (bottom) of the tour length legs of the optimal tour, both for the evolved easy and hard instances for Chris- tofider	56
6.2	Boxplots of the mean values angle between adjacent cities on the optimal tour for Christofides.	57
6.3	Scatterplots of exemplary feature combinations classifying easy and hard in- stances for Christofides.	57
6.4	Distance features (top) and Cluster features (bottom): approximation quality and feature values for different α levels of all conducted morphing experiments for Christofides.	59
6.5	Angle (top) and Centroid Features (bottom): approximation quality and feature values for different α levels of all conducted morphing experiments for Christo-fides.	60
6.6	Convex Hull (top) and Mode (bottom) features: approximation quality and feature values for different α levels of all conducted morphing experiments for Christofides.	61
6.7	MST features: approximation quality and feature values for different α levels of all conducted morphing experiments for Christofides.	63
6.8	Nearest neighbour distance features: approximation quality and feature values for different α levels of all conducted morphing experiments for Christofides.	64
6.9	Some contrast patterns observed for Christofides (top) and RLS (bottom)	64
6.10	Some contrast patterns observed for 2-Approximation (top) and Christofides (bottom)	65
6.11	Performance of the RLS (top) and Christofides algorithm (bottom) on the easy	00
6.12	(grey) and hard (black) instances of the 2-Approximation algorithm	65
6.13	rithm (bottom) on the easy (grey) and hard (black) instances of RLS Performance of RLS algorithm (top) and the 2-Approximation algorithm (bot-	66
	tom) on easy (grey) and hard (black) instances of Christofides algorithm	67
7.1	Instance examples	74

7.2	Boxplots of the standard deviations of the angles between adjacent cities on the optimal tour for parameter setting 2 ($\alpha = 0$, $\beta = 4$) on the left and setting 3 ($\alpha = 4$, $\beta = 0$) on the	
	right	75
7.3	Hard and easy classification with two exemplary features for parameter setting 2 ($\alpha = 0, \beta = 4$) on the top and parameter setting 3 ($\alpha = 4, \beta = 0$) at the bottom.	76
7.4	Feature variation with instance difficulty for some exemplary features from dis- tance (top) and minimum spanning tree (bottom) feature groups for the default parameter setting ($\alpha = 1, \beta = 2$).	77
7.5	Feature variation with instance difficulty for mean (left) and standard deviation (right) of distances for the three parameter settings 1 (top), 2 (middle) and 3 (bottom).	78
7.6	Performance of the second parameter setting (top) and the third (bottom) on the easy (grey) and hard (black) instances of the first parameter setting.	78
7.7	Performance of the first parameter setting (top) and the third (bottom) on the easy (grey) and hard (black) instances of the second parameter setting.	79
7.8	Boxplots of the means and the standard deviations of the angles between neighbor cities	80
7.9 7.10	Boxplots of the means(top) and the standard deviations(bottom) of the distances Prediction Model 1. It predicts the algorithm performance based on the problem	81
7.11	features c_i , $1 \le i \le p$ and the possible algorithm parameters θ_j , $1 \le j \le q$ Prediction Model 2. It predicts the algorithm parameters θ_i , $1 < j < q$ based on	82
	the problem features c_i , $1 \le i \le p$ on optimal performance.	84
8.1	Edges that intersect at a point p form the diagonals of a convex quadrilateral in the plane. Interior edges define nondegenerate triangles with given angles.	93
8.2	Comparison of solution quality (minimum tour length values) of (1+1) EA_e^k , (1+1) EA_i^k and (1+1) EA_j^k obtained within 15 seconds on 30 instances of size 100 and inner point percentage 40	105
9.1 9.2	Example instance with two interior points	112 120
9.3	Comparison of solution quality of classical MMAS and the new version (XPMMAS ₁ obtained within 10000 iterations for parameters $\alpha = 1$ and $\beta = 2$ for 100 instances of size 100 and inner point percentage 30) 121

List of Tables

4.1	Expected fitness gain in <i>t</i> iterations for RLS and (1+1) EA for Manhattan and Euclidean instances due to single-step and consecutive-steps analysis. The former applies for any time span <i>t</i> ; the latter requires $t = \Omega(n^3)$. The consecutive-steps analysis was formally proven for the (1+1) EA* and transfers to the (1+1) EA if, as conjectured, the latter does not perform worse. All fitness gains assume that no local optimum is reached. Otherwise the expected approximation ratio	
	is $O(\sqrt{\phi})$.	42
4.2	The solution quality in <i>t</i> iterations for RLS and for Manhattan and Euclidean instances due to single-step and consecutive-steps analysis if the current solution is not locally optimal. Otherwise, the approximation ratio is $O(\sqrt{\phi})$.	43
4.3	The solution quality in t iterations for (1+1) EA or (1+1) EA* and for Manhattan and Euclidean instances due to single-step and consecutive-steps analysis if the current solution is not locally optimal. Otherwise, the approximation ratio is	
	$O(\sqrt{\phi})$	43
5.1	Expected fitness gain in <i>t</i> iterations for $(1+\lambda)$ RLS and $(1+\lambda)$ EA for Manhattan and Euclidean instances due to single-step and consecutive-steps analysis. The former applies for any time span <i>t</i> : the latter requires $t = O(r^3/\min(\lambda r^2))$	
	Otherwise the expected approximation ratio is $O(\sqrt{\phi})$.	50
5.2	Expected approximation ratio in <i>t</i> iterations for $(1+\lambda)$ RLS and for Manhattan and Euclidean instances due to single-step and consecutive-steps analysis.	50
5.3	Expected approximation ratio in t iterations for $(1+\lambda)$ EA and for Manhattan and Euclidean instances due to single-step analysis.	51
7.1	Predicted and actual approximation ratios for 26 TSPLIB instances of size in range 51–264. Note, that the underlying model is based only on our analysis of	
7.2	instances of size 100	83
	of size in range 51–264. Note, that the underlying model is based only on our analysis of instances of size 100	85
7.3	Results of the Wilcoxon signed rank tests on the predicted and actual approx- imation ratios for all the parameter combinations of the TSPLib instances, for	00
	the hypothesis "predicted > actual", positive rank sum (W) and confidence (p) values are displayed accordingly.	86
7.4	Predicted and actual best parameter settings (α , β , n and ρ) for 26 TSPLIB in- stances of size in range 51–264 from the prediction model 2a. Note, that the	00
75	underlying model is based only on our analysis of instances of size 100 Predicted and actual parameter settings (α , β , n and α) for 26 TSPI IB instances	88
	of size in range 51–264 from the prediction model 2b. Note, that the underlying model is based only on our analysis of instances of size 100.	89

