



## ANNUAL PROGRESS REPORT: 2003-04

# **BioInformatics Research Centre (BIRC)**

Nanyang Technological University, Singapore

### I. INTRODUCTION

The BioInformatics Research Centre (BIRC) was established on March 1, 2002, under NTU's partnership with Hewlett-Packard Asia to jointly establish a center of excellence in bioinformatics. The BIRC is the focus of the education, research and development, and human-resource training in bioinformatics at NTU. BIRC is an inter-school research centre hosted by the School of Computer Engineering (SCE). Currently 23 staff members from SCE, SBS, NIE, MPE, and EEE are affiliated and based their research projects at BIRC. It has 7 full-time researchers and 19 Ph.D. students.

Bioinformatics is the field of analyzing biological data, such as sequences, expressions, phenotypes, images, and literature, to discover biological knowledge leading to discover novel drugs and therapeutics. The mission of BIRC is to provide the interdisciplinary environment and training for students and researchers to engage in leading and cutting edge research in bioinformatics at NTU, and thereby become a part of the life sciences workforce in Singapore and elsewhere. BIRC brings together scientists and engineers, who are interested in bioinformatics modeling and computation, and fosters cross-disciplinary interactions among different schools to perform advanced research in bioinformatics. It also facilitates the teaching and research projects of the MSc. (Bioinformatics) offered by SCE.

*Mission*: The BioInformatics Research Centre (BIRC) has a mission to provide interdisciplinary environment and training for students and researchers to engage in leading and cutting edge research in bioinformatics in NTU, and thereby become a part of the life sciences workforce in Singapore and elsewhere.

*Vision*: The Centre's vision is to dedicate itself to the advancement of bioinformatics through education, research, and scientific breakthroughs, leading to discoveries of new medical drugs and therapies.

#### **II. RESEARCH INTERESTS**

BIRC research interests are currently focussed on the following research areas:

#### a) **GENOMICS**

Computational genomics, gene structure prediction, comparative genomics, phylogenetic studies, gene expression analysis

### b) STRUCTURAL GENOMICS AND PROTEOMICS

Protein structure prediction, protein-protein interactions, protein classification, modeling, and docking, mass spectroscopy.

c) **BIOLOGICAL DATABASES, MINING, AND VISUALIZATION** Biological data integration, storage, and query processing, 3-D visualization.

#### d) FUNCTIONAL AND MOLECULAR IMAGING

Functional brain imaging, molecular imaging, microarray and electrophorosis image analysis, bioimaging databases.

### e) COMPUTING SYSTEMS FOR BIOINFORMATICS

Immunoinformatics, modeling human immune system

#### f) DRUG DISCOVERY AND TRIAL DESIGN

Parallel algorithms and architectures for bioinformatics, grid computing, embedded systems for bioinformatics.

The interests of staff in the center are distributed across its research areas:



# III. RESEARCH FUNDING

List of current research projects					
S/No	Project Title	Source Of Funding	Principle Investigators/ Collaborators	Amount Of Funding S (\$)	Duration (Date)
01	Bio-visualisation	A*Star	A/P Cai Yiyu	\$748,000	2003-2006
02	Elucidation of Expression Profiles of Genes in Alpha- fetoprotein Positive and Alpha-fetoprotein Negative Hepatocellular Carcinoma by cDNA Microarray Analysis	BMRC & NMRC	A/P Lin Feng (collaborator)	\$113,000	2004
03	Design and Simulation of Artificial Bone Implantation	MOE & ARF	A/P Lin Feng	\$17,402	2001-2004
04	Analysis of functional brain images	RGM11/03	A/P Jagath Rajapakse	\$140,000	Oct 2003 – Oct 2006
05	Neural systems modeling using functional MRI	MOE & A*STAR	A/P Jagath Rajapakse	\$658,320	Oct 2002 – May 2006
06	Strategic research initiative at TechnoPlaza	RGM 4/03	A/P Wong Kok Cheong (PI)/ A/P Jagath Rajapakse	\$150,000	Jul 2003 – Dec 2004
07	Markov Random Field based spatial regularization for fMRI detection	CE – SUG 2/04	Asst Prof Vitali Zagorodnov	\$15,625	Oct 2004 – Oct 2005

The research funding for the centre comprises of the following:

### **IV. RESEARCH PROJECTS**

#### Signal Detection in Genomic Sequences

Detection of signals in genomic sequences is important in inferring transcription and translational processes and finding gene annotation. BIRC has developed a Markov/hybrid method to detect three types of signals, namely, splice sites, transcription initiation sites, and transcription start sites. This approach uses a Markov encoding method as inputs to the neural networks, which has given better accuracies over the conventional orthogonal coding.



Figure 1: Markov/neural hybrid model for the detection of signals in genomic sequences

#### Inferring Molecular Evolution of PD and AD Genes with Comparative Genomes

BIRC has taken a comparative genomic approach to infer the evolution of the genes affecting Parkinson's Disease (PD) and Alzheimer's Disease (AD), including the variants of PARK genes. The study used relative rate tests to determine synonymous and nonsynomous substitutions. Comparative genomics of human, chimp, mouse, chicken, and fugu revealed most of the genes did not provide evidence of rate heterogeneity, thereby inferring most of them are undergoing neutral or nearly neutral mutation.



Figure 2: The framework for phylogenetic studies on Parkinson's and Alzheimer's Disease genes.

#### Neural Network Based Analysis of DNA Microarry Gene Expression Data

DNA microarry technologies provide gene expression data on a massive scale involving thousands of genes. Exploratory data analyses in the form of clustering analysis with a goal to group the genes into meaningful sets are investigated using neural networks and machine learning approaches: Kohonen's self-organizing map (SOM), PCA and ICA algorithms, and SVMs. Our development leads to identify the genes whose transcript profiles response to specific stimuli such as timing, cell type, temperature, or drug dosage. The objective is to estimate pertinent parameters for individual transcripts, with a goal of testing specific hypotheses concerning transcript response to the stimulus.

#### Computational Approaches for Reconstructing Gene Regulatory Networks

The rapid accumulation of complete genome sequences and the application of microarray technology to genome-wide gene expression profiling have made computational approaches to the regulatory motif discovery and the study of transcriptional regulatory networks feasible. DNA-binding transcription factors (TFs) are one of the important components of transcription regulatory network. TFs usually bind to specific, short DNA sequence motifs in the cis-regulatory region of a gene to activate or repress its expression in response to changes in the environment. This project looks in to the development of novel methods or the improvement of the current methods for identifying transcription factor binding sites by analyzing time course microarray data. We also use expression profiling to identify sets of co-regulated genes and correlate these to regulatory motif search. The underlying assumption of using microarray data in regulatory region analysis is that a set of co-regulated genes usually share a similar set of regulatory motifs.



Figure 3: Gene expression profile data was used to identifying coordinate regulated genes in Arabidopsis genome

### Predicting Protein-Protein Interfaces Directly from Amino-acid Sequences

Protein-protein interactions are fundamental biochemical reactions in the organisms and play an important role in determining the biological processes. A novel information theory based algorithm is being developed for predicting protein-protein interfaces directly from amino-acid sequences. Each type of interface corresponds to a different functional or structural association between residues. With this method and using amino acid composition alone, we expect to predict statistically which of the six different types of interfaces a pool of 1000 residues at a better accuracy. The six types of interfaces include intra-domain, domain–domain, homo-obligomer, homo-complex, heteroobligomer, and hetero-complex.



Figure 4: Illustration of a protein-to-protein interaction network

#### Cancer Classification with Mass Spectra Data

BIRC has addressed the problem of cancer classification with mass spectra data and used Support Vector Machine Recursive Feature Elimination (SVM-RFE) to select a small subset of peaks as input variables for classification. We found that SVM-RFE always selects the best peak subset which has the top ranked peaks detected by T-statistics. Our finding supports that selecting a small subset of peaks not only improves the efficiency of the algorithm, but also improves the cancer classification accuracy.



Figure 5: Average test error rates at different sizes of peak subsets, selected by T-statistics and SVM-RFE, on Lung Cancer dataset

#### Computer Simulations Modeling Electrostatic Attraction of Nucleosomal DNA Mediated by Charged Histone Tails

The fundamental unit of DNA packed in chromatin in eukaryotic cells is the nucleosome core particle (NCP), composed of a histone protein octamer core with DNA wrapped around it and flexible positively charged histone tails protruding out. The net negatively charged NCPs also show counterion induced aggregation *in vitro*. DNA-histone tail interactions are important for the mechanisms which are responsible for transcription and replication. Molecular dynamics (MD) computer simulations of charged tail – DNA interactions in systems mimicking NCPs are performed modeling simplified systems of the NCP as flexible polycationic histone tails attached to the negatively charged spherical particle, with a dielectric model of the aqueous solvent. The size, charge and distribution of the tails relative to the core were built mimicking real NCP. Results are in good agreement with experimental data. More detailed mechanisms of the histone tail – DNA binding and dynamics have been obtained from all-atom MD simulations (including water) comprising three parallel DNA oligomers and fragments of the H4 histone tail We found correlation of the DNA-DNA distance with the presence and binding of the histone

tail between the DNA molecules. Future comparison of the results for unmodified and modified (reduced positive charge on the tails corresponding to transcriptionally active states of chromatin) could help to understand molecular mechanisms behind epigenetic control of transcriptional regulation.



Figure 6: Initial configuration of NCPs in dielectric continuum MD simulations (left); aggregation in the presence of  $Mg^{2+}$  (middle); DNA - DNA interaction mediated by positively charged peptide histone tails from all atom MD (water not shown) (right).

#### BioWare: A Warehouse of Biological Data

We build a biological data integration system, BioWare, that is build on XML data model and supports novel query optimization techniques. We first generate a relational schema. Second, we transform data from various sources to XML format by creating valid XML documents of the corresponding data. Third, we parse XML documents created from the previous step and load them into tuples of relational tables in a standard commercial DBMS (in our case, SQL Server). We support a visual XML-based query interface. Through the interface, DTD/schema of stored XML documents are displayed, and users can formulate queries by clicking the relevant data elements and entering conditions. Such queries are transformed into SQL queries over the corresponding relational data. The results are formatted as XML documents and returned back to the user or passed to another application for further processing. The novelties of our system are as follows: it creates an illusion of a fully XML-based data management system as the underlying relational system remains hidden from the users; the storage structure does not need to be maintained when the structure of remote sources evolve; it allows bioinformatics researchers to concentrate on gathering and analysis of data and relieving them of the burden of learning new query languages; it expedites query processing greatly; our approach provides us with the flexibility to ``plug" it on top of any existing optimization technique for processing biological data in relational environment; there does not exist any additional cognitive overhead to the users while they formulate their queries using the GUI; Finally, our optimization techniques noticeably improve the performance of XML query execution.

#### Neural Systems Modeling with functional MRI

The project seeks to find a general framework for modeling interactions among neural populations involved in sensory or cognitive tasks and thus studying brain disorders by mimicking lesion studies. BIRC has developed techniques to analyze brain connectivity using Independent Component Analysis and Graphical Models. These techniques have applied to analyze data obtained from language and memory experiments and from normal as well as patients.



Figure 7: Neural systems derived form (a) normal subject and (b) stroke patient.

### High Performance Computing Technologies for Computational Biology

A High Performance Computing (HPC) system for analysis and visualization of biological and clinical data has been developed. Various parallel algorithms for computational biology have been studied and implemented on a cluster of multiple compute nodes, using an industrial standard message passing package, MPI; for examples, BLAST for searching similar sequences, dynamic programming for local alignment, ClustalW for multiple sequence alignment, hierarchical clustering and supervised machine learning algorithms for gene expression analysis, and homology modelling for protein secondary structure prediction. The execution of these parallelised programs on centre's Alpha SC-45 Supercomputer has shown a great improvement of speed and accuracy, due to the methods used in maximizing the utilisation of the computing resources.



Figure 8: BIRC has developed a parallel algorithm for protein structure prediction on its Alpha supercomputer.

### Toolkit for First Phase Clinical Trial Design

In collaboration with the National Cancer Center (NCC), Singapore, and University of Sheffield, we have been developing novel techniques for 1<sup>st</sup> phase clinical trial design. A window-based software system called CDT explorer is developed as well and is currently under NCC's evaluation.

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Figure 9: A toolkit for first phase clinical trial design

#### Feature Selection in Gene Expression Data

Gene expression data from DNA microarrays is a great source for scientists to understand the simultaneous activities of thousands of genes. One of the characteristics of gene expression data is that the number of genes (often more than 1000) far exceeds the number of samples (often less than 100). Furthermore, it has been shown that the large proportion of the genes in a microarray are not relevant to the discrimination of disease types Hence the identification of those important genes that have the most discriminate power is of considerable interest to both biologists and medical professionals, where the research can be concentrated on small set of those important genes. In BIRC, we implemented a algorithm inspired by wrapper approach and LS-SVM to our feature selection problem. We implemented a fast Leave-One-Out (LOO) Guided Feature Selection (LGFS) implementation address this problem. The classification accuracies were notably increased while the number of genes required was drastically decreased to just a few and the timely improved as compare to other implementations.

#### *In silico* Modelling of Hormone-regulated Gene Expression Network

The molecular effect of estrogen and progesterone are reflected by their receptor regulated gene expression. It is, therefore, important to identify the direct target genes of estrogen and progesterone receptors and the down-stream targets of these genes. A list of potential progesterone-regulated human genes consists of about 200 (microarray data), but not all of them are regulated by progesterone receptor directly. If a particular gene is progesterone-regulated, its product may, in turn, regulate expression of another gene, and so on. This project is aimed at reconstruction of such "progesterone-regulated" gene expression network for clinical trial and cancer counteraction. Existing information on progesterone receptor DNA-specificity allows us to define potential PRE target genes using complete human genome sequence and different methods for statistical prediction of gene regulatory elements (promoters, PRE binding sites). Then, using gene description databases (OMIM, GeneOntology), it would be possible to establish entire pathway of hormone-induced effect on gene expression. This project is to define direct target genes for progesterone receptor on basis of experimental microarray data, to develop a method and the corresponding software for prediction of new potential progesterone-regulated human genes, to create progesterone-regulated gene expression network, and finally to extend described results over the whole family of steroid hormones.

### V. STAFF PUBLICATIONS AND IMPACT FACTOR

### Books

No.	Books
1	Limsoon Wong, editor, "The Practical Bioinformatician", Imperial College
	Press, London, December 2003. (In press.)
2	Louxin Zhang, Limsoon Wong, editors, "Selected Topics in Post-Genome Knowledge Discovery", <i>Singapore University Press</i> , Singapore, September 2003. (In press.)
3	J. C. Rajapakse and L. Wang, (eds.) "Neural Information Processing: Research and Development", <i>Springer - Verlag</i> , March 2004, ISSN 1434-9922, pp. 478.
4	Feng Chu and Lipo Wang, "Bio-medical data mining using neural networks", in <i>Encyclopedia of Data Warehousing and Mining</i> , John Wang (Editor), Information Sciences Publishing, 2005.

### **Journals**

No.	Journals
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3	Korolev, N.; Lyubartsev, A. P.; Laaksonen , A.; & Nordenskiöld, L. "A
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9	J. C. Rajapakse and M. N. Nguyen, "General framework for two-stage
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10	J. C. Rajapakse, "Book review: adaptive blind signal and image processing,"
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11	Guang-Bin Huang, "Learning Capability and Storage Capacity of Two-Hidden-
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10	no. 2, pp. $2/4-281$ , 2003.
12	Wu, Z. K., Lin, F. and Sean, H. S., Topology Preserving Voxelisation of Detional Degion and NUDDS Curves" Computing & Curves
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19	Jinyan Li, Huiqing Liu, See-Kiong Ng, Limsoon Wong, "Discovery of
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56	Zonglin Zhou, Chee Keong Kwoh, Stan Z. Li, "The Nearest Feature Midpoints -
	a Novel Approach for Pattern Classification", Accepted to be published in
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57	SH. Tan, Z. Zhang, SK. Ng, "ADVICE: Web Service for Automated Detection
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# **Book Chapters**

No.	Book Chapters
1	Feng Chu and Lipo Wang, "Gene expression data analysis using support vector
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	Asia-Pacific Bioinformatics Conference (APBC2004), Dunedin, New Zealand,
	18 - 22 Jan 2004.
33	M. P. Rajapakse, J. Tan, and J. C. Rajapakse, "Color channel encoding with
	NMF for face recognition, <i>IEEE International Conference on Image</i> Processing (ICIP04) Singapore October 2004 (accepted)
34	M. N. Nguyen and J. C. Rajapakse. "Two-stage support vector machines to
01	protein relative accessibility prediction," <i>IEEE Symposium on Computational</i>
	Intelligence in Bioinformatics and Computational Biology, San Diego, 2004
	(accepted)
35	X. Yang, and J. C. Rajapakse, "Graphical approach for motif recognition in
	DNA sequences," IEEE Symposium on Computational Intelligence in
	<i>Bioinformatics and Computational Biology</i> , San Diego, 2004 (accepted)
36	K. Duan and J. C. Rajapakse, "A variant of SVM-RFE for gene selection in
	cancer classification with expression data," <i>IEEE Symposium on Computational</i>
	Intelligence in Bioinformatics and Computational Biology, San Diego, 2004
	(accepted)

No.	Conference
37	G. Pang and J. C. Rajapakse, "Inferring neutral evolution from Parkinson's
	disease genes," IEEE Symposium on Computational Intelligence in
	Bioinformatics and Computational Biology, San Diego, 2004 (accepted)
38	S. L. Ho and J. C. Rajapakse, "High sensitive technique for translation initiation
	site detection," IEEE Symposium on Computational Intelligence in
• •	Bioinformatics and Computational Biology, San Diego, 2004 (accepted)
39	J. C. Rajapakse, D. Srinivasan, M. J. Er., GB. Huang, and L. Wang, "Excerpts
	of research in brain sciences and neural networks in Singapore," International
	<i>Joint Conjerence on Neural Networks (IJCNN2004)</i> , Budapest 2004, pp. 509-
40	X Zhang and L C Rajanakse "Graphical models for brain connectivity from
ŦV	functional imaging data" International Joint Conference on Neural Networks
	(LICNN2004). Budapest 2004. pp. 531-536.
41	K Yang and I C Rajanakse. "An exploratory approach to modeling effective
••	connectivity." <i>IEEE International Symposium on Biomedical Imaging</i> .
	Arlington, Virginia, April 2004, pp. 844-847
42	Jinyan Li, Huiqing Liu, Limsoon Wong, "Use of Built-in Features in the
	Interpretation of High-dimensional Cancer Diagnosis Data", Proceedings of
	2nd Asia Pacific Bioinformatics Conference, pages 6774, Dunedin, New
	Zealand, January 18-22, 2004.
43	SHU Jian Jun, Ouw Li Shan, 2004, "Pairwise alignment of DNA sequence
	using hypercomplex number representation", The 1st International Conference
	From Scientific Computing to Computational Engineering, Athens, Greece, 8–
4.4	10 September 2004, Greece.
44	Du, Z. H. and Lin, F., Using Blocks+ Database in Needleman-wunsch Algorithm" The 23rd International Conference of the North American Fuzzy
	Information Processing Society (NAFIPS 2004) Canada June 2004
45	Du Z H and Lin F. "Improvement of the Needleman-Wunsch Algorithm".
	Fourth International Conference on Rough Sets and Current Trends in
	Computing 2004 (RSCTC 2004), Sweden, June 2004.
46	Du, Z. H. and Lin, F., "Using Prior Knowledge for Sequence Alignment, The
	8th World Multiconference on Systemics", Cybernetics and Informatics (SCI
	2004), USA, Accepted for Publication in 2004
47	Qi, Y. T. and Lin, F., "mpiPSSP: Parallelized Protein Secondary Structure
	Prediction", IASTED International Conference on Biomedical Engineering
	( <i>BioMED 2004</i> ), Canada, Accepted for publication in 2004
48	Yan, R. A., Cheang, P. and Lin, F., "Spline-based Volumetric Modeling and
	Printing for Bioceramic Implants", (VRCAI 2004), Singapore, 16 – 18 June
40	
49	Lin, F., Du, Z. H. and Qi, Y. T., "HPTC for Sequence Analyses in
	DIOIIIIOIIIIaucs, <i>HP</i> -CASI 2004, Australia, 28-31 March 2004
50	Qi, Y. T. and Lin, F., "Parallelized Protein Secondary Structure Prediction",
	The 3rd International Conference on Machine Learning and Cybernetics
	(ICMLC 2004), China, 26-29 August 2004

No.	Conference
51	Yan, R. A., Cheang, P. and Lin, F., "Customized Body Parts: Computerized and
	Printing of Bioceramic Based Porous Scaffold for Clinical Implants", <i>The 6th</i>
	Asia Symposium on Biomedical Materials (ASBM 2004), China, 19-22 July
52	2004. Narendra S. Chaudhari, and Nirmal Dagdee, "Turing Machine Simulation using
32	Hard-limiter Neurons" International Joint Conference on Neural Networks
	( <i>IJCNN 2004</i> ), Budapest, Hungary (26-29 July 2004).
53	Jinmiao Chen, and Narendra S. Chaudhari, "Improvement of Bidirectional
	Recurrent Neural Network for Learning Long Term Dependencies",
	International Conference on Pattern Recognition (ICPR-2004), Cambridge,
54	U.K. (23-26 Aug. 2004). Wajgua Liu B. Sahmidt "A Canaria Parallal Pattern based System for
54	Bioinformatics", <i>Proceedings of Euro-Par'04, 2004</i> , to appear.
55	Tong Liu, B.Schmidt, "Parallel RNA Sequence-Structure Alignment",
	Proceedings of IPDPS'04, IEEE, 2004
56	Chen Chunxi, B. Schmidt, "Performance Analysis of Computational Biology Applications on Hierorchical Crid Systems", Proceedings of CCCrid(04, IEEE
	2004
57	SCH Wong, Y Cai, et al, "Knowledge enhanced cellular visualization using 3D
	confocal images", Focus on Microscopy 2004, Philadelphia, USA, 2004.
58	Huiging Liu, Jinyan Li, Limsoon Wong, "Selection of Patient Samples and
	Genes for Outcome Prediction", IEEE Bioinformatics Proceedings (CSB2004),
	Stanford, CA, August 2004.
59	Rickard Liow S. J., Tham W. Lim W.E.H. Ng S.E.S. Ho G. L., Tan K.,
	"Neurolinguistic Correlates in Chinese-English Bilingual Biscriptals: An fMRI
	Study", American Association for Applied Linguistics (AAAL), Portland,
	Oregon, 1-4 May 2004.
60	Su Li, B Lu, and Y Cai, "VR-enhanced Modeling and Visualization of Cystine
	Knot Proteins", ACM SIGGRAPH International Conference on Virtual Reality
	Continnum and its Applications in industry, VRCAI 2004, 15-18 Jun 2004.
61	Jianhui Zhao* Ling Li* CKKwoh "A Model-based Approach for Human
	Motion Reconstruction from Monocular Images", 2nd International Conference
	on Information Technology for Application (ICITA 2004).
62	Zhang Yan*, Jia Yiyu*, C.K.Kwoh, Liu Jianjun*, "Comparison of four
	algorithms for haplotype inference problem", 2nd RECOMB satellite workshop
	on computational methods for SNPs and Haplotypes, 2004, pp. 113-123
63	YY Jia*, Y Zhang*, C.K.Kwoh, V Gopalan*, "Length Distributions Of Exons
	And Introns Imply The Evolutionary Constraints For Exon/Intron Length",
	2004)
64	ZL Zhou*, C.K.Kwoh, "The SVM Classification of Light Regulated
	Arabidopsis Genome Expression Profiles," Biotech China 2004.

