



# Towards a Better Understanding of Search Algorithms

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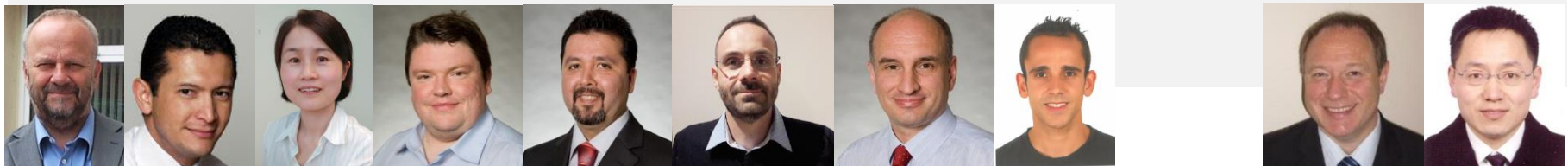
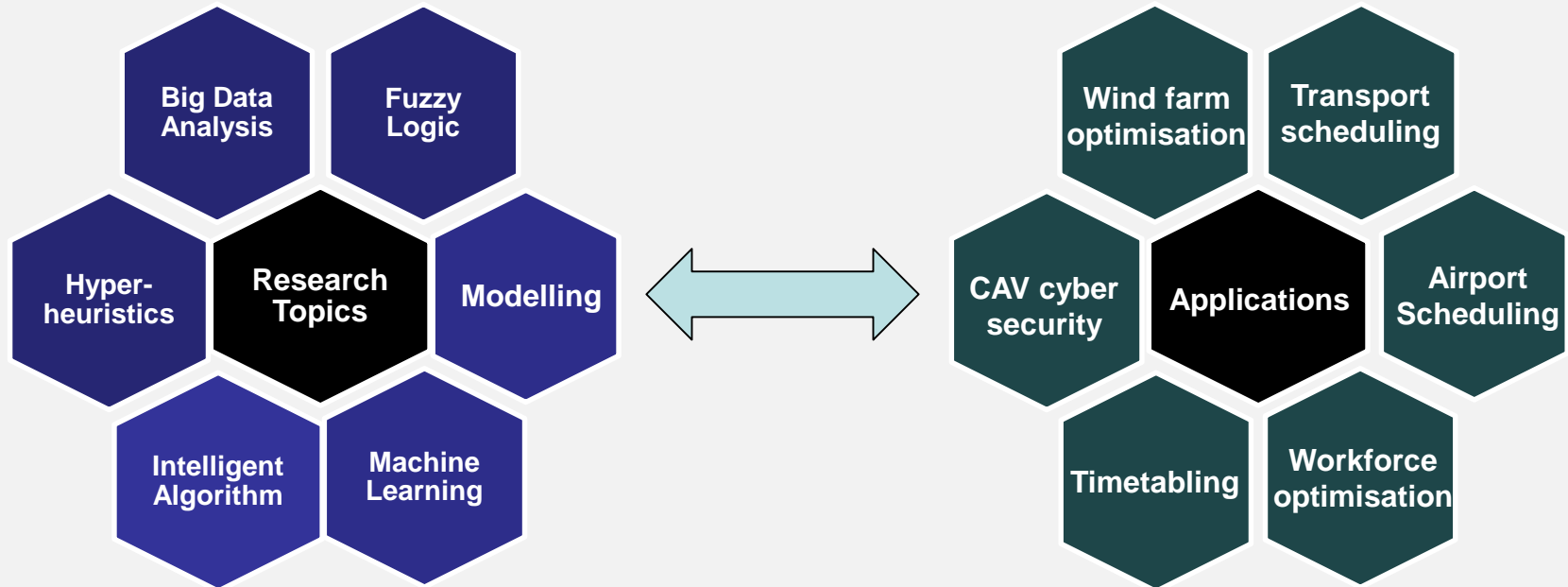
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# COL Lab – Research & Applications



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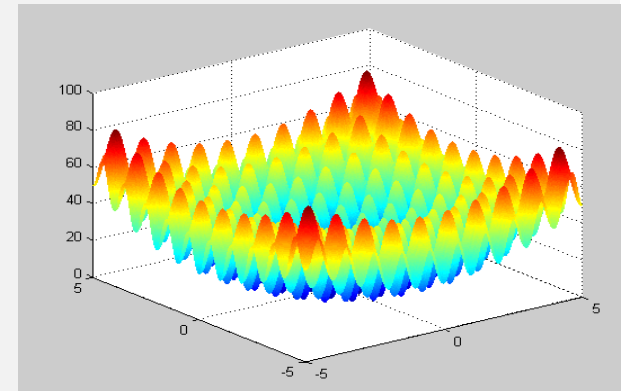
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# Algorithm Design - An Overview



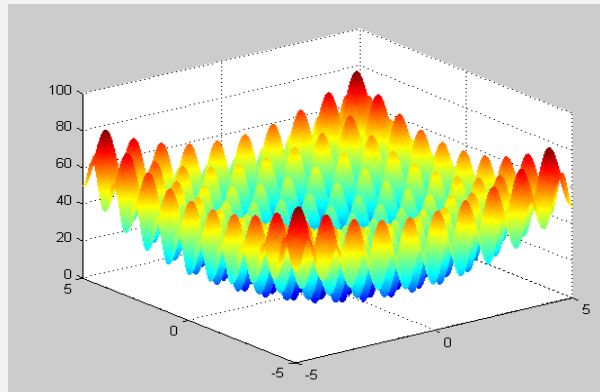
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- **Decisions** to make when designing algorithms
  - **Algorithm specific** decisions
    - Simulated annealing, Tabu search, Variable neighbourhood search, etc.
    - Genetic algorithms, Estimation of distribution algorithm, Swarm Algorithms (i.e. Particle swarm optimisation, Ant colony, etc.)
  - **General** decisions
    - Solution representation
    - Evaluation function
    - Initialisation
    - Stopping condition
    - Acceptance criteria



- Recent / advanced research developments
  - **Integration** of computational intelligence techniques
    - Hybridisation of evolutionary and local search algorithms
    - Machine learning and optimisation
    - Data-driven optimisation
    - Hyper-heuristics
  - **Automated** algorithm design
    - Automated **configuration**
    - Automated **selection**
    - Automated **composition**

- Automated algorithm design: search space:
  - Automated configuration: parameters of target algorithms
  - Automated selection: target algorithms
  - Automated composition: components of algorithms
- Most current meta-heuristics operate directly on problem solutions
  - Requires extensive experience, time consuming



- **Search space:** parameter configurations of target algorithms
- **Objective:** To automatically **configure** parameters of target algorithms **offline** against a given set of **training instances**
  - **Target algorithms:** stochastic local search [Pag19], multi-objective evolutionary algorithms [Lop12]
  - **Parameters:** numerical, categorical
  - **COPs:** TSP, VRP, flowshop scheduling
- **Platforms:** **automatically search** for the configuration of **parameters** for target algorithms
  - **ParamILS<sup>1</sup>:** [Hut09]
  - **F-Race/I-Race<sup>2</sup>:** [Bir10]

1. <http://www.cs.ubc.ca/labs/beta/Projects/ParamILS/>

2. <http://iridia.ulb.ac.be/irace/>



- **Search space:** a portfolio of **algorithms/solvers**
- **Objective:** according to the clustering **training instances** against certain features, to automatically **select** from the given target algorithms **offline**
  - **Target algorithms:** evolutionary algorithms [Aka17], solvers [Liu19]
  - **COPs:** TSP, function optimisation
- **Platforms**
  - **Population-based Algorithm Portfolios (PAP):** [Tan14]
  - **Hydra:** [Xu10]





- **Search space:** a set of basic building blocks/components of algorithms
- **Objective:** to automatically **compose** new algorithms **online** by searching for the **best composition of components** for solving the given problem instances **online**
  - **Algorithms:** evolutionary algorithms [Bez14], generic new algorithms, i.e. hyper-heuristics [Bur13,Pil18]
  - **COPs:** timetabling, NRP, TSP, job shop scheduling, VRP
- **Platforms:**
  - **HyFlex<sup>3</sup>:** [Bur11]
  - **EvoHyp<sup>4</sup>:** timetabling, NRP, TSP, job shop scheduling, VRP

3. <http://www.asap.cs.nott.ac.uk/external/chesc2011/>

4. <http://titancs.ukzn.ac.za/EvoHyp.aspx>

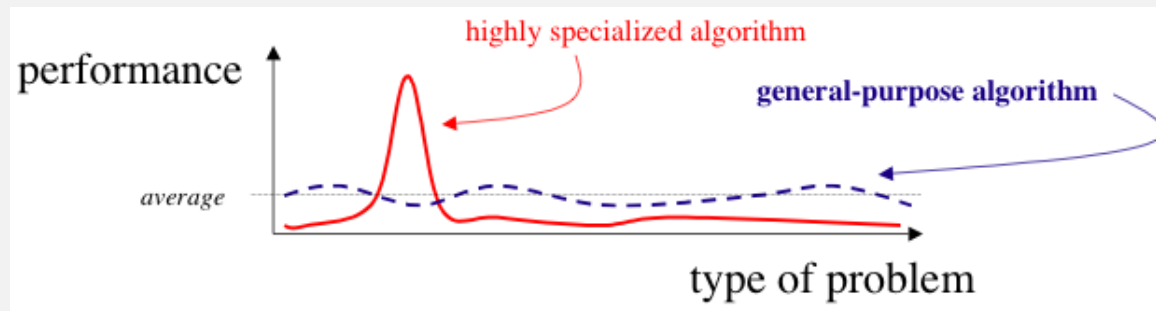
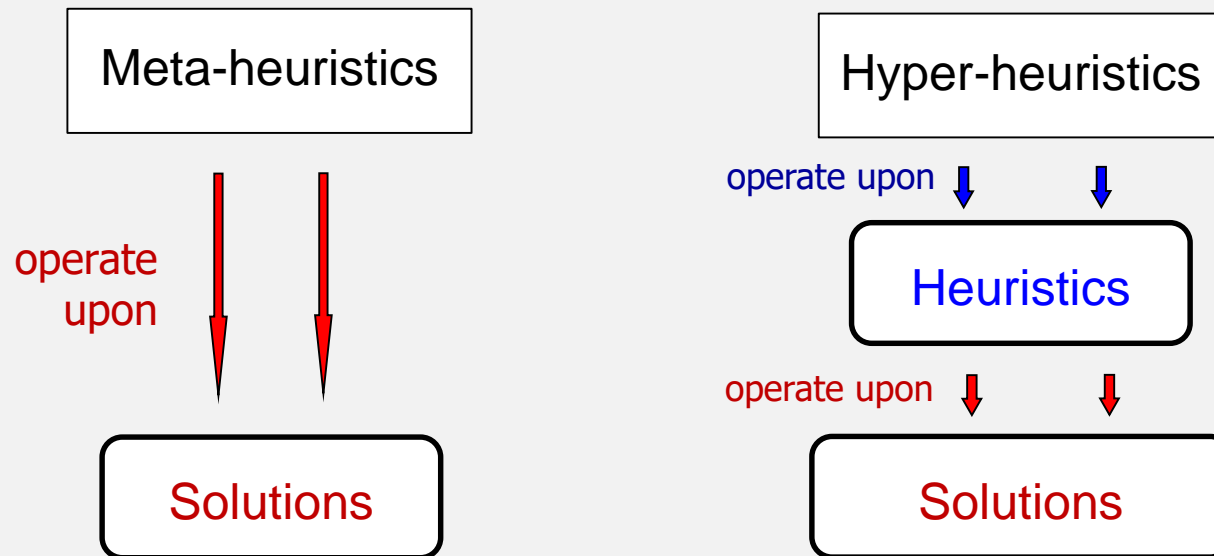




# **Automated Algorithm Composition - A General Graph Based Hyper-heuristic Framework (GHH)**



# Hyper-heuristics vs. Meta-heuristics



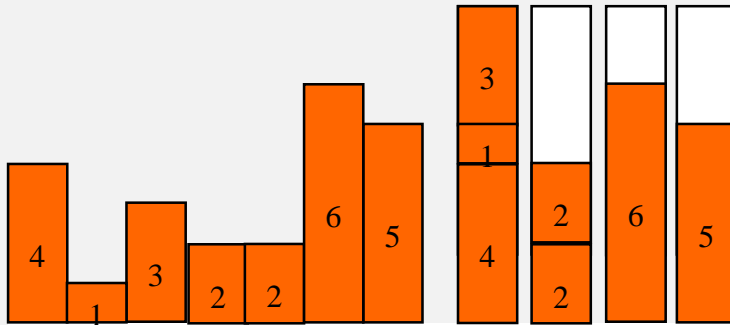
- Hyper-heuristics operate on a **search space of heuristics**
  
- **High level** heuristics
  - Selection
    - Search methods: evolutionary algorithms, tabu search, simulated annealing, etc.
    - Selection methods: case based reasoning, fuzzy techniques, choice function, etc.
  - Generation
    - Genetic programming, Gene expression programming



- Hyper-heuristics operate on a **search space of heuristics**
  
- **Low level** heuristics
  - Constructive heuristics: construct solutions step by step
    - Graph colouring heuristics, dispatching rules, etc.
  - Improvement heuristics: improve initial solutions by using different strategies iteratively
    - Move operators: swap, insert, destroy and repair



# Hyper-heuristics: Applications



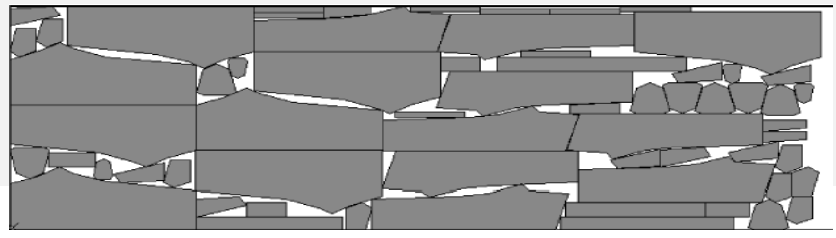
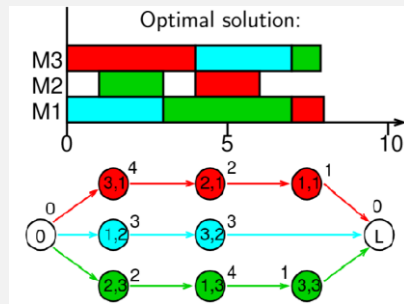
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Minimum Cover

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Programme: Computer Science 12 month PG (Session start) Full time/1 Weeks: 1-18 w1 - w/c Mon 25/09/2017-w18 - w/c Mon 22/01/2018  
 6405 MSC Computer Science

Year	Module	Level	Prerequisites	Corequisites	Excluded Modules
1st	6405L001	Level 1	None	None	None
2nd	6405L002	Level 2	6405L001	6405L003	6405L004
3rd	6405L003	Level 3	6405L002	6405L004	6405L005
4th	6405L004	Level 4	6405L003	6405L005	6405L006
5th	6405L005	Level 5	6405L004	6405L006	6405L007
6th	6405L006	Level 6	6405L005	6405L007	6405L008
7th	6405L007	Level 7	6405L006	6405L008	6405L009
8th	6405L008	Level 8	6405L007	6405L009	6405L010
9th	6405L009	Level 9	6405L008	6405L010	6405L011
10th	6405L010	Level 10	6405L009	6405L011	6405L012



- **Graph-based hyper-heuristic (GHH)**
  - **High level methods**
    - Steepest Descent (hill climbing)
    - Variable Neighbourhood Search
    - Iterated Search
    - Tabu Search
  
    - Same no. of total iterations
    - “walks” (same quality neighbourhood) allowed
  - **Problems: educational timetabling (exam / course); graph colouring**



- **Graph-based hyper-heuristic (GHH)**
  - **Low level heuristics**
    - Five graph colouring heuristics
    - Constructive methods that order events by the difficulties of assigning them (descending order)
    - Random ordering strategy

<b>Low Level Heuristics</b>	<b>Ordering strategies</b>
Largest degree	Number of clashed events
Largest weighted degree	LD with number of common students
Saturation degree	Number of valid remaining time periods
Largest enrolment	Number of students
Colour degree	Number of clashed event that are scheduled
Random ordering	Randomly





- Educational timetabling
  - A number of **events**  $\{e_1, e_2, \dots, e_e\}$ , taken by different **students**  $\{s_1, s_2, \dots, s_s\}$ , need to be scheduled to a limited **time period**  $\{t_1, t_2, \dots, t_3\}$  and certain **rooms**  $\{r_1, r_2, \dots, r_3\}$
  - **Hard** constraints
    - Events with common students can't be assigned to the same time period
    - Room capacity can't be exceeded
  - **Soft** constraints
    - Spread of exams / no single course on one day
    - Large exams assigned earlier



- Educational timetabling
  - Objectives:
    - Minimise timeslots / colours used
    - Minimise violations of soft constraints, i.e. weighted sum
  - Benchmark problems
    - Widely tested in the last decade
    - <http://www.cs.nott.ac.uk/~rxq/data.htm>
    - 1st International Timetabling Competition - <http://www.idsia.ch/Files/ttcomp2002/>



- Exam timetabling
  - **Hard constraints**: conflicts between exams
  - **Soft constraints**: spread out exams over slots
  
- Course timetabling
  - **Hard constraints**: room capacity; conflicts
  - **Soft constraints**
    - Courses scheduled consecutively (students)
    - More than two classes or no class a day
    - Courses can't be combined into one room
    - Last timeslot of the day
    - Preferred time periods, day-off (lecturers)
  - Courses associated with by **lecturers**, **time periods** usually on weekly basis, and **rooms** with certain features



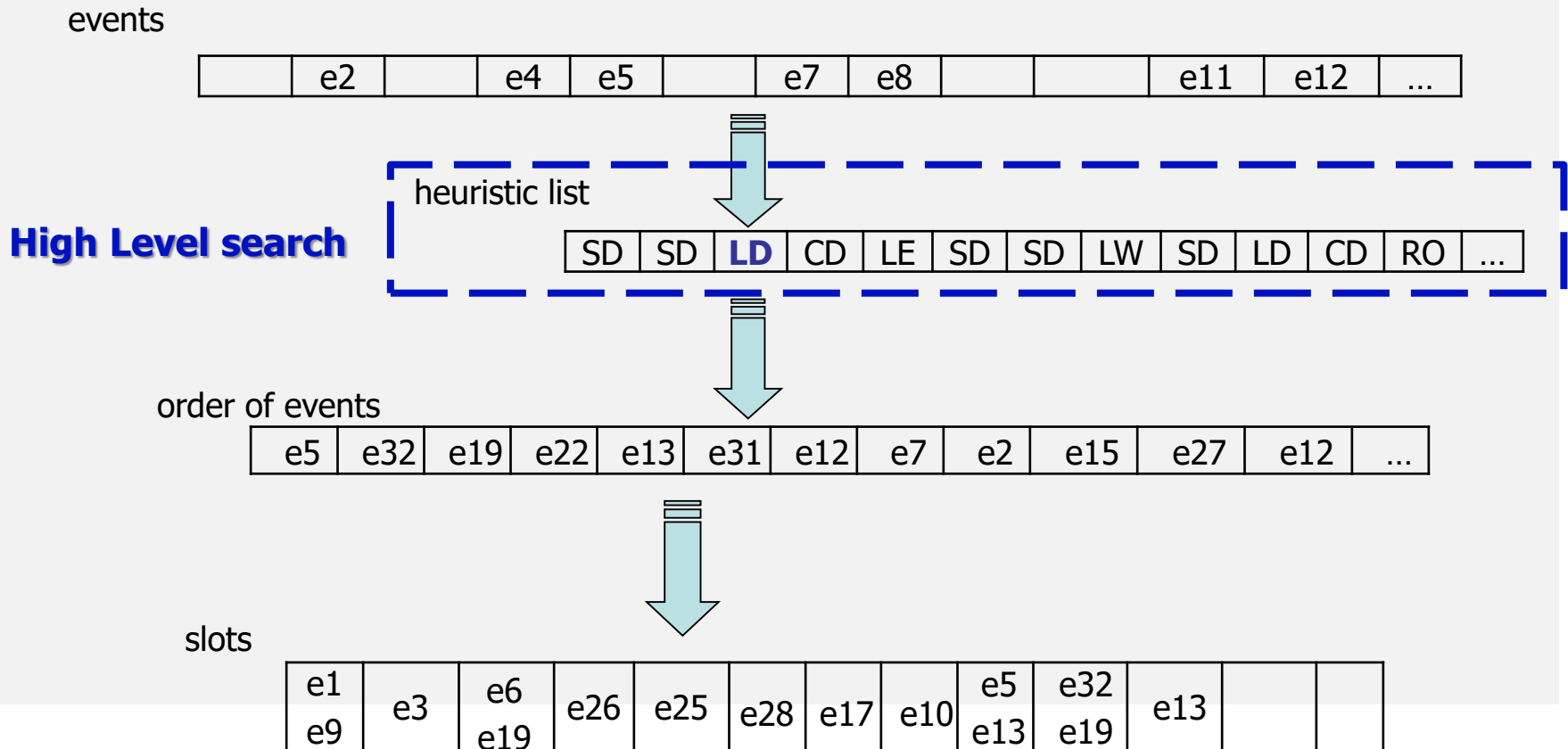




# GHH: A General Framework



- Graph-based hyper-heuristic (GHH)



- **Graph-based hyper-heuristic (GHH)**
  - VNS performs better than iterated search, both better than hill climbing and tabu search
  - **Iterated search** performs generally well
  - Search space of GHH for some instances: large **areas of plateau**
  - Same quality heuristic lists don't always produce same solutions
  - Greedy local search (almost always) further improve the solutions generated by heuristic lists; however, time increases significantly
  - **High level search cannot reach local optima in the solution space**





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# Automated Algorithm Composition - Understanding the Search Algorithms



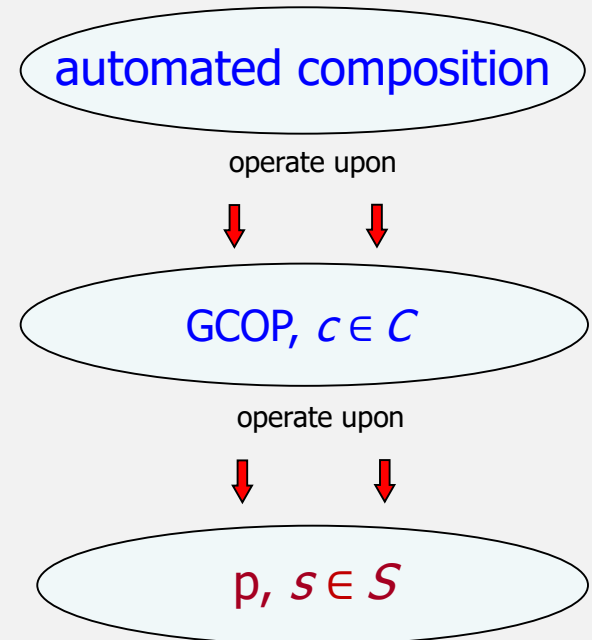
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# GCOP: A New Standard