8.1	Average minimum tour length values (rounded) obtained by the six algorithms ((1+1) $\text{EA}_{e'}^n$ (1+1) $\text{EA}_{e'}^n$ (1+1) $\text{EA}_{i'}^n$ (1+1) $\text{EA}_{$	
	value by Concorde (from left to right) for the set of 30 instances in each category	104
8.2	Results of Wilcoxon signed rank tests for minimum tour length values within	. 104
	time limits (2, 3 and 15 seconds for 25, 50 and 100 sizes accordingly) for (1+1) EA_e^n > (1+1) EA_e^k (exchanges), (1+1) EA_i^n > (1+1) EA_i^k (inversions) and (1+1) EA_i^n >	
	(1+1) EA_i^k (jumps), positive rank sums (W) and confidence (p) values are dis-	
	played accordingly. A * denotes $p < 0.001$. 106
8.3	Results of Wilcoxon signed rank tests for minimum tour length values within time limits (2, 3 and 15 seconds for 25, 50 and 100 sizes accordingly) for (1+1) EA_i^k	
	< (1+1) EA ^{<i>k</i>} _{<i>j</i>} (test 1), (1+1) EA ^{<i>k</i>} _{<i>j</i>} < (1+1) EA ^{<i>k</i>} _{<i>e</i>} (test 2), positive rank sums (<i>W</i>) and	100
	confidence (p) values are displayed accordingly. A * denotes $p < 0.001$. 108
9.1	Results for different construction procedures with $\alpha = \beta = 0$. 115
9.2	Results of Wilcoxon signed rank tests for solution quality (minimum tour length)	
	within 10000 iterations for XPMMAS ₁ $<$ MMAS (<i>test</i> ₁), MMAS $<$ XPMMAS ₂	
	$(test_2)$ and XPMMAS ₁ < XPMMAS ₂ $(test_3)$, positive rank sums (W) and confi-	100
0.2	dence (<i>p</i>) values are displayed accordingly	. 122
9.5	obtained by MMAS_XPMMAS, and XPMMAS_ within 10000 iterations for each	
	set of 100 instances having sizes 25, 50, 100 and 200 and inner point percentages	
	5%, 10%, 20%, 30% and 40%	. 123
9.4	Results of Wilcoxon signed rank tests for solution quality within 10000 iterations	
	without local search for XPMMAS ₁ > MMAS ($test_1$), XPMMAS ₂ > MMAS ($test_2$)	
	and XPMMAS ₂ > XPMMAS ₁ (<i>test</i> ₃), positive rank sums (W) and confidence (p)	
0 5	values are displayed accordingly	. 123
9.5	Average minimum tour length values (rounded to the nearest whole number)	
	set of 100 instances having sizes 25–50–100 and 200 and inner point percentages	
	5%, 10%, 20%, 30% and 40%	. 124
9.6	Results of Wilcoxon signed rank tests for the number of iterations to achieve a	
	1.1 approximation ratio for XPMMAS ₁ < MMAS ($test_1$), XPMMAS ₂ < MMAS	
	$(test_2)$ and XPMMAS ₂ > XPMMAS ₁ $(test_3)$ without local search, positive rank	
	sums (<i>W</i>) and confidence (<i>p</i>) values are displayed accordingly	. 124

Abbreviations

TSP	Traveling Salesperson Problem
MST	Minimum Spanning Tree
EA	Evolutionary Algorithm
GA	Genetic Algorithm
ACO	Ant Colony Optimization
RLS	Randomized Local Ssearch
RSH	Randomized Search Heuristics
MMAS	Max Min Ant System
NP	Nondeterministic Polynomial
FPT	Fix Parameter Tractable
ХР	eXPonential
PTAS	Polynomial Time Approximation Scheme
w. l. o. g.	without loss of generality
i. e.	id est (that is)
cf.	c onfer (compare)
e. g.	e xempli g ratia (for example)

In loving memory of Blacks and Pinky (2003 - 2014) ...