No.	Conference
65	YY Jia*, Y Zhang*, C.K.Kwoh, M K Sundaram*, "Intron/exon: which one tells
	us more about coding of life? - evidence from statistical analysis of length
	distribution", Genomic Signal Processing and Statistics (GENSIPS 2004).
66	Y Zhang*, JJ Liu*, C.K.Kwoh, YY Jia*, "The sensitivity and rationality of
	pairwise linkage disequilibrium measures - a practical analysis," Genomic
	Signal Processing and Statistics (GENSIPS 2004).
67	ZL Zhou*, C.K.Kwoh, "An evolutionary lineage for intron loss/gain in five
	eukayotic genomes," The Fourth International Conference on Bioinformatics of
	Genome Regulation and Structure (BGRS'2004).
68	Y Zheng*, C.K.Kwoh, "Dynamic Algorithm For Inferring Qualitative Models
	of Gene Regulatory Networks," IEEE Computer Society Bioinformatics
	Conference, CSB2004.
69	Zhao Ying*, C.K.Kwoh, "Fast Leave-one-out Evaluation and Improvement on
	Inference for LS-SVMs," International Conference on Pattern Recognition
=0	(ICPR), 2004
70	Zhou Zonglin <sup>*</sup> , C.K.Kwon, <sup>*</sup> The Pattern Classification Based on the Nearest
	Peature Midpoints, International Conference on Pattern Recognition (ICPR),
71	2004 Vun Zhang * C.K.Kuuch "Deconstructing Declean Naturals from Noisy Cone
/1	Function Date " Fighth International Conference on Control Automation
	Production and Vision (ICARCV 2004)
72	Vang Song* S B Souray "BioDiff: An Effective East Change Detection
12	Algorithm for Genomic and Proteomic Data "Proceedings of the 13th ACM
	International Conference on Information and Knowledge Management (ACM
	CIKM 2004).
73	L. Shen and E. C. Tan. "Gene Selection for Cancer Classification from
	Microarray Data using PLS-RLSC", 1 <sup>st</sup> International BioEngineering
	Conference 2004 (IBEC 2004), 8-10 Sep 2004, Singapore.
74	Shen L. and Tan E.C., "PLS and SVD based Penalized Logistic Regression for
	Cancer Classification using Microarray Data", APBC 2004, in press.
75	Shen L. and Tan E.C., "Nonlinear Kernel MSE Methods for Cancer
	Classification", <i>ICARCV 2004</i> , accepted.
76	Shen L. and Tan E.C., "Kernel PLS-SVM and Kernel SVD-SVM for Cancer
	Classification using Microarray Data, <i>ICMLC 2004</i> , accepted.
//	Sheh L. and Tah E.C., Efficient Algorithm for Gene Selection using PLS- RISