

Evolutionary Computation for Feature Selection and Feature Construction

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<http://www.sigevo.org/gecco-2016/>


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GECCO'16 Companion, July 20–24, 2016, Denver, CO, USA.
ACM 978-1-4503-4323-7/16/07.
<http://dx.doi.org/10.1145/2908961.2927002>



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Instructors

 **Mengjie Zhang** is a Professor of Computer Science at the School of Engineering and Computer Science, Victoria University of Wellington (VUW), New Zealand. His research is mainly focused on evolutionary computation, particularly genetic programming, particle swarm optimization and learning classifier systems with application areas of image analysis, multi-objective optimization, classification with unbalanced data, feature selection and reduction, and job shop scheduling. He has published over 400 academic papers in refereed international journals and conferences. He has been serving as an associated editor or editorial board member for five international journals (including IEEE Transactions on Evolutionary Computation and the Evolutionary Computation Journal) and as a reviewer of over fifteen international journals. He has been serving as a steering committee member and a program committee member for over eighty international conferences.

 **Bing Xue** is a Lecturer at Victoria University of Wellington. She is with the Evolutionary Computation Research Group at VUW, and her research focuses mainly on evolutionary computation, machine learning and data mining, particularly, evolutionary computation for feature selection, feature construction, dimension reduction, symbolic regression, multi-objective optimisation, bioinformatics and big data. Bing is has been organising special sessions and issues on evolutionary computation for feature selection and construction. She is also the Chair of IEEE CIS Task Force on Evolutionary Computation for Feature Selection and Construction. Bing is a committee member of Evolutionary Computation Technical Committee, and Emergent Technologies Technical Committee, IEEE CIS. She has been serving as a guest editor, associated editor or editorial board member for international journals, and program chair, special session chair, symposium/special session organiser for a number of international conferences, and as reviewer for top international journals and conferences in the field.

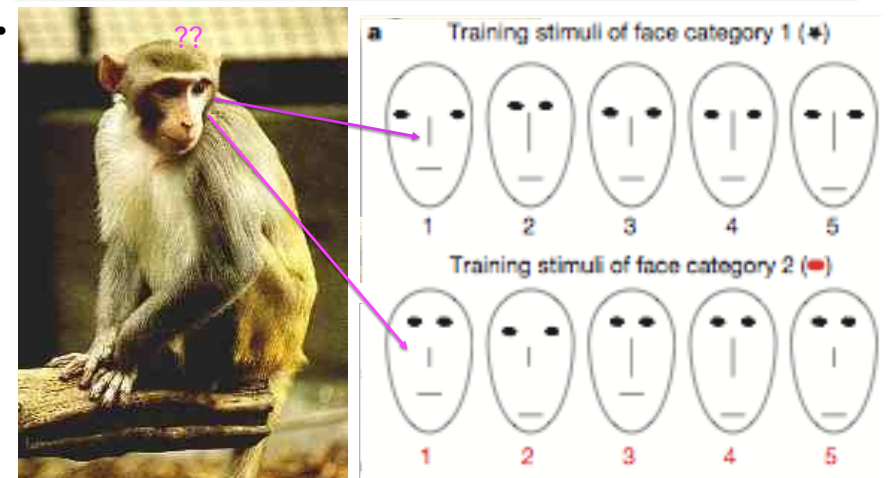
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Outline

- Feature Selection and Feature Construction
- Evolutionary Computation (EC) for Feature Selection
- Feature Selection Methods
- Feature Construction Methods
- Application on Images
- Application on Biology
- Issues and Challenges

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Feature Selection: Example from Biology



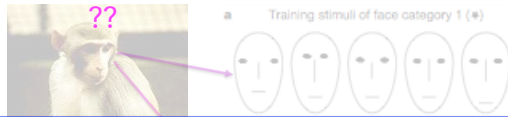
Monkeys performing a classification task

[Acknowledgement: Nathasha Sigala, Nikos Logothetis: Visual categorization shapes feature selectivity in the primate visual cortex. Nature Vol. 415(2002)]

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Feature Selection: Example from Biology

- Monkeys performing classification task
 - Diagnostic features:



“The data from the present study indicate that neuronal selectivity was shaped by **the most relevant subset of features** during the categorisation training.”

—Nathasha Sigala, Nikos Logothetis

(52/44) were selective to one or both of the diagnostic features (and not for the non-diagnostic features)



[Acknowledgement: Nathasha Sigala, Nikos Logothetis: Visual categorization shapes feature selectivity in the primate visual cortex. Nature Vol. 415(2002)]

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Data set (Classification) — Example 1

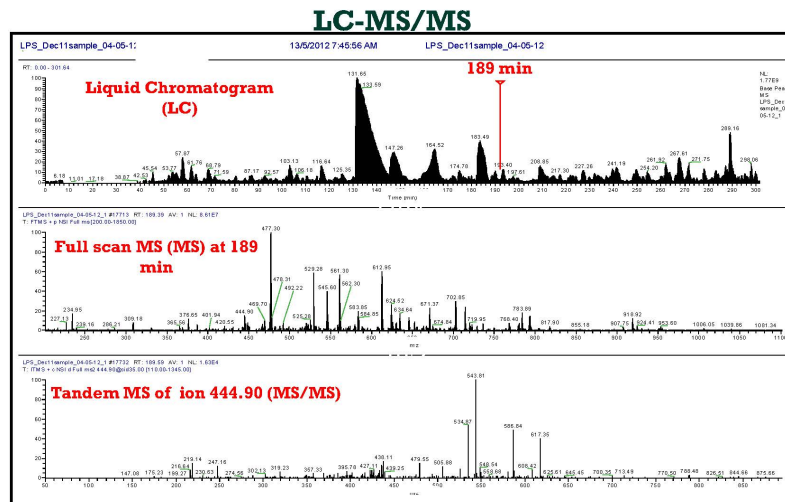
Credit card application:

- 7 applicants (examples/instances/observations)
- 2 classes: Approve, Reject
- 3 features/variables/attributes

	Job	Saving	Family	Class
Applicant 1	true	high	single	Approve
Applicant 2	false	high	couple	Approve
Applicant 3	true	low	couple	Reject
Applicant 4	true	low	couple	Approve
Applicant 5	true	high	children	Reject
Applicant 6	false	low	single	Reject
Applicant 7	true	high	single	Approve

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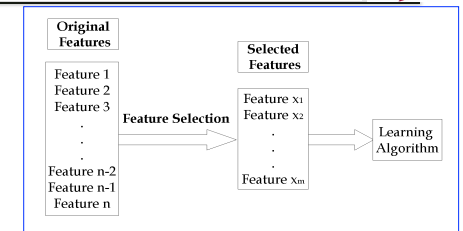
Cancer Diagnosis— Example 2



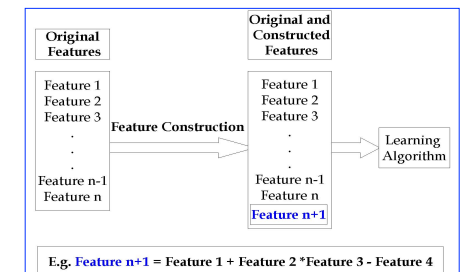
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Feature Selection and Feature Construction

- Feature selection aims to pick a subset of relevant features to achieve similar or better classification performance than using all features.



- Feature construction is to construct new high-level features using original features to improve the classification performance.



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Why Feature Selection ?



- "Curse of the dimensionality"
 - Large number of features: 100s, 1000s, even millions
- Not all features are useful (relevant)
- Redundant or irrelevant features may reduce the performance (e.g. **classification accuracy**)
- Costly: time, memory, and money
- **Feature selection**
 - to select a **small subset** of **relevant** features from the original large set of features in order to **maintain or even improve** the performance

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Why Feature Construction?



- The **quality of input features** can drastically affect the learning performance.
- Even if the quality of the original features is good, transformations might be required to make them usable for **certain types of classifiers**.
- A large number of classification algorithms are unable of **transforming** their **input space**.
- Feature construction **does not add to the cost of extracting** (measuring) original features; it only carries computational cost.
- In some cases, feature construction can lead to **dimensionality reduction or implicit feature selection**.
- **Why Feature Selection ? what Feature Selection can do ?**

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What can FS/FC do ?



- Reduce the dimensionality (No. of features)
- Improve the (classification) performance
- Simplify the learnt model
- Speed up the processing time
- Help visualisation and interpretation
- Reduce the cost, e.g. save memory
- and ?

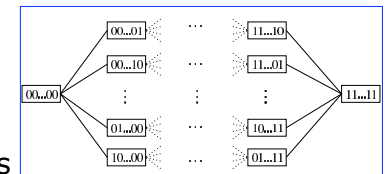
Multi-objective Problems — challenging

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Challenges in FS and FC



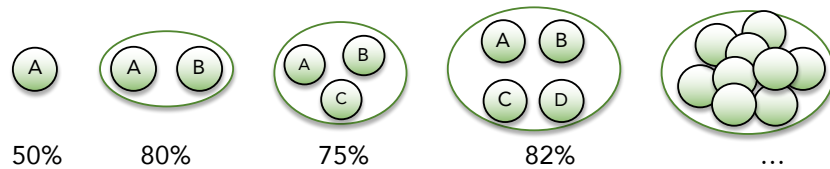
- **Large search space:** 2^n possible feature subsets
 - 1990: $n < 20$
 - 1998: $n \leq 50$
 - 2007: $n \approx 100s$
 - Now: 1000s, 1 000 000s
- **Feature interaction**
 - Relevant features may become redundant
 - Weakly relevant or irrelevant features may become highly useful
- **Slow** processing time, or even not possible



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Challenges in FS and FC

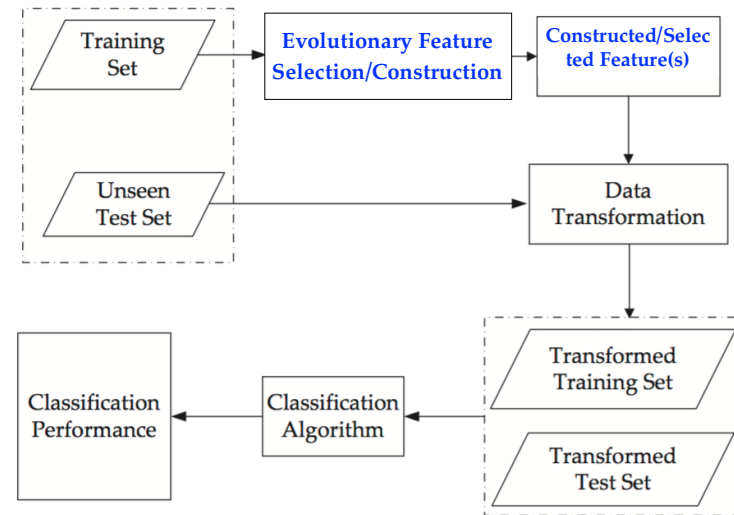
- Large search space 2^n
- Feature interaction
 - Weakly relevant or irrelevant features may become highly useful
 - Relevant features may become redundant



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General FS/FC System

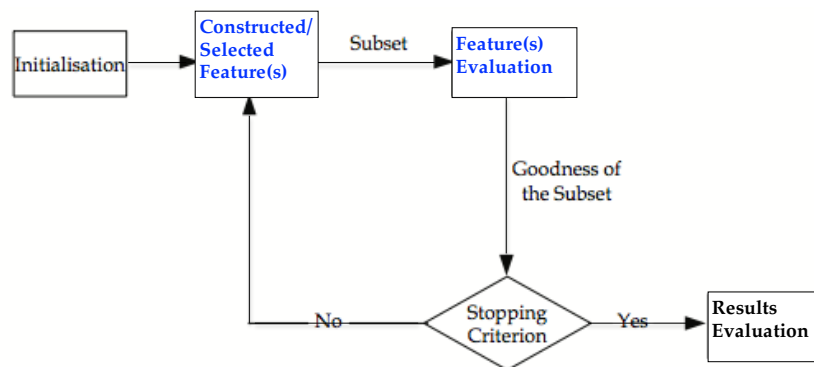
- Avoid bias



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Feature FS/FC Process

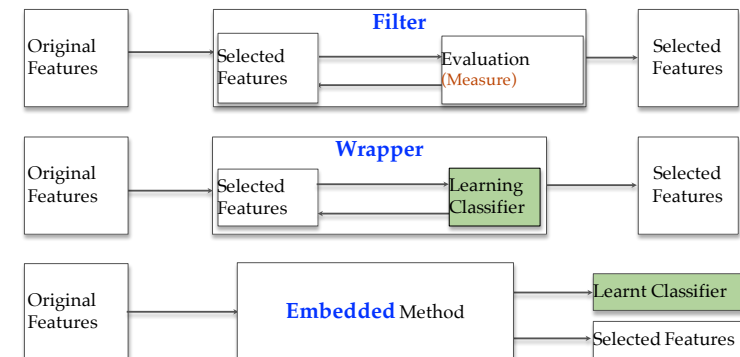
- On training set:



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Feature Selection Approaches

- Based on Evaluation ——— learning algorithm
 - Three categories: Filter, Wrapper, Embedded
 - Hybrid (Combined)



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- Generally:

	Classification Accuracy	Computational Cost	Generality (different classifiers)
Filter	Low	Low	High
Embedded	Medium	Medium	Medium
Wrapper	High	High	Low

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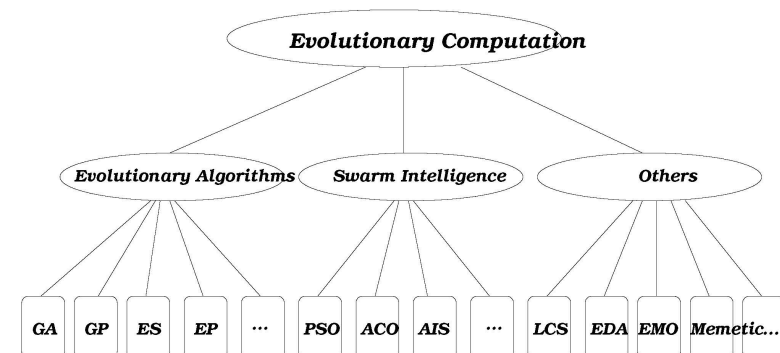
Feature Selection

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- Conventional approaches
 - The Relief algorithm
 - Feature ranking method
 - The FOCUS algorithm
 - Sequential forward/backward selection
 - Sequential forward/backward floating selection
- Evolutionary Computation (EC) based approaches

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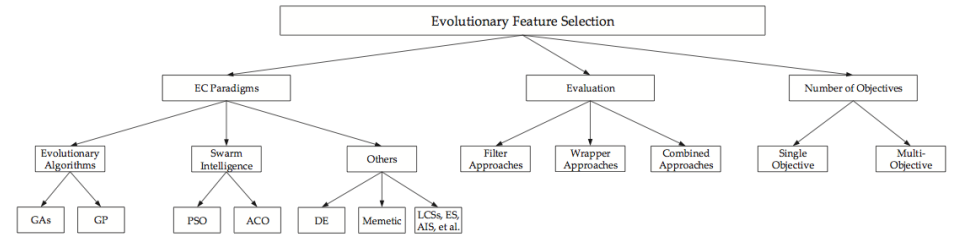
- A group of techniques inspired by the principles of biological evolution



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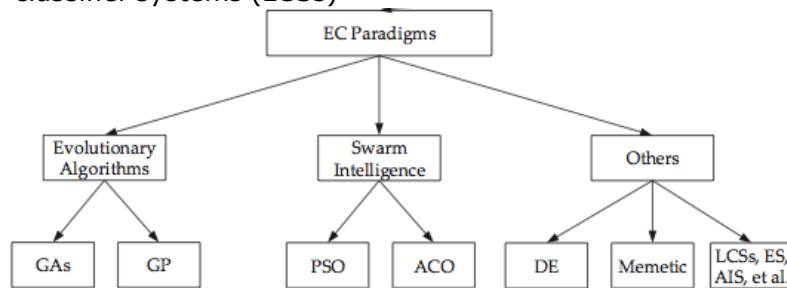
- Don't need domain knowledge
- Don't make any assumption
 - e.g. differentiable, linearity, separability, equality
- Easy to handle constraints
- EC can simultaneously build model structures and optimise parameters
- Population based search is particularly suitable for **multi-objective** optimisation

- EC Paradigms
- Evaluation
- Number of Objectives

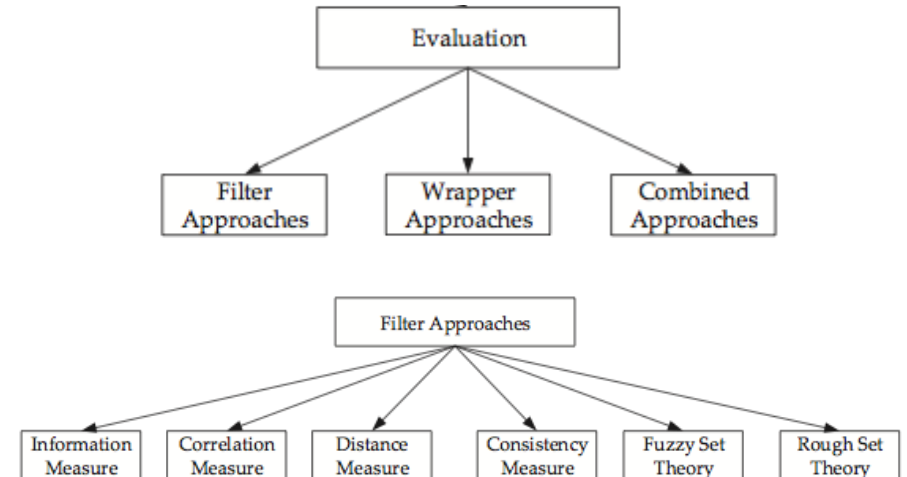


Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selecti

- Genetic algorithms (GAs), Genetic programming (GP)
- Particle swarm optimisation (PSO), ant colony optimisation(ACO)
- Differential evolution (DE), memetic algorithms, learning classifier systems (LCSs)



Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selection", IEEE Transaction on Evolutionary Computation, doi: 10.1109/TEVC.2015.2504420, published online on 30 Nov 2015



Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selection", IEEE Transaction on Evolutionary Computation, doi: 10.1109/TEVC.2015.2504420, published online on 30 Nov 2015

- Over 25 years ago, first EC techniques
 - Filter, Wrapper, Single Objective, Multi-objective
- Representation
 - Binary string
- Search mechanisms
 - Genetic operators
- Multi-objective feature selection
- Scalability issue

1	0	1	1	0	0	1	0	0	1	1	0	0
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R. Leardi, R. Boggia, and M. Terrile, "Genetic algorithms as a strategy for feature selection," *Journal of Chemometrics*, vol. 6, no. 5, pp. 267–281, 1992.

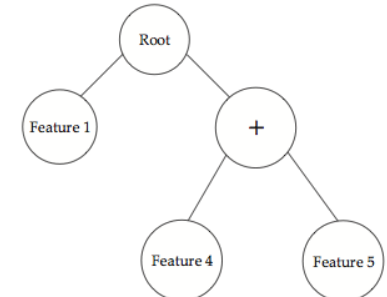
Z. Zhu, Y.-S. Ong, and M. Dash, "Markov blanket-embedded genetic algorithm for gene selection," *Pattern Recognition*, vol. 40, no. 11, pp. 3236–3248, 2007.

W. Sheng, X. Liu, and M. Fairhurst, "A niching memetic algorithm for simultaneous clustering and feature selection," *IEEE Transactions on Knowledge and Data Engineering*, vol. 20, no. 7, pp. 868–879, 2008.

Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selection", *IEEE Transaction on Evolutionary Computation*, doi: 10.1109/TEVC.2015.2504420, published online on 30 Nov 2015

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- Implicit feature selection
 - Filter, Wrapper, Single Objective, Multi-objective
- Embedded feature selection
- Feature construction
- Computationally expensive



L. Jung-Yi, K. Hao-Ren, C. Been-Chian, and Y. Wei-Pang, "Classifier design with feature selection and feature extraction using layered genetic programming," *Expert Systems with Applications*, vol. 34, no. 2, pp. 1384–1393, 2008.

Purohit, N. Chaudhari, and A. Tiwari, "Construction of classifier with feature selection based on genetic programming," in *IEEE Congress on Evolutionary Computation (CEC)*, pp. 1–5, 2010.

M. G. Smith and L. Bull, "Genetic programming with a genetic algorithm for feature construction and selection," *Genetic Programming and Evolvable Machines*, vol. 6, no. 3, pp. 265–281, 2005.

Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selection", *IEEE Transaction on Evolutionary Computation*, doi: 10.1109/TEVC.2015.2504420, published online on 30 Nov 2015

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- Very popular in recent years
 - Filter, Wrapper, Single Objective, Multi-objective
- Representation, continuous PSO vs Binary PSO
- Search mechanism
- Fitness function
- Scalability

0.7	0.12	0.84	0.69	0.25	0.06	0.92	0.45	0.36	0.80	0.67	0.30	0.41
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1	0	1	1	0	0	1	0	0	1	1	0	0
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E. K. Tang, P. Suganthan, and X. Yao, "Feature selection for microarray data using least squares SVM and particle swarm optimization," in *IEEE Symposium on Computational Intelligence in Bioinformatics and Computational Biology (CIBCB)*, pp. 1–8, 2005.

L. Y. Chuang, H. W. Chang, C. J. Tu, and C. H. Yang, "Improved binary PSO for feature selection using gene expression data," *Computational Biology and Chemistry*, vol. 32, no. 29, pp. 29–38, 2008.

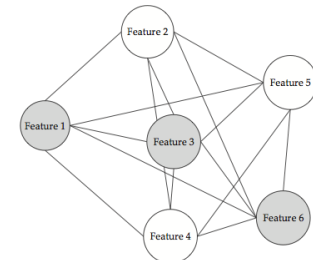
C. L. Huang and J. F. Dun, "A distributed PSO-SVM hybrid system with feature selection and parameter optimization," *Application on Soft Computing*, vol. 8, pp. 1381–1391, 2008.

B. Xue, M. Zhang, and W. N. Browne, "Multi-objective particle swarm optimisation (PSO) for feature selection," in *Proceeding of the 14th Annual Conference on Genetic and Evolutionary Computation Conference (GECCO)*, pp. 81–88, ACM, 2012.

Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selection", *IEEE Transaction on Evolutionary Computation*, doi: 10.1109/TEVC.2015.2504420, published online on 30 Nov 2015

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- Start from around 2003
 - Filter, Wrapper, Single Objective, Multi-objective
- Representation
- Search mechanism
- Filter approaches
- Scalability



S. Kashef and H. Nezamabadi-pour, "An advanced ACO algorithm for feature subset selection," *Neurocomputing*, 2014.

S. Vieira, J. Sousa, and T. Runkler, "Multi-criteria ant feature selection using fuzzy classifiers," in *Swarm Intelligence for Multi-objective Problems in Data Mining*, vol. 242 of *Studies in Computational Intelligence*, pp. 19–36, Heidelberg, 2009.

C.-K. Zhang and H. Hu, "Feature selection using the hybrid of ant colony optimization and mutual information for the forecaster," in *International Conference on Machine Learning and Cybernetics*, vol. 3, pp. 1728–1732, 2005.

R. Jensen, "Performing feature selection with aco," in *Swarm Intelligence in Data Mining*, vol. 34 of *Studies in Computational Intelligence*, pp. 45–73, / Heidelberg, 2006.

L. Ke, Z. Feng, and Z. Ren, "An efficient ant colony optimization approach to attribute reduction in rough set theory," *Pattern Recognition Letters*, vol. 29, no. 9, pp. 1351–1357, 2008.

Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selection", *IEEE Transaction on Evolutionary Computation*, doi: 10.1109/TEVC.2015.2504420, published online on 30 Nov 2015

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- DE: since 2008
 - potential for large-scale
- LCSs:
 - implicit feature selection
 - embedded feature selection
- memetic:
 - population search + local search
 - Wrapper + filter

A. Al-Ani, A. Alsukker, and R. N. Khushaba, "Feature subset selection using differential evolution and a wheel based search strategy," *Swarm and Evolutionary Computation*, vol. 9, pp. 15–26, 2013.

Z. Li, Z. Shang, B. Qu, and J. Liang, "Feature selection based on manifold-learning with dynamic constraint handling differential evolution," in *IEEE Congress on Evolutionary Computation (CEC)*, pp. 332–337, 2014.

I.-S. Oh, J.-S. Lee, and B.-R. Moon, "Hybrid genetic algorithms for feature selection," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. 26, no. 11, pp. 1424–1437, 2004.

S. Palanisamy and S. Kanmani, "Artificial bee colony approach for optimizing feature selection," *International Journal of Computer Science Issues (IJCSI)*, vol. 9, no. 3, pp. 432–438, 2012.

Z. Zhu, S. Jia, and Z. Ji, "Towards a memetic feature selection paradigm [application notes]," *IEEE Computational Intelligence Mag-azine*, vol. 5, no. 2, pp. 41–53, 2010.

Y. Wen and H. Xu, "A cooperative coevolution-based pittsburgh learning classifier system embedded with memetic feature selection," in *IEEE Congress on Evolutionary Computation*, pp. 2415–2422, 2011.

Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selection", *IEEE Transaction on Evolutionary Computation*, doi: 10.1109/TEVC.2015.2504420, online on 30 Nov 2015 29

- Biological and biomedical tasks
 - gene analysis, biomarker detection, cancer classification, and disease diagnosis
- Image and signal processing
 - image analysis, face recognition, human action recognition, EEG brain-computer-interface, speaker recognition, handwritten digit recognition, personal identification, and music instrument recognition.
- Network/web service
 - Web service composition and development, network security, and email spam detection.
- Business and financial problems
 - Financial crisis, credit card issuing in bank systems, and customer churn prediction.
- Others
 - power system optimisation, weed recognition in agriculture, melting point prediction in chemistry, and weather prediction.

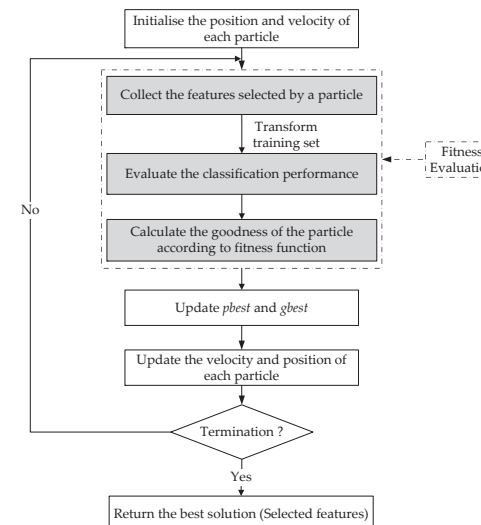
Bing Xue, Mengjie Zhang, Will Browne, Xin Yao. "A Survey on Evolutionary Computation Approaches to Feature Selection", *IEEE Transaction on Evolutionary Computation*, doi: 10.1109/TEVC.2015.2504420, published online on 30 Nov 2015

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Feature Selection

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PSO for FS: initialisation and updating



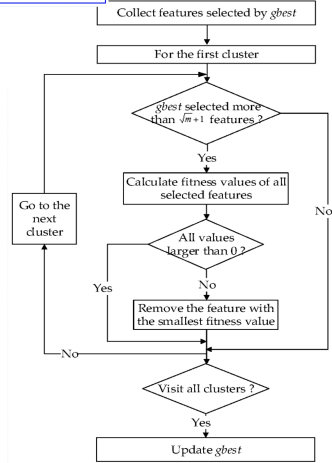
- Initialisation:
 - Forward selection
 - Backward selection
 - Mixture of both
- Updating:
 - Consider the number of features in the best and gbest updating

Bing Xue, Mengjie Zhang, Will N. Browne. "Particle Swarm Optimisation for Feature Selection in Classification: Novel Initialisation and Updating Mechanisms". *Applied Soft Computing*. Vol 18, PP. 261–276, 2014

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PSO FS: with backward elimination

Backward Elimination



Filter Measure

$$f'(s_i) = \frac{1}{x_i} (Rel(s_i) - \frac{1}{|s| - 1} Red(s_i))$$

x_i : the position value in the i th dimension

By adding $\frac{1}{x_i} f'(s_i)$ ensures that if two features have the same $f(s)$ value, the one with a smaller position value (i.e. smaller probability) will be removed

s_i is removed only when $f'(s_i) < 0$ and $f'(s_i)$ is the smallest value

$$f(s_i) = (Rel(s_i) - \frac{1}{|s| - 1} Red(s_i))$$

where,

$$Rel(s_i) = I(s_i; c)$$

$$Red(s_i) = \frac{1}{|S| - 1} \sum_{s_i, s_j \in S, s_i \neq s_j} I(s_i; s_j)$$

$Rel(s_i)$: relevance contribution of s_i in S

$Red(s_i)$: redundancy in S caused by s_i

s_i should be removed if $f(s_i) < 0$

Bach Hoai Nguyen, Bing Xue, Ivy Liu and Mengjie Zhang. "Filter based Backward Elimination in Wrapper based PSO for Feature Selection in Classification". Proceedings of 2011 IEEE Congress on Evolutionary Computation. Beijing, China. 6-11 July, 2014. IEEE Press. PP.3111--3118. 2015

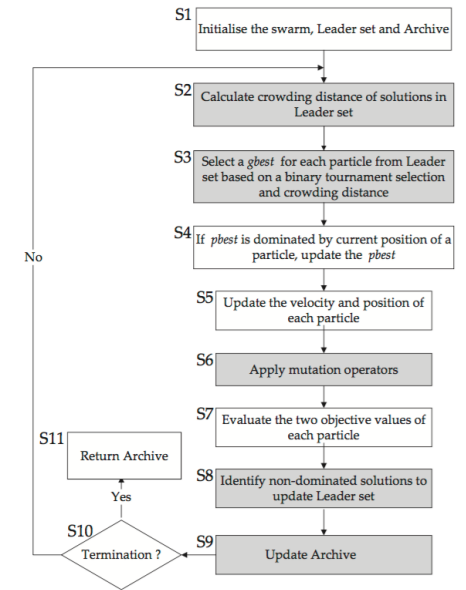
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Multi-objective PSO for FS

- Introduce and develop the **first multi-objective PSO** approach to feature selection

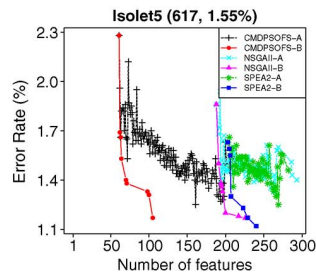
- Simultaneously minimise the number of features and the error rate
- ~105 citations since June 2013

Bing Xue, Mengjie Zhang, Will Browne. "Particle swarm optimization for feature selection in classification: A multi-objective approach, IEEE Transactions on Cybernetics, vol. 43, no. 6, pp. 1656-1671, 2013. [ARC/ERA Tier A, IF 3.783]



Multi-objective PSO for FS

- Introduce and develop the **first multi-objective PSO** approach to feature selection
- Simultaneously minimise the number of features and the error rate
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T-TEST ON HYPERVOLUME RATIOS ON TRAINING ACCURACY

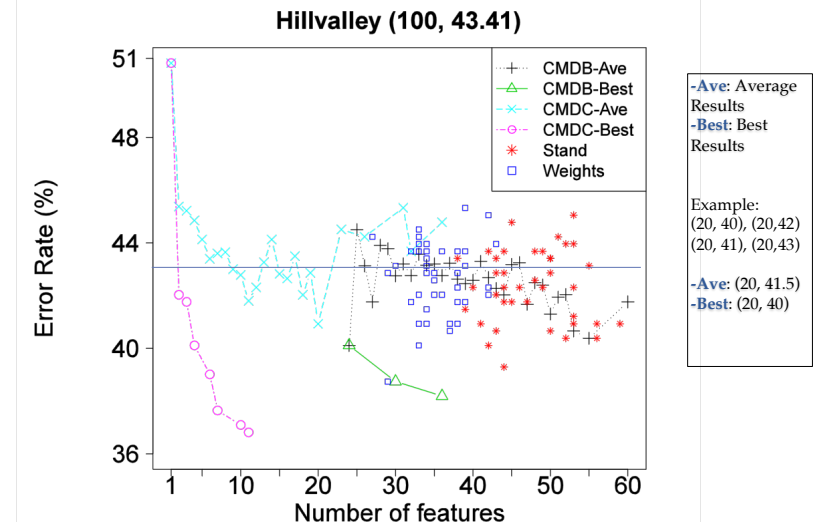
Dataset	Wine	Australian	Zoo	Vehicle	German	WBCD
	NS	CMD	NS	CMD	NS	CMD
NSPSOFS	+	+	+	+	+	+
CMDPSOFS	-	-	-	-	-	-
NSGAII	-	-	-	-	-	-
SPEA2	-	-	-	-	-	-
PAES	-	-	-	-	-	-

Dataset	Lung	Ionosphere	Hillvalley	Musk1	Madelon	Isolet5
	NS	CMD	NS	CMD	NS	CMD
NSPSOFS	+	+	+	+	+	+
CMDPSOFS	-	-	-	-	-	-
NSGAII	-	-	-	-	-	-
SPEA2	-	-	-	-	-	-
PAES	-	-	-	-	-	-

Bing Xue, Mengjie Zhang, Will Browne. "Particle swarm optimization for feature selection in classification: A multi-objective approach, IEEE Transactions on Cybernetics, vol. 43, no. 6, pp. 1656-1671, 2013. [ARC/ERA Tier A, IF 3.783]

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Multi-objective PSO for FS : Binary VS continuous



Bing Xue, Mengjie Zhang, Will N. Browne. "Multi-Objective Particle Swarm Optimisation (PSO) for Feature Selection". Proceedings of 2012 Genetic and Evolutionary Computation Conference (GECCO 2012). ACM Press, Philadelphia, USA. 7-11 July 2012. pp. 81-88

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- Updating equations:

$$x_{id}(t+1) = \begin{cases} 1 - x_{id}(t), & \text{if } \text{rand}() < p_{id} \\ x_{id}(t), & \text{otherwise} \end{cases}$$

$$p_{id} = p_0 + p_{pd} + p_{gd}$$

$$p_{pd} = \begin{cases} p_1, & \text{if } x_{id}(t) \neq y_{id}(t) \\ 0, & \text{otherwise} \end{cases}$$

$$p_{gd} = \begin{cases} p_2, & \text{if } x_{id}(t) \neq \hat{y}_{id}(t) \\ 0, & \text{otherwise} \end{cases}$$

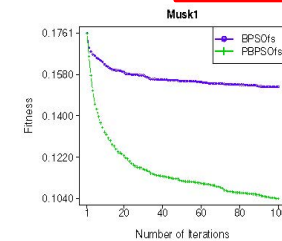
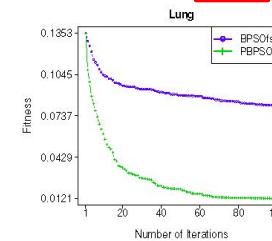
where $y_{id}(t)$ represents $pbest$, and \hat{y}_{id} represents $gbest$

$$p_0 + p_1 + p_2 = 1$$

Bing Xue, Su Nguyen, Mengjie Zhang, "A New Binary Particle Swarm Optimisation Algorithm for Feature Selection". Proceedings of the 17th European Conference on Applications of Evolutionary Computation (EvoApplications 2014). Lecture Notes in Computer Science, Vol. 8602. Granada, Spain 23rd - 25th April 2014. pp. 501-513

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Dataset	Method	AveSize	BestAcc	AveAcc ± StdAcc	Test 1	Test 2	Time
Hillvalley	All	100	56.59				
	BPSOfs	39.35	60.16	56.88 ± 1.6322	=		50.28
	PBPSOfs	31.08	61.26	58.25 ± 1.6952	+	+	46.1
Musk1	All	166	83.92				
	BPSOfs	75.52	90.91	84.21 ± 2.8401	=		13.96
	PBPSOfs	69.3	88.81	85.38 ± 1.8087	+	+	12.7
Arrhythmia	All	279	94.46				
	BPSOfs	99.7	95.14	94.21 ± 0.3937	-		16.97
	PBPSOfs	63.42	95.48	94.71 ± 0.3405	+	+	12.44
Madelon	All	500	70.9				
	BPSOfs	243.85	78.59	75.81 ± 1.4905	+		991.6
	PBPSOfs	212.42	81.15	78.91 ± 1.2565	+	+	953.63
Isolet5	All	617	98.45				
	BPSOfs	225.15	98.59	98.25 ± 0.1354	-		384.16
	PBPSOfs	169.35	98.87	98.61 ± 0.1248	+	+	328.34
Multiple Features	All	649	98.63				
	BPSOfs	237.05	99.1	98.89 ± 0.0923	+		692.54
	PBPSOfs	176.15	99.27	99.01 ± 0.1043	+	+	551.44



Bing Xue, Su Nguyen, Mengjie Zhang, "A New Binary Particle Swarm Optimisation Algorithm for Feature Selection". Proceedings of the 17th European Conference on Applications of Evolutionary Computation (EvoApplications 2014). Lecture Notes in Computer Science, Vol. 8602. Granada, Spain 23rd - 25th April 2014. pp. 501-513

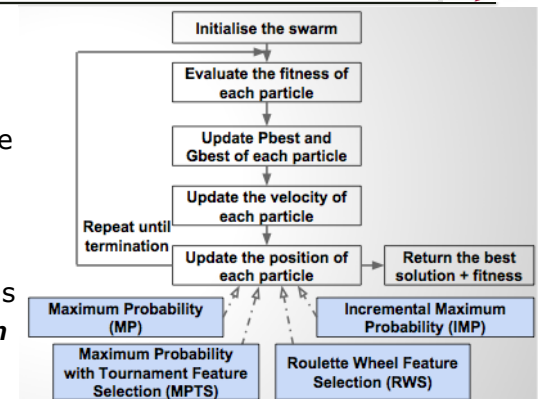
38

- Introduce **statistical feature clustering** to feature selection and develop the first approach
 - reduce the size of the search space
 - #features: from 600 to ~12
 - implicitly consider feature interaction
 - Example:
 - our method achieved accuracy 100%: {10, 7, 3}
 - Single feature ranking: 7, 10, 12, 1, 9, 11, 6, 2, 13, 5, 4, 3

Bing Xue, Mitchell C. Lane, Ivy Liu, Mengjie Zhang, "Particle Swarm Optimisation for Feature Selection Based on Statistical Clustering", Evolutionary Computation (Journal, MIT Press), Passed first round review with positive comments [ARC/ERA Tier A]

39

- Development of four new particle position update algorithms that automatically select a single feature from each feature cluster
- As features are grouped by similarity, a single feature is expected to provide **enough** information about its feature cluster



Mitchell C. Lane, Bing Xue, Ivy Liu, Mengjie Zhang, "Gaussian Based Particle Swarm Optimisation and Statistical Clustering for Feature Selection". Proceedings of the 14th European Conference on Evolutionary Computation in Combinatorial Optimisation (EvoCOP 2014). Lecture Notes in Computer Science, Volume 8600, Granada, Spain 23rd - 25th April 2014. pp. 133-144
 Mitchell C. Lane, Bing Xue, Ivy Liu and Mengjie Zhang, "Particle Swarm Optimisation and Statistical Clustering for Feature Selection". Proceedings of the 26th Australasian Joint Conference on Artificial Intelligence (AI2013) Lecture Notes in Computer Science, Vol. 8272. Springer, Dunedin, New Zealand, December 2013. pp. 214-220

40

- Information theory in evolutionary feature selection
 - Fast algorithm – mutual information
 - New measures, evaluate multiple features
 - Evolutionary multi-objective filter feature selection

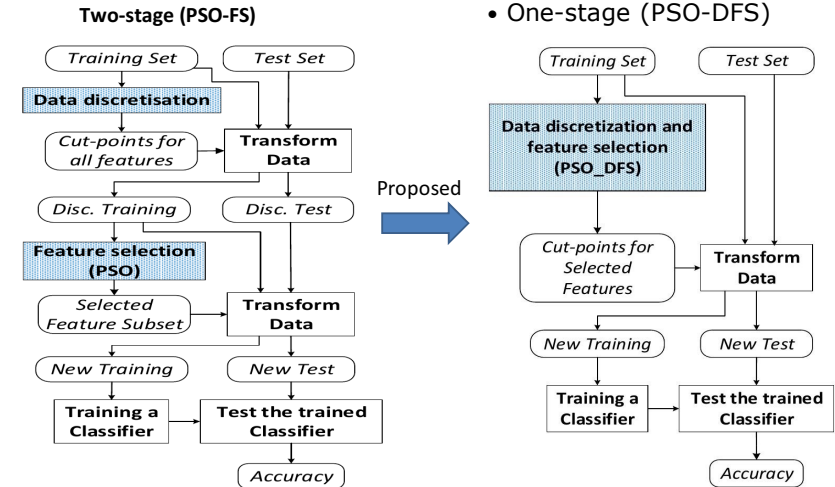
F-MI	0.05	0.05	0.05	0.06	0.07	0.09	0.15	0.18
F-E	2.88	97.7	8.64	27.95	9.85	256.57	2.96	236.42
F-RS	2.07	2485.61	8.21	55.3	14.81	1372.93	0.69	928.25
F-PRS	2.86	2766.29	8.28	38.36	9.95	1827.06	0.68	911.3
W-SVM	24.41	5143.18	53.28	270.64	118.37	2441.21	5.4	10937.87
W-SNN	6.12	9311.59	18.89	264.51	72.72	4095.07	1.68	1936.67
W-DT	5.19	189.43	10.53	43.15	47.87	244.55	3.82	529.7
W-NB	13.46	304.08	15.89	150.37	19.42	377.24	4.13	706.23

Bing Xue, Liam Cervante, Lin Shang, Will Browne, Mengjie Zhang. "A Multi-Objective Particle Swarm Optimisation for Filter Based Feature Selection in Classification Problems". Connection Science. Vol. 24, No. 2-3, pp. 91-116, 2012.

Bing Xue, Liam Cervante, Lin Shang, Will N. Browne, Mengjie Zhang. "Evolutionary Algorithms and Information Theory for Filter Based Feature Selection in Classification". International Journal on Artificial Intelligence Tools. Vol. 22, Issue 04, August 2013. pp. 1350024 – 1 - 31. DOI: 10.1142/S0218213013500243.

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Bare-Bone Particle Swarm Optimisation



Binh Tran Ngon, Mengjie Zhang, Bing Xue. "Bare-Bone Particle Swarm Optimisation for Simultaneously Discretising and Selecting Features For High-Dimensional Classification". Proceedings of the 19th European Conference on the Applications of Evolutionary Computation (EvoApplications 2016, EvoIASP 2016). Lecture Notes in Computer Science. Vol. 9597. Porto, Portugal, March 30 - April 1, 2016. pp. 701-718

42

	F₁	F₂	F₃	F₄	F₅	...	F_D
Min	5.5	-9.2	7.6	-8.5	6.9	...	-9.3
Max	10.2	20.5	12.7	4.5	50.1	...	-1.6
Particle's Position	7.2	10.4	12.7	-3.8	6.9	...	-4.5

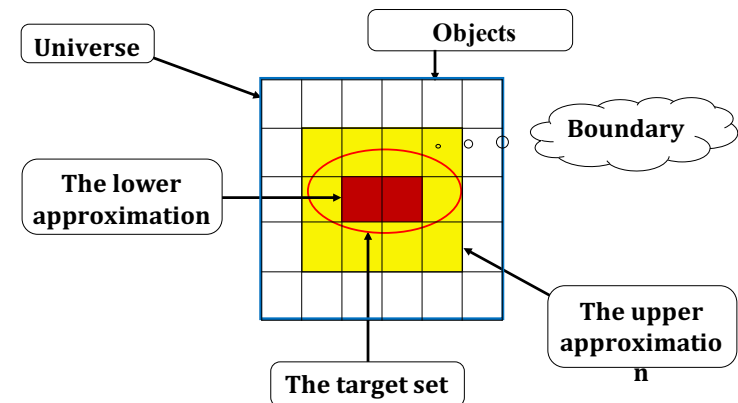
Not selected

Candidate solution

Binh Tran Ngon, Mengjie Zhang, Bing Xue. "Bare-Bone Particle Swarm Optimisation for Simultaneously Discretising and Selecting Features For High-Dimensional Classification". Proceedings of the 19th European Conference on the Applications of Evolutionary Computation (EvoApplications 2016, EvoIASP 2016). Lecture Notes in Computer Science. Vol. 9597. Porto, Portugal, March 30 - April 1, 2016. pp. 701-718

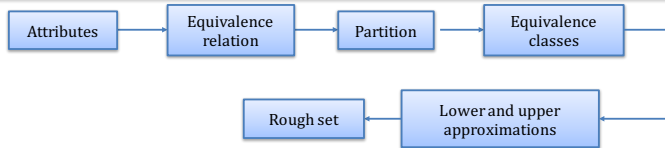
43

- Promote rough set theory for feature selection
 - Others': mainly < 200 features
 - Ours: more than 600 features



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FS based on Rough Set



$$Fitness = \frac{\sum_{i=1}^n |aprP U_i|}{|U|} + \frac{\sum_{x \in \{EqC\}} \frac{|x|}{|U|}}{|EqC|}$$

- U is the universe or the **whole dataset**
- U_i is **one class** in the dataset
- EqC : *equivalence classes*
- $aprP$ is the **lower approximation in probabilistic rough set theory**
- A parameter α to relax the definition of $aprP$

Bing Xue, Liam Cervante, Lin Shang, Will Browne and Mengjie Zhang. "Binary PSO and rough set theory for feature selection: a multi-objective filter based approach". International Journal of Computational Intelligence and Applications (IJCIA), Vol. 13, No. 2 (2014). pp. 1450009(1-34)

Liam Cervante, Bing Xue, Lin Shang, Mengjie Zhang. "A Multi-Objective Feature Selection Approach Based on Binary PSO and Rough Set Theory". Proceedings of the 13th European Conference on Evolutionary Computation in Combinatorial Optimisation (EvoCOP 2013). Lecture Notes in Computer Science. Vol. 7832. Vienna, Austria. 3-5 April 2013. pp. 25-36

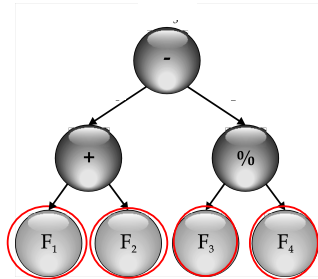
Liam Cervante, Bing Xue, Lin Shang and Mengjie Zhang. "A Dimension Reduction Approach to Classification Based on Particle Swarm Optimisation and Rough Set Theory". Proceedings of the 25th Australasian Joint Conference on Artificial Intelligence. Lecture Notes in Artificial Intelligence. Vol. 7691. Springer. Sydney, Australia, December 2012. pp. 313-325

45

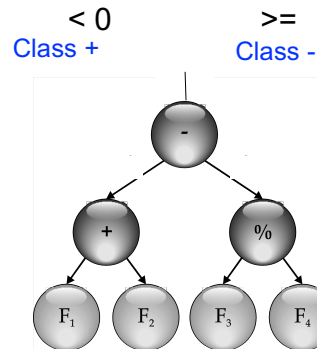
46

GP for Embedded Feature Selection

Feature Selection



Classification



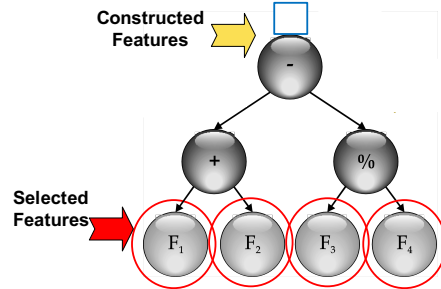
Feature Construction

Soha Ahmed, Mengjie Zhang, Lifeng Peng and Bing Xue. "Genetic Programming for Measuring Peptide Detectability". Proceedings of the 10th International Conference on Simulated Evolution and Learning (SEAL 2014). Lecture Notes in Computer Science. Vol. 8886. Dunedin, New Zealand. December 15-18, 2014. pp. 593-604

47

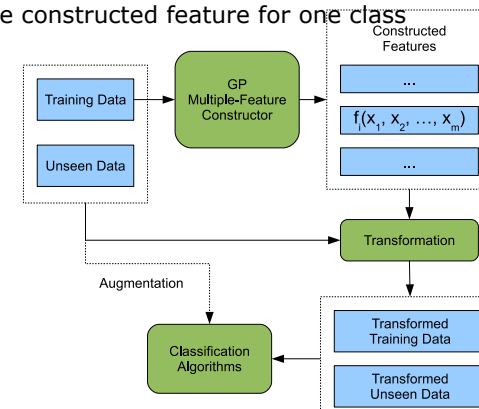
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- GP is **flexible** in making mathematical and logical functions
- There **isn't much structural (topological) information** in the search space of possible functions, so using a meta-heuristic approach (such as evolutionary computation) seems reasonable.



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- One constructed feature for one class



Neshatian, K.; Mengjie Zhang; Andrae, P., "A Filter Approach to Multiple Feature Construction for Symbolic Learning Classifiers Using Genetic Programming," in *Evolutionary Computation, IEEE Transactions on*, vol.16, no.5, pp.645-661, Oct. 2012

50

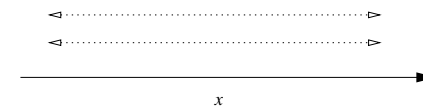
Defining a measure of goodness for a single feature:

- The interval of a **class** along a feature is determined by the dispersion of the instances of that class along the feature axis. The dispersion of instances themselves is related to the distribution of data points in that class.
- An interval **I** is represented with a pair (*lower, upper*) which shows the lower and upper boundaries of the interval. **I_c** is used to indicate an interval for class **c**.
- The interval of class **c** could be formulated as follows if the class distributions were normal.

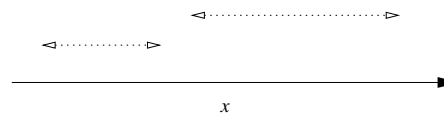
$$I_c = [\mu_c - 3\sigma_c, \mu_c + 3\sigma_c]$$

- However, the normality assumption is not always satisfied.

- Overlapping intervals



- Non-overlapping intervals



- Given a discrete or categorical random variable C (the class label) which can take values c_1, c_2, \dots, c_L with probabilities $p(c_1), p(c_2), \dots, p(c_L)$, the entropy of C is defined by:

$$H(C) = -\sum_{i=1}^L p(c_i) \log_b p(c_i)$$

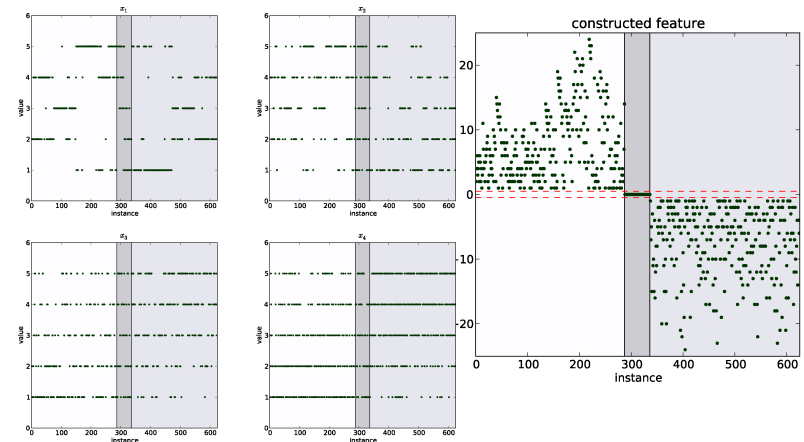
where b is base of the logarithm and is usually 2.

- A class interval establishes a new probability space. Therefore, the probability of classes in the above equation should be conditioned on the values of the feature that fall in the interval.
- Given X , a feature, C , the set of all class labels, and c^* , the class of interest with corresponding interval I_{c^*} , the entropy of the interval of class c^* is

$$H(I_{c^*}) = -\sum_{c \in C} p(c|X \in I_{c^*}) \log_2 p(c|X \in I_{c^*})$$

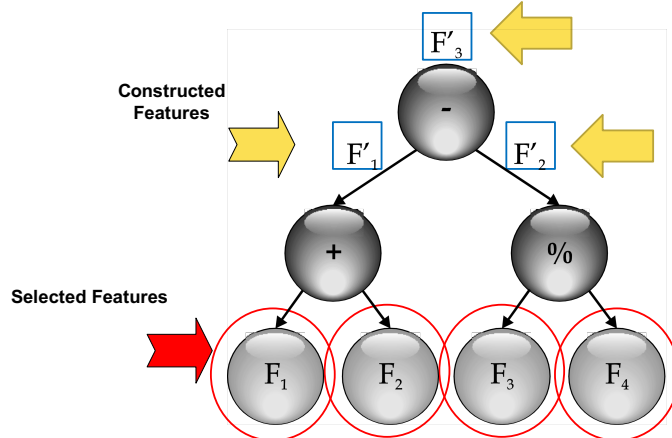
Neshatian, K.; Mengjie Zhang; Andrae, P., "A Filter Approach to Multiple Feature Construction for Symbolic Learning Classifiers Using Genetic Programming," in *Evolutionary Computation, IEEE Transactions on*, vol.16, no.5, pp.645-661, Oct. 2012 53

- 4 features, 3 classes



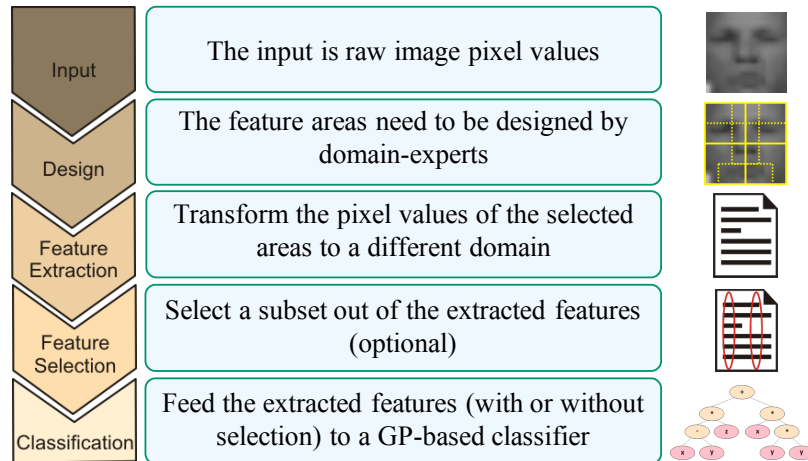
Neshatian, K.; Mengjie Zhang; Andrae, P., "A Filter Approach to Multiple Feature Construction for Symbolic Learning Classifiers Using Genetic Programming," in *Evolutionary Computation, IEEE Transactions on*, vol.16, no.5, pp.645-661, Oct. 2012 54

- Construct multiple features from a single tree

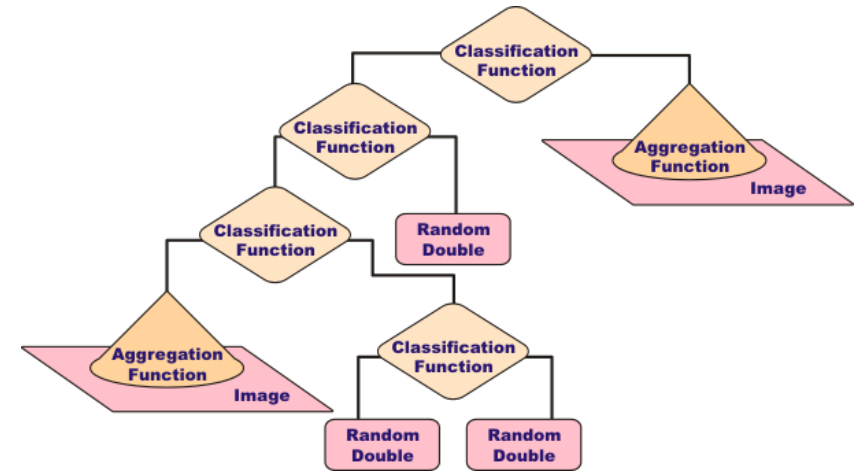


Soha Ahmed, Mengjie Zhang, Lifeng Peng and Bing Xue. "Multiple Feature Construction for Effective Biomarker Identification and Classification using Genetic Programming". Proceedings of 2014 Genetic and Evolutionary Computation Conference (GECCO 2014). ACM Press. Vancouver, BC, Canada. 12-16 July 2014. pp.249-256

- The traditional way
- Domain-specific pre-extracted features approach (DS-GP)



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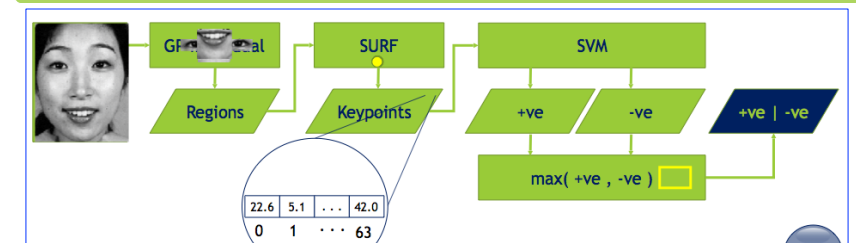
- **Method:** DWST
- **Dataset:** Faces
- **Accuracy**
 - Training: 97.23%
 - Test: 97.27%



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- Improve domain-independent object classification in images by using GP techniques.

- **Designing** a program representation that is capable of detecting sub-regions of the image that are rich in features;
- **Constructing** a classification system to extract features from the selected regions and then use a SVM classifier and voting scheme to predict the class label; and
- **Investigating** whether the regions detected by the new method are similar to those designed by domain experts.

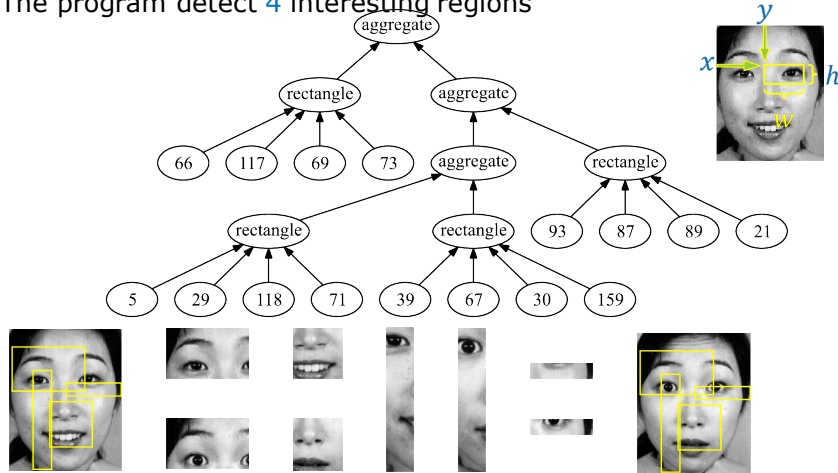


Andrew Lensen, Harith Al-Sahaf, Mengjie Zhang and Bing Xue. "A Hybrid Genetic Programming Approach to Feature Detection and Image Classification". Proceedings of 2015 the 30th International Conference on Image and Vision Computing New Zealand (IVCNZ 2015). IEEE Press. Auckland. 23 - 24 Nov 2015. pp. (to appear)

60

Images: GP-Surff

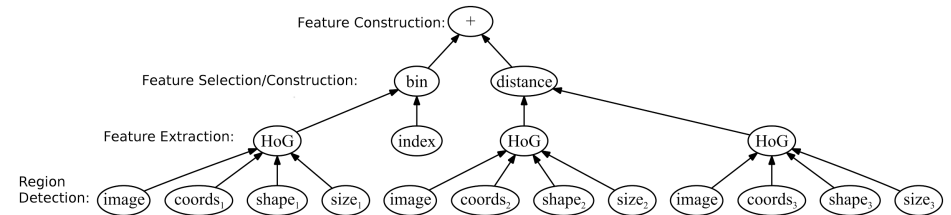
- A program evolved on JAFFE, average over 95% test accuracy
- The program detect 4 interesting regions



Andrew Lensen, Harith Al-Sahaf, Mengjie Zhang and Bing Xue. "A Hybrid Genetic Programming Approach to Feature Detection and Image Classification". Proceedings of 2015 the 30th International Conference on Image and Vision Computing New Zealand (IVCNZ 2015). IEEE Press. Auckland. 23 - 24 Nov 2015. pp. (to appear)

Images: GP-HoG Method

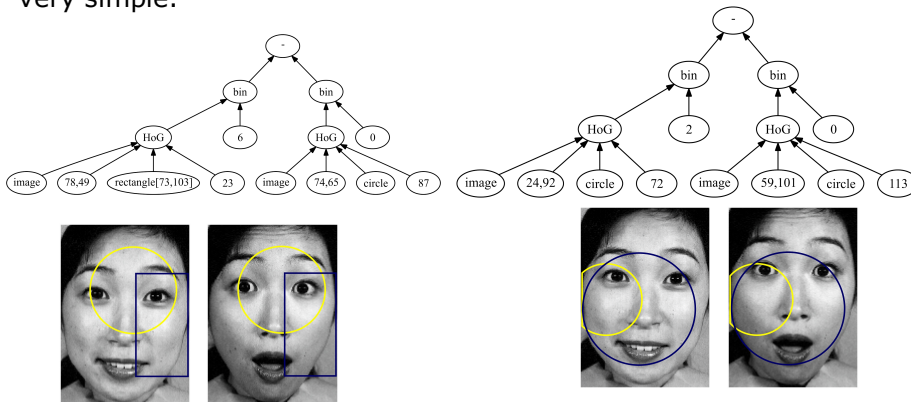
- GP-HoG uses strongly typed GP to perform three tasks in the same tree structure.
- All layers are trained simultaneously and coherently.
- Output of the tree is thresholded.



Andrew Lensen, Harith Al-Sahaf, Mengjie Zhang, Bing Xue. "Genetic Programming for Region Detection, Feature Extraction, Feature Construction and Classification in Image Data". Proceedings of the 19th European Conference on Genetic Programming (EuroGP 2016). Lecture Notes in Computer Science. Vol. 9594. Porto, Portugal, March 30 - April 1, 2016. pp. 51-67

Images: GP-HoG Method

- The below tree has 98% training and 95% test performance on the Jaffe dataset despite being very simple.
- The below tree has 95% training and 100% test performance on the Jaffe dataset.



Andrew Lensen, Harith Al-Sahaf, Mengjie Zhang, Bing Xue. "Genetic Programming for Region Detection, Feature Extraction, Feature Construction and Classification in Image D

Biology

- Due to the nature, the MS data production process is very expensive (costs around 2,000 NZD daily) and time consuming (around two weeks to produce a single sample).
- The number of samples available is very small and the number of features in each sample is extremely large.
- Moreover, the features of interest are too small.
- The classification of MS data is so challenging.

Data set	# Features	# Samples	# Classes
Pancreatic Cancer	6771	181	2
Ovarian Cancer1	15154	253	2
Ovarian Cancer 2	15000	216	2
Prostate Cancer	15000	322	4
Toxpath	7105	115	4
Arcene	10,000	200	2
Apple-plus	773	40	4
Apple-minus	365	40	4

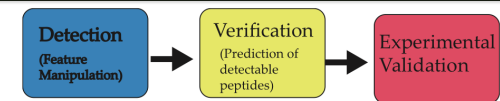
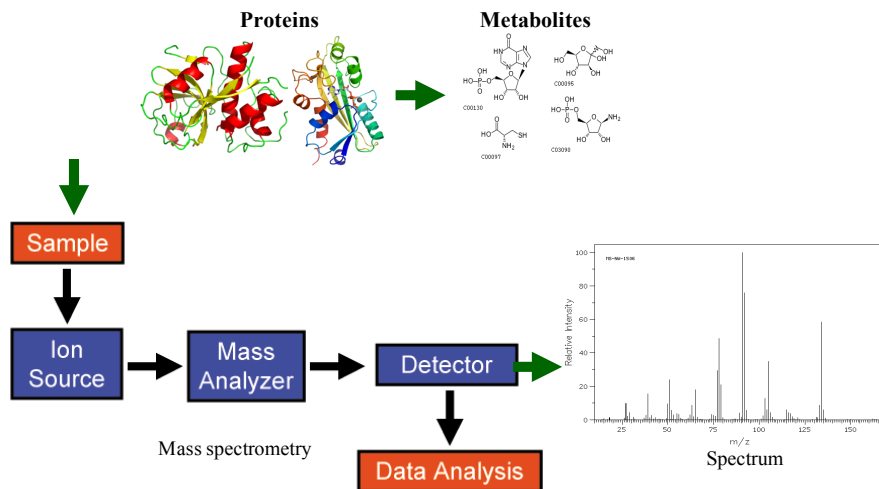
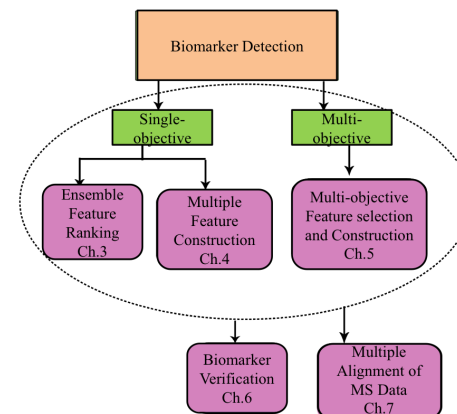


Figure 1.1: Stages of the biomarker identification process



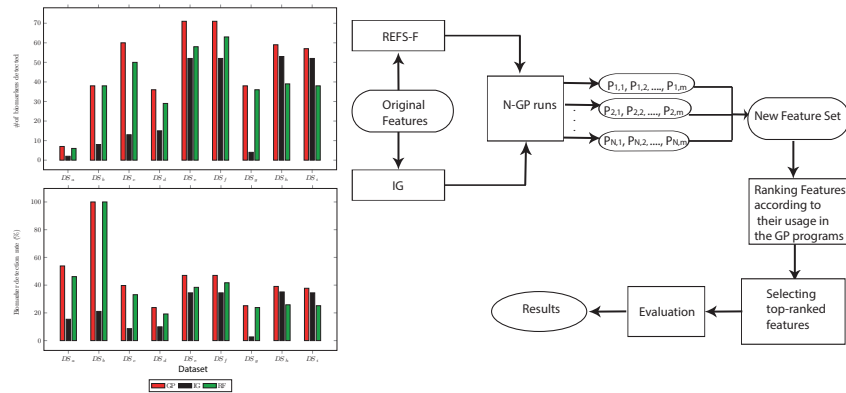


Figure 3.6: Biomarker detection of the proposed method in comparison with IG and RF.

Soha Ahmed, Mengjie Zhang, Lifeng Peng. "Improving Feature Ranking for Biomarker Discovery in Proteomics Mass Spectrometry Data using Genetic Programming". Connection Science. Vol. 26, Issue 3, 2014. pp. 215-243

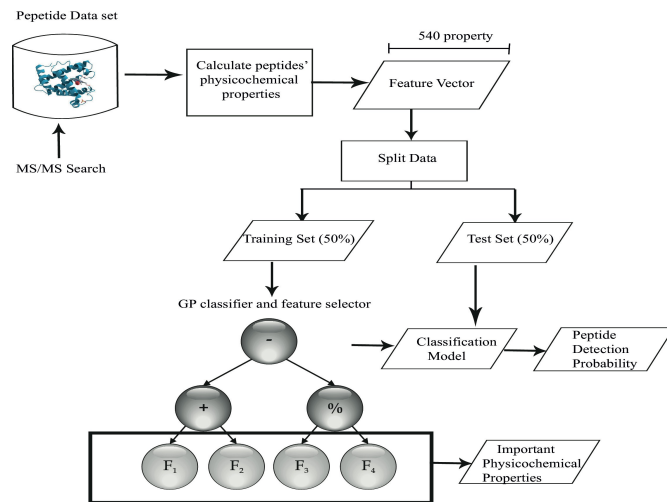
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m/z values in Apple-plus data set (12 biomarkers)	New Method (9 ✓)	Method 2 (3✓)
331.21	×	✓
471.09	✓	✓
107.05, 169.05, 238.05, 275.09, 456.11, 459.13	✓	×
456.62, 475.10	×	×
449.11	✓	✓
229.09	✓	×

Apple minus m/z (5 biomarkers)	New Method (5 ✓)	Method 2 (2✓)
463.0	✓	×
447.09	✓	✓
273.03	✓	✓
435.13	✓	×
227.07	✓	×

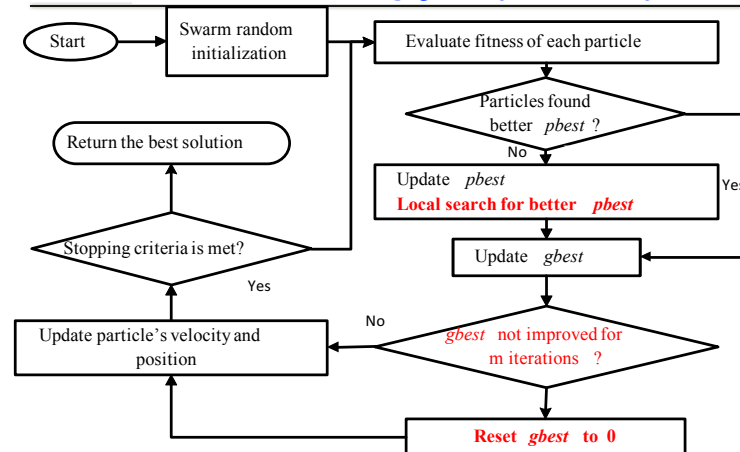
Soha Ahmed, Mengjie Zhang, Lifeng Peng and Bing Xue. "Multiple Feature Construction for Effective Biomarker Identification and Classification using Genetic Programming". Proceedings of 2014 Genetic and Evolutionary Computation Conference (GECCO 2014). ACM Press. Vancouver, BC, Canada. 12-16 July 2014. pp.249-256

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Soha Ahmed, Mengjie Zhang, Lifeng Peng and Bing Xue. "Genetic Programming for Measuring Peptide Detectability". Proceedings of the 10th International Conference on Simulated Evolution and Learning (SEAL 2014). Lecture Notes in Computer Science. Vol. 8886. Dordrecht, New Zealand. December 15-18, 2014. pp. 593-604

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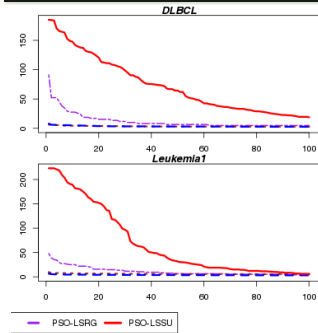


- Use a filter measure to identify:
 - Relevant features: correlated to the class label.
 - Redundant features: correlated with each other.
- Symmetric uncertainty (SU) is a normalised version of information gain (IG).

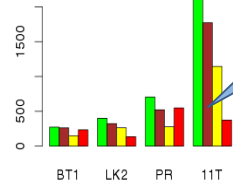
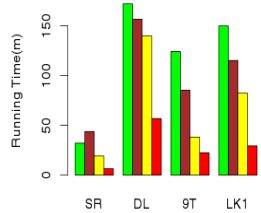
Binh Tran, Mengjie Zhang and Bing Xue, "A PSO Based Hybrid Feature Selection Algorithm For High-Dimensional Classification". Proceedings of 2016 IEEE World Congress on Computational Intelligence/ IEEE Congress on Evolutionary Computation (WCCI 2016 / CEC2016). Vancouver, Canada. 24-29 July, 2016. pp(to appear)

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Biology: PSO with local search on *pbest* and resetting *gbest* (PSO-LSRG)



- A PSO based hybrid FS algorithm for high-dimensional classification.
- PSO-LSSU combines wrapper and filter measures:
 - The fitness function.
 - The local search.
- PSO-LSSU achieved much smaller feature subsets with significantly better classification performance than the compared methods in most cases.



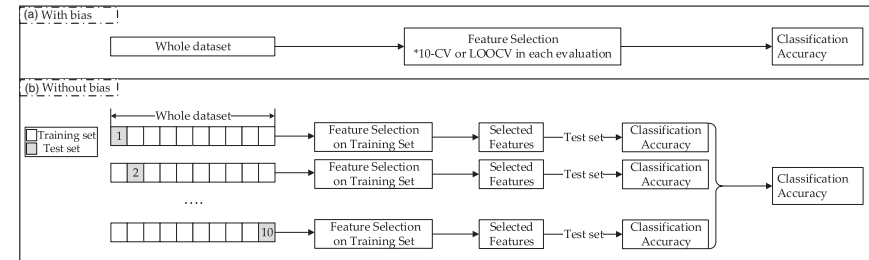
5 - 6 times faster than PSO

Binh Tran, Mengjie Zhang and Bing Xue, "A PSO Based Hybrid Feature Selection Algorithm For High-Dimensional Classification", Proceedings of 2016 IEEE World Congress on Computational Intelligence/IEEE Congress on Evolutionary Computation (WCCI2016/CEC2016), Vancouver, Canada, 24-29 July, 2016, pp.(to appear)

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Feature Selection Bias

- Many works on bio-data containing feature selection
 - which leads to biased results
 - conclusion might change



Binh Tran, Bing Xue and Mengjie Zhang, "Investigation on Particle Swarm Optimisation for Feature Selection on High-dimensional Data: Local Search and Selection Bias", Connection Science, Accepted April 2016

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GP for FS and FC

- Subset 1: Constructed feature only;
- Subset 2: Original feature set augmented by the constructed feature;
- Subset 3: Terminal features used to construct the new feature;
- Subset 4: The combination of subset 2 and 3;
- Subset 5: Multiple features constructed from all possible subtrees of the best GP individual;
- Subset 6: The combination of subset 3 and 5;

Figure 1: Leukemia constructed feature

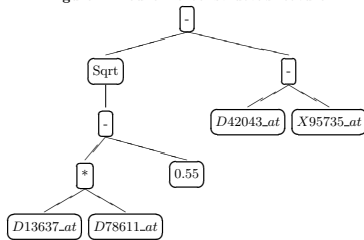


Figure 2: Feature X95735_at and D42043_at

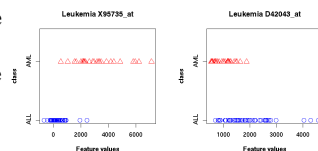


Figure 3: D13637_at and D78611_at

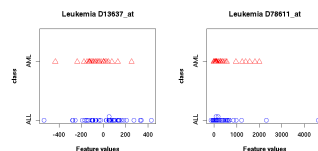
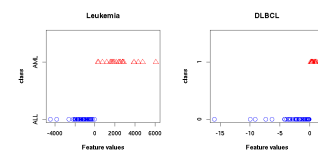


Figure 4: Constructed Features



Binh Tran, Bing Xue and Mengjie Zhang, "Genetic Programming for Feature Construction and Selection in Classification on High-dimensional Data", Memetic Computing, vol 8, Issue 1, pp3-15, 2016

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GP for FS and FC

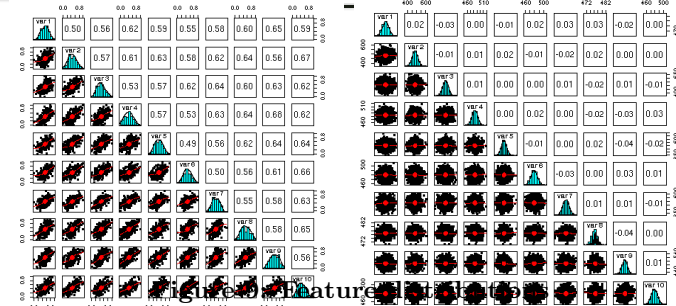
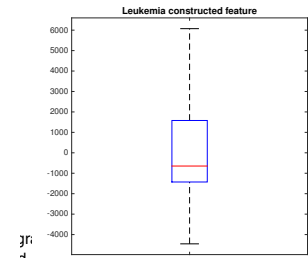
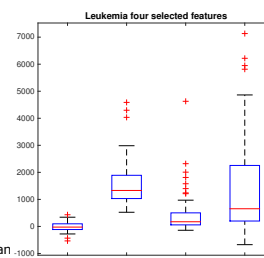


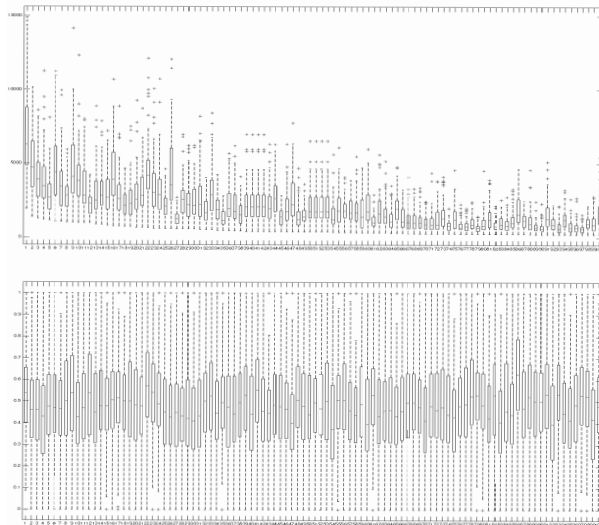
Figure 5: Feature values



Binh Tran, Bing Xue and Mengjie Zhang, "Genetic Programming for Feature Construction and Selection in Classification on High-dimensional Data", Memetic Computing, vol 8, Issue 1, pp3-15, 2016

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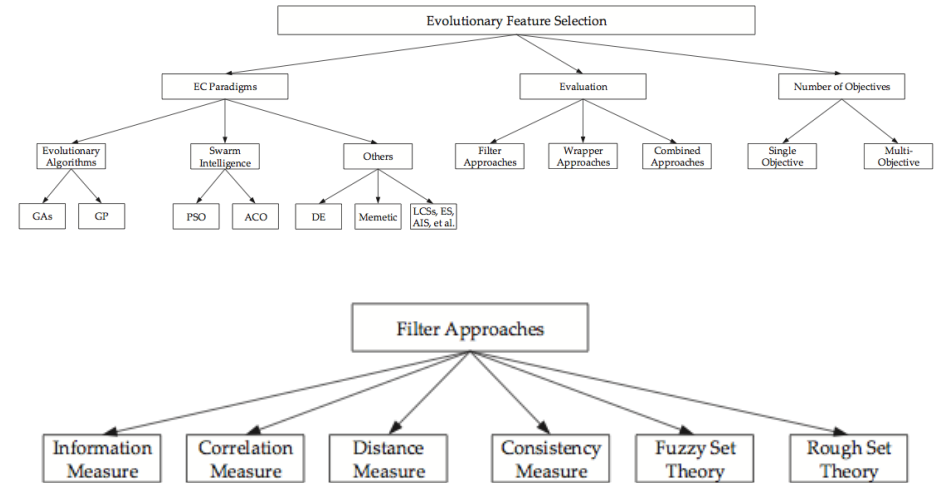
GP for FS and FC



Binh Tran, Bing Xue and Mengjie Zhang. "Genetic Programming for Feature Construction and Selection in Classification on High-dimensional Data", Memetic Computing, vol 8, Issue 1, pp3-15. 2016

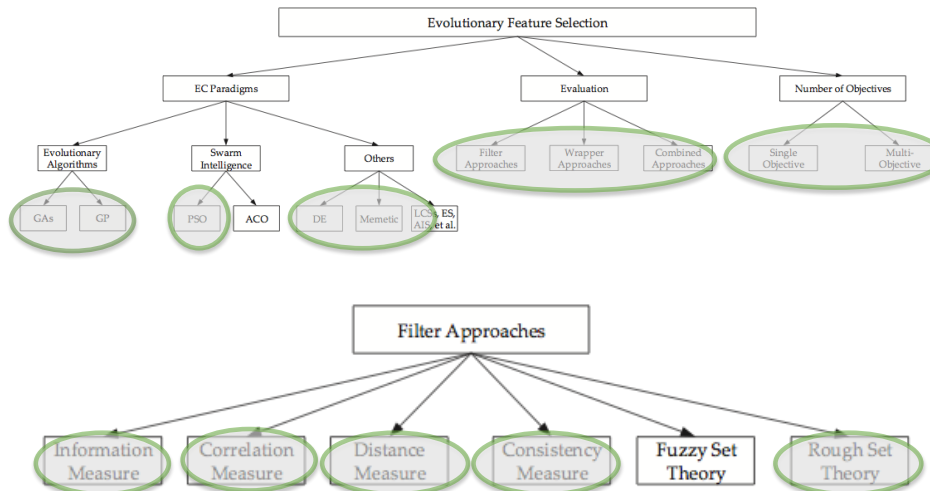
77

Work from ECRG



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Work from ECRG



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Issues and Challenges

- Scalability Problem
 - thousands, tens of thousands, and even millions
- Computational Cost
- Search Mechanisms
- Measures
- Representation
- Multi-Objective Feature Selection
- Feature Construction
- Number of Instances

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Acknowledgement

- Thanks A/Prof Will Browne, A/Prof Peter Andreae, A/Prof Ivy (I-Ming) Liu, A/Prof Lin Shang, Dr Lifeng Peng, Dr Kourosh Neshatian, Dr Su Nguyen, Dr Yi Mei, Dr Soha Ahmed, Harith Al-Sahaf, Liam Cervante, Andrew Lensen, Hoai Bach Nguyen, Binh Tran, Qi Chen, Emrah Hancer, and others
- Funding Agents:
 1. Marsden Fund of New Zealand award number(s): VUW1209
 2. University Research Fund at Victoria University of Wellington award number(s): 210375/3557, 209861/3580

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Thank you

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Acknowledgement

- Thanks everyone in the Evolutionary Computation Research Group at Victoria University of Wellington, New Zealand