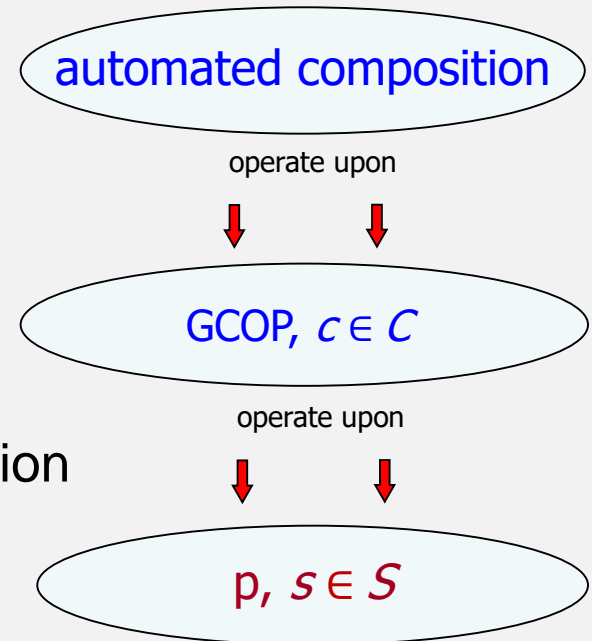
- A **General Combinatorial Optimisation Problem GCOP**, whose **decision variables** are **algorithmic components** rather than **direct solution variables** in the **optimisation problem  $p$**
- To solve  $p$ , composition methods explores at a **algorithm compositions  $c$**  in a **component space  $C$** , which map **direct solutions  $s$**  in the **solution space  $S$**  for  $p$
- **GCOP**: automated algorithm composition



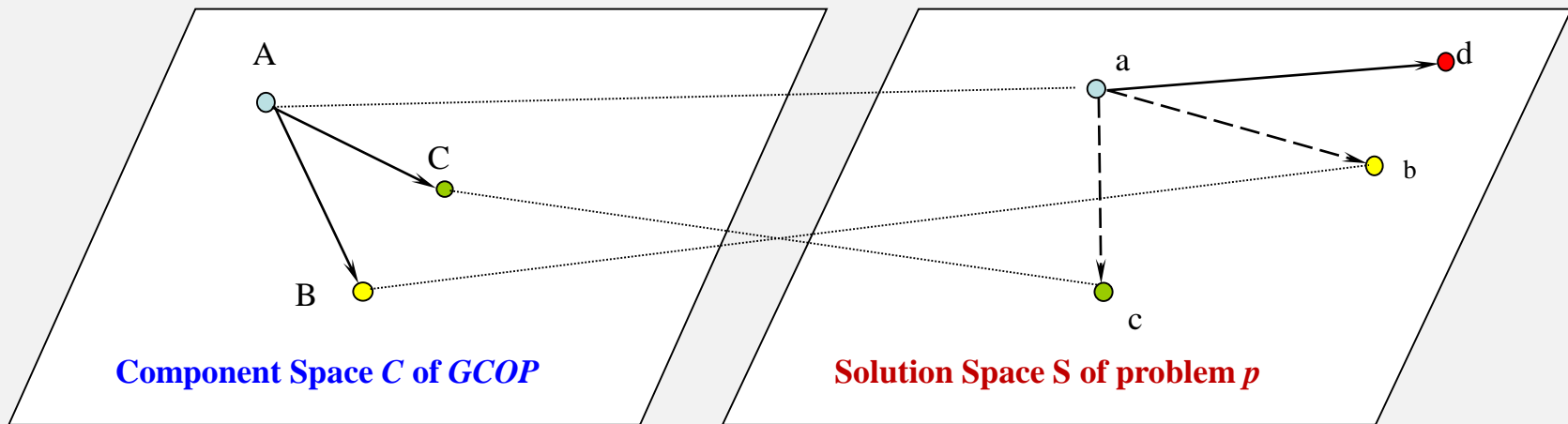
# GCOP: A New Standard



- The algorithm compositions  $c \in \mathbf{C}$  are measured by objective function  $F(c) \rightarrow R$   
The direct solutions  $s \in \mathbf{S}$  are measured by objective function  $f(s) \rightarrow R$
- $s$  are obtained using  $c$ , i.e.  $c \rightarrow s$   
Let mapping function  $M: f(s) \rightarrow F(c)$
- The objective of GCOP is to find optimal  $c^*$
- Therefore, two spaces are under consideration
  - an **algorithmic component space**  $\mathbf{C}$  and
  - a **solution space**  $\mathbf{S}$



- Graph-based hyper-heuristic (GHH)
  - Two search spaces
    - high level: sequences of low level heuristics (components)
    - low level: actual problem solutions



**Search is upon heuristics (components), not direct solutions: are all the solutions in solution space reachable?**

# GCOP: Two Search Spaces



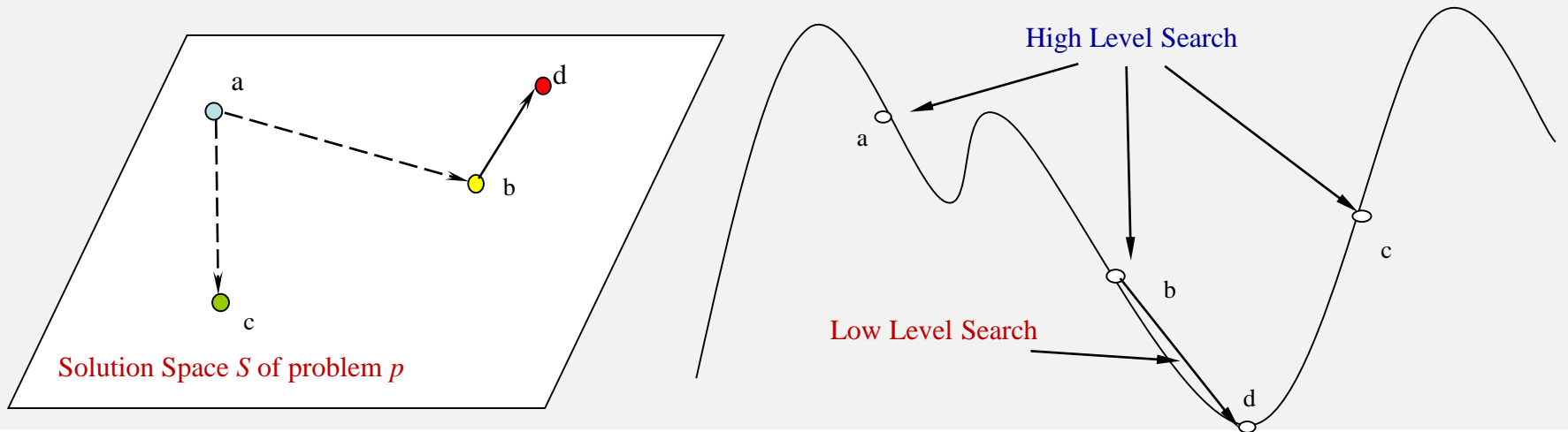
**Heuristic (component) space  $C$**    **Solution space  $S$**

<b>Representa- tion</b>
<b>Size (Upper Bound)</b>
<b>Neighbor- hood Operator</b>
<b>Objective Function</b>

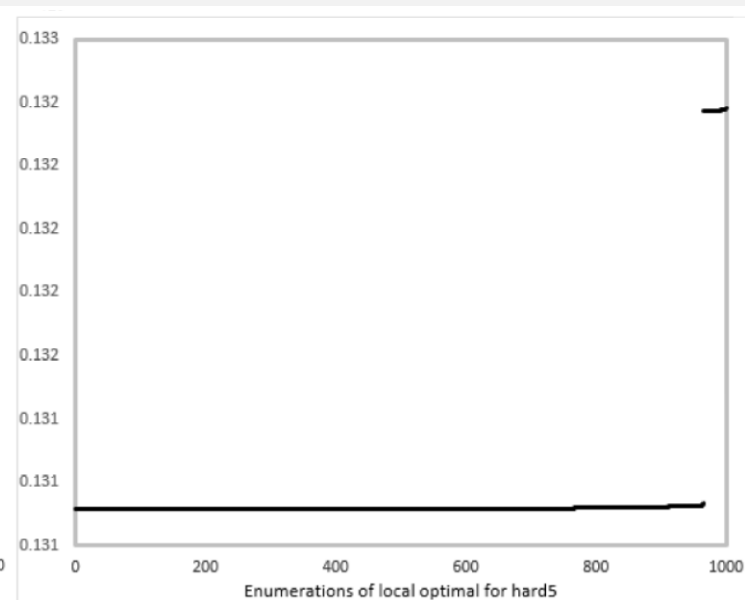
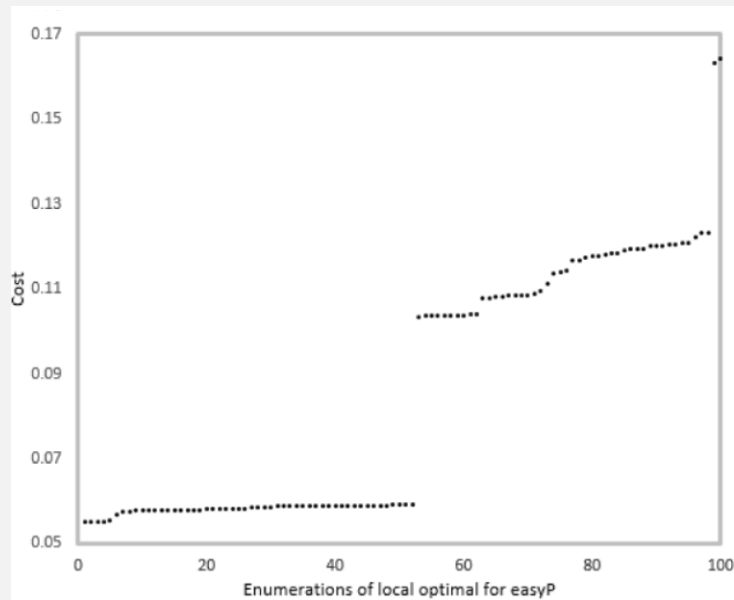
# GCOP: Two Search Spaces



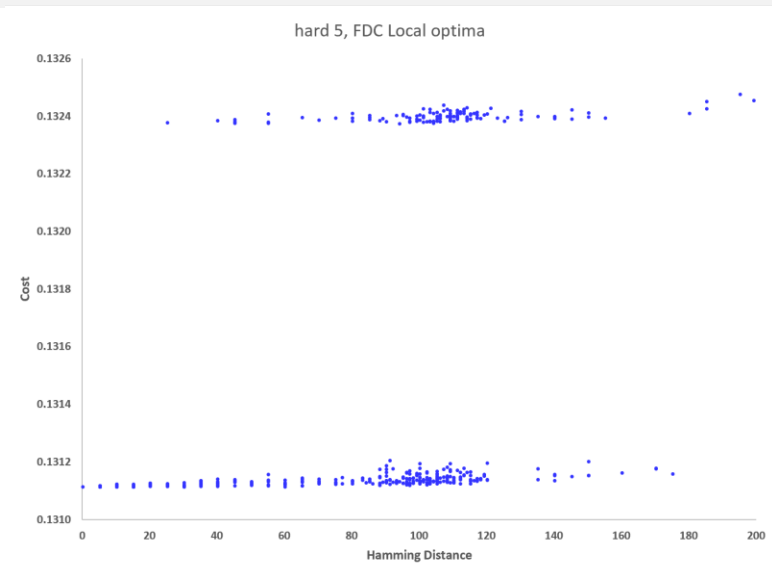
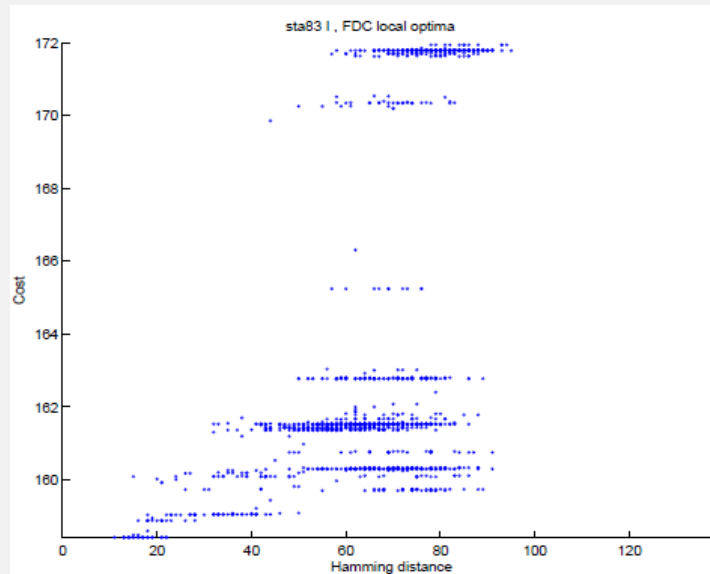
- Search within the two search spaces  $C$  and  $S$ 
  - **Hypothesis**: search upon heuristics (components) not solutions, not all solutions are **reachable**
  - Component space  $C$ : matched solutions  $a, b, c, \dots$
  - Solution space  $S$ :  $b \rightarrow d, \dots$ 
    - Coverage of all solutions in  $S$



- Landscape Analysis on high level heuristic compositions  $c$ 
  - Distribution of costs for local optimal  $c$



- Landscape Analysis on high level heuristic compositions  $c$ 
  - Fitness distance correlation ( $fdc$ ) of local to global optimum



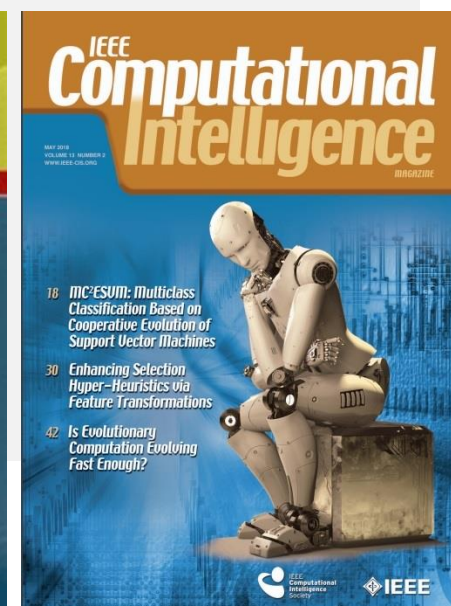
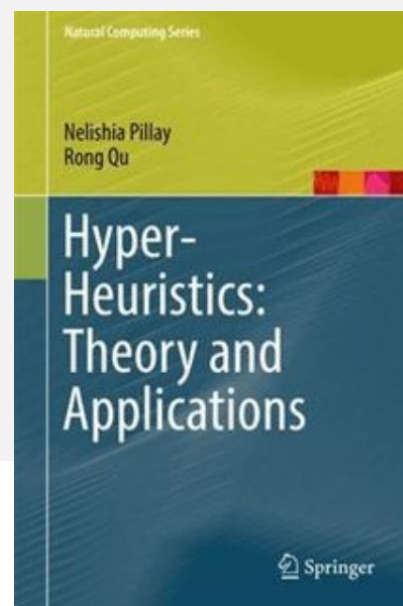
# Related Activities



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- N. Pillay, R. Qu, << [Hyper-heuristics: Theory and Applications](#)>>, Springer, ISBN [978-3-319-96514-7](#), December, 2018
- N. Pillay, R. Qu (ed.), [Automated Design of Machine Learning and Search Algorithms](#), [Special Issue](#) at Computational Intelligence Magazine, 13(2), June 2018.
- IEEE Computational Intelligence Society [Task Force on Hyper-heuristics](#)
- IEEE Computational Intelligence Society [Task Committee on Evolutionary Computation](#)



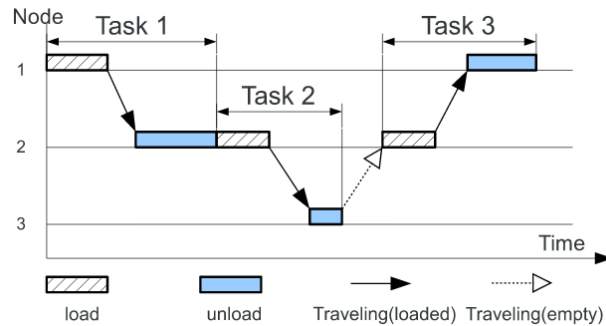




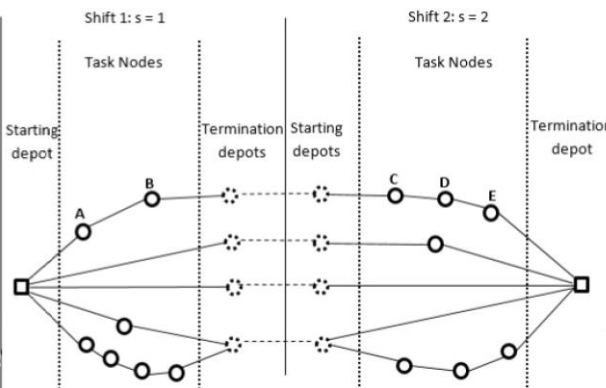
# Modelling and Optimisation of other COPs



Extended new problem model with inland dry ports  
**Mixed shift types** with non-linear driver costs  
 Bi-objective optimization by hybrid **hyper-heuristics**



ge international port.



R Qu and R Bai

# Logistic Transport Scheduling @ Ningbo

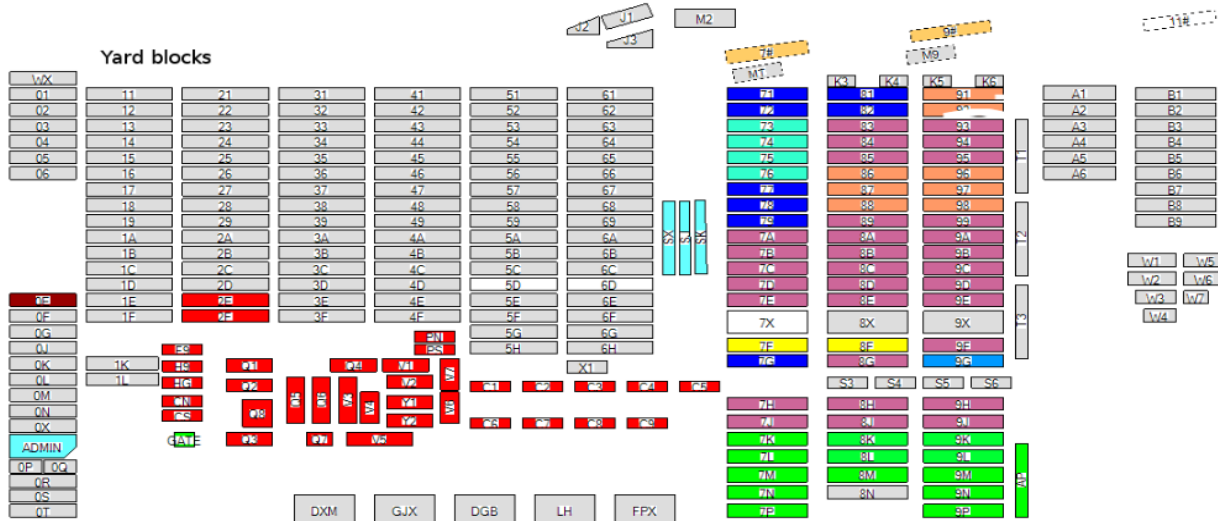
B. Chen, R. Qu, R. Bai, W. Laesanklang, "A hyper-heuristic with two guidance indicators for bi-objective mixed-shift vehicle routing problem with time windows", in press, *Applied Intelligence*, 2018.

Real time **crane scheduling** at container terminals  
 Complex **dynamic truck dispatching** for containers' transfer  
 - Robust hyper-heuristics hybridising three dynamic heuristics



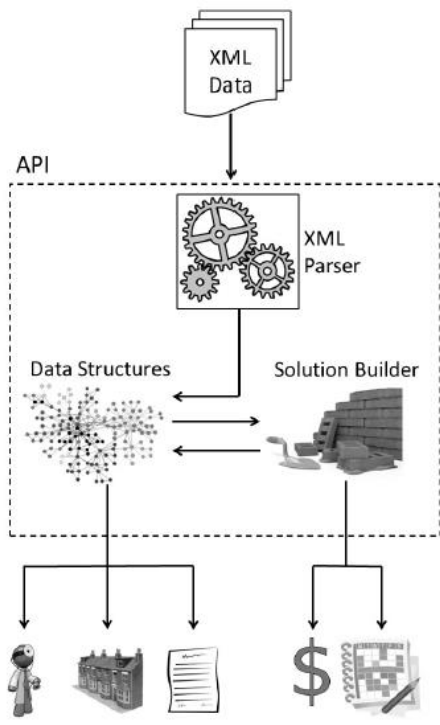
Large international port.

R Qu and R Bai



# Logistic Transport Scheduling @ Ningbo

J Chen, R Bai, H Dong, R Qu and G Kendall, "A Dynamic Truck Dispatching Problem in Marine Container Terminal"  
 The 2016 Symposium on Computational Intelligence in Scheduling and Network Design (IEEE CISND'16), Dec 6-9, 2016



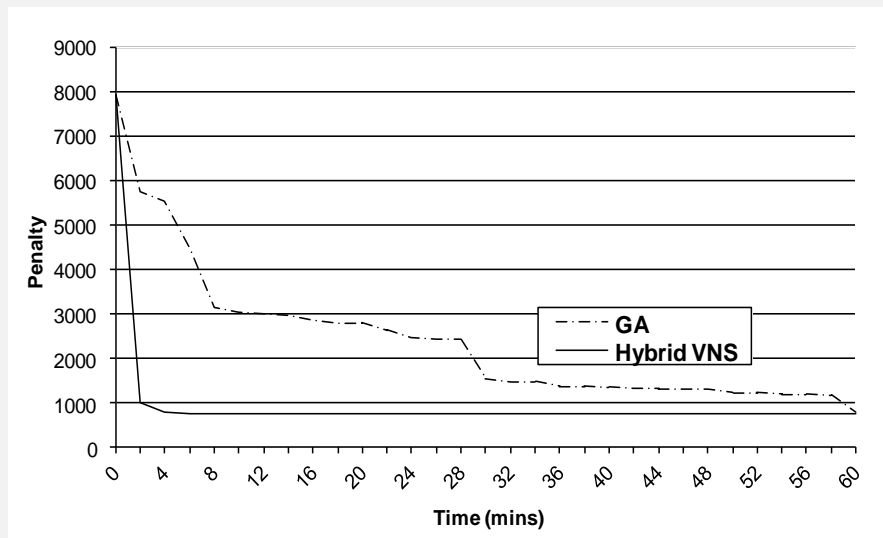
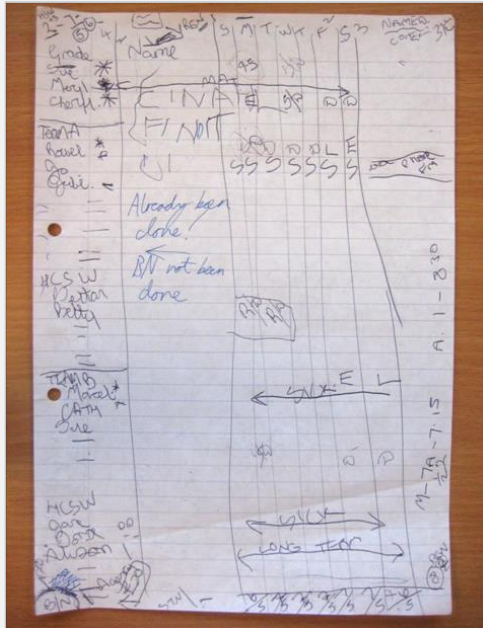
- Routing + Rostering in healthcare
- Optimisation engine demonstrated at roadshows
- “Outstanding” award at KTP, Innovate UK
- Automated heuristic algorithms
- UK SME: Webroster®



# Healthcare Rostering & Routing

J. Arturo Castillo-Salazar, Dario Landa-Silva, Rong Qu, "Computational Study for Workforce Scheduling and Routing Problems" The 3rd International Conference on Operations Research and Enterprise Systems (ICORES 2014), pp. 434-444, Angers France, March 2014

- Different grades / skill, shift types, coverage
- **Constraints**
  - Hard: Coverage
  - Soft: work/rest hours, complete weekends, preferences, etc.
- Evolutionary algorithms, hybrid VNS



# Nurse Rostering Problems

E.K. Burke, T. Curtois, R. Qu and G. Vanden Berghe. "A Time Predefined Variable Depth Search for Nurse Rostering".  
INFORMS Journal on Computing, 25: 411-419, 2013

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H	E	E	E			D	D			E	E	E	E			D	D	D		N	N	N	N			L	L		26

Too few resting time (10)

Too few consecutive late shifts (5)

Too few consecutive night shifts (5)

Total Penalty 176  
Unassigned Shifts 0

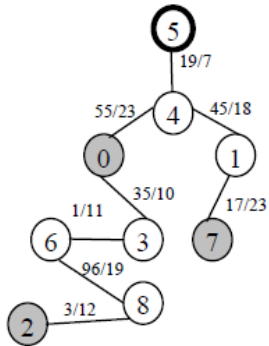
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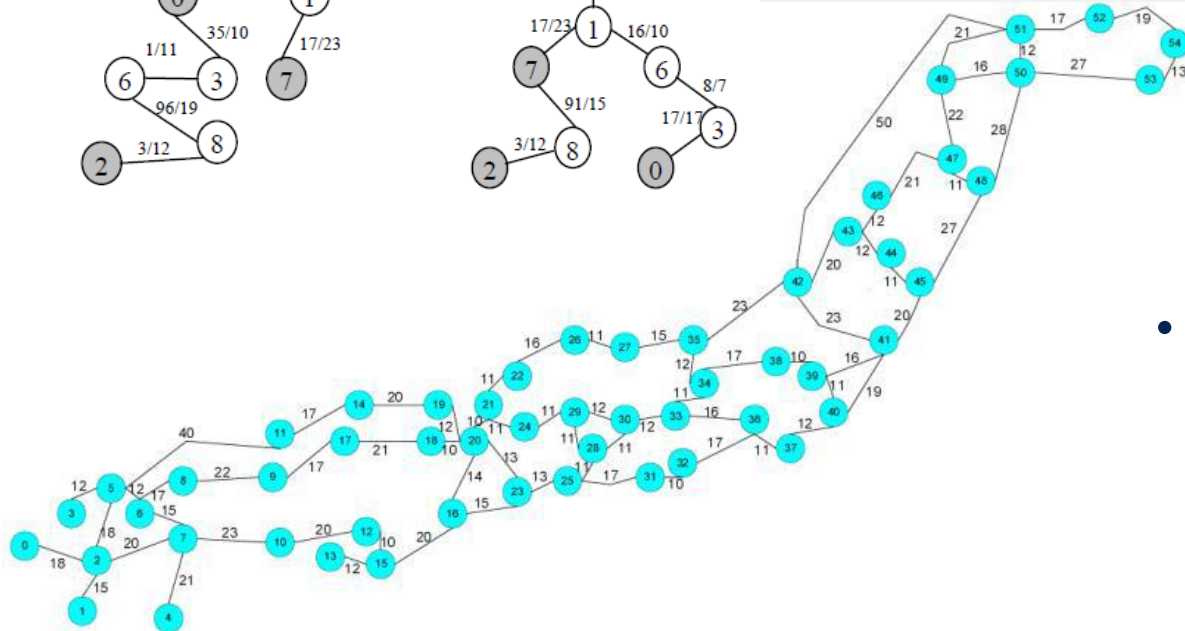
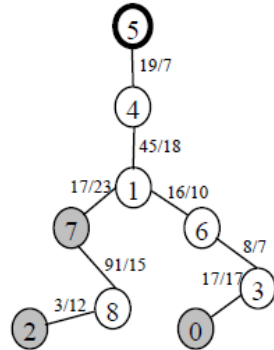
# Nurse Rostering Problems

NRP benchmark datasets:  
<http://www.schedulingbenchmarks.org/>

Current tree  $T_0$   
Cost( $T_0$ ) = 271  
Delay( $T_0$ ) = 82



Attractor tree  $T_a$   
Cost( $T_a$ ) = 216  
Delay( $T_a$ ) = 75



- Find the multicast tree serving all terminals, satisfying delay bound
- **Multiple objectives**
  - Minimal costs
  - Maximal end-to-end delay
  - Maximal link utilisation
  - Average delay
- **Applications**
  - Video conferencing
  - e-learning, etc.

# Multicast Routing

R. Qu, Y. Xu, J. Castro, D. Landa-Silva.  
"Particle Swarm Optimization for the Steiner Tree in Graph and Delay-Constrained Multicast Routing Problems.", Journal of Heuristics, 19(2): 317-342, 2013



The cost of the multicast tree:

$$C(T) = \phi \cdot \sum_{(i,j) \in T} c_{ij}$$

The maximal end-to-end delay of the multicast tree:

$$DM(T) = \text{Max}\{d(p_T(s, r_d))\}, r_d \in R$$

The maximal link utilisation:

$$\alpha(T) = \text{Max}\left\{\frac{\phi + t_{ij}}{z_{ij}}\right\}, (i, j) \in T$$

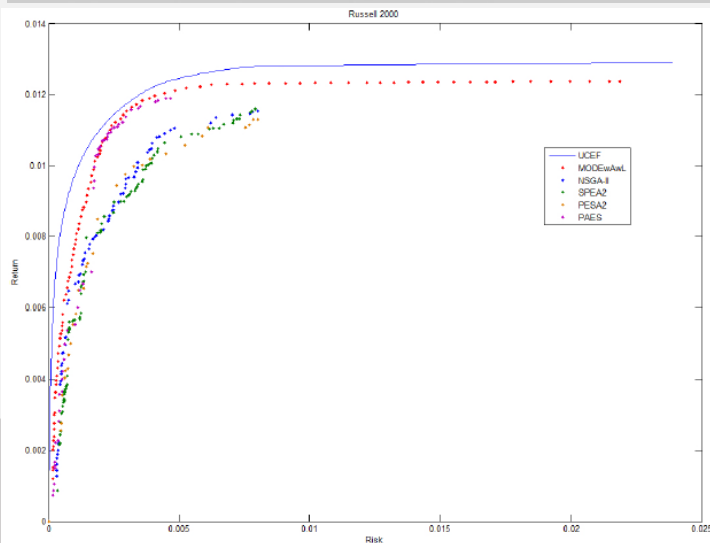
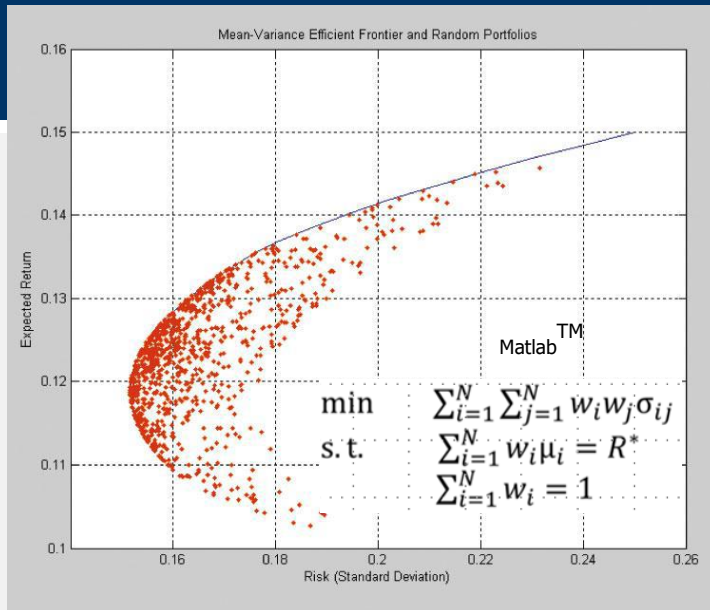
The average delay of the multicast tree:

$$DA(T) = \frac{1}{|R|} \sum_{r_d \in R} d(p_T(s, r_d))$$

- **Quality of Service (QoS)** constraints
  - Bandwidth, Delay, Cost, Delay variations
- Various **multi-objective** evolutionary algorithms
  - Scatter search, PSO, iterative local search
- Future extension: problems with uncertainties

# Multicast Routing

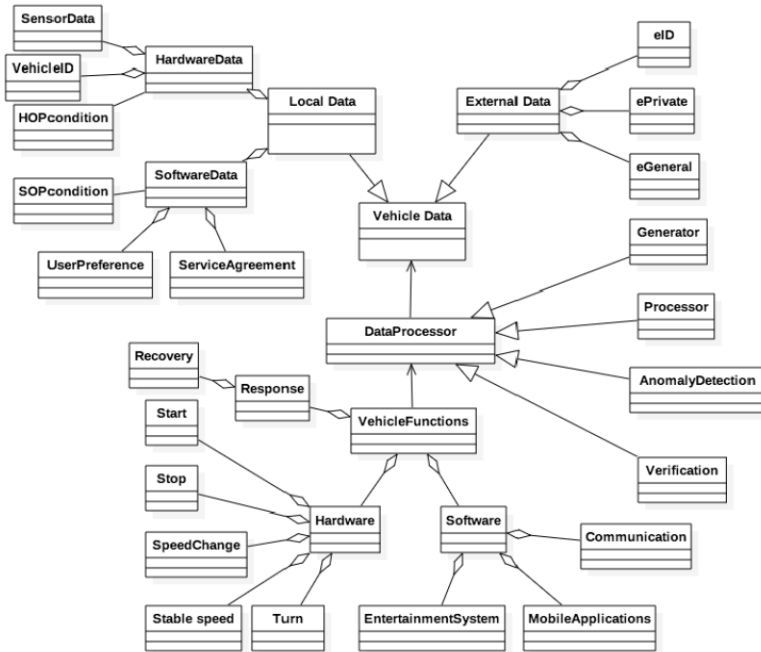




- Allocate capital to selected assets
- **Objective:** to find the portfolio with
  - the highest expected return or
  - the lowest risk for the expected return
- **Markowitz's portfolio theory**
  - Mean-Variance model
  - Efficient frontier: risk vs. return
- **Real world constraints**
  - Cardinality  $\sum_{i=1}^N s_i = K$
  - Boundary  $\epsilon_i s_i \leq w_i \leq \delta_i s_i, i = 1, \dots, N$
  - Round lot  $w_i = y_i \cdot v_i, i = 1, \dots, N, y_i \in \mathbb{Z}_+$
  - Pre-assignment  $s_i \geq z_i, i = 1, \dots, N$

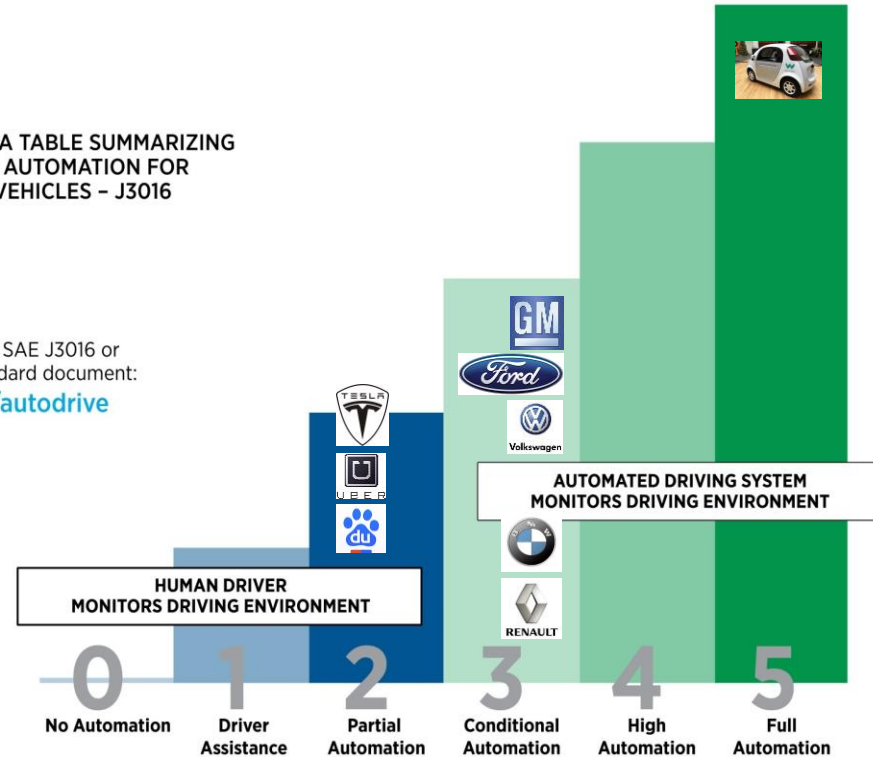
# Portfolio Optimisation

Khin Lwin, Rong Qu, Bart MacCarthy, "Mean-VaR Portfolio Optimization: A Nonparametric Approach", European Journal of Operational Research, 260(2): 751-766, 2017



▶ OVER FOR A TABLE SUMMARIZING LEVELS OF AUTOMATION FOR ON-ROAD VEHICLES - J3016

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# CAV Cyber Security

Q. He, X. Meng, R. Qu, A New Framework for Assessing CAV Cyber Security, under review, 2019.



- **KDD99**
  - A benchmark dataset: online intrusion / attack detection
  - 5m data records, **42 attributes**, labelled with **four major types of 39 sub-attacks** (only 22 sub-attacks in the training dataset)
- **CAV-KDD: new dataset for CAVs cyber security**
  - Three types attack points: **hardware, software, data**
  - KDD99 training and testing datasets processed against characteristics of CAVs, compatible to the new framework
  - **Four major types of 14 sub-attacks**

Amount of Normal and Attack Data in the Training Datasets

	10% KDD99 Data	CAV-KDD Data
Attacks	396743	13274
Normal	97278	58716
Total	494021	71990

Accuracy and Runtime of J48 and Naive Bayes

	Accuracy on the Testing Dataset	Time to Build Model (s)	Time on the testing Dataset (s)
Naive Bayes	76.2%	0.04	3.95
J48	76.3%	1.4	0.94

# CAV Cyber Security

Q. He, X. Meng, R. Qu, A New Framework for Assessing CAV Cyber Security, under review, 2019.

- **ITS / Traffic Network Simulation & Optimisation**
  - Machine Learning
    - CAV cyber security
    - Image recognition
    - Traffic data analysis
  - Optimisation in Intelligent Transport Systems
  - CAV real time testing with Engineering
- **Automated Algorithm Design**
  - General search algorithm framework
    - Easy to implement and use
    - Data collection on algorithm compositions
  - Theory: landscape analysis
  - Machine learning: patterns of algorithm design / compositions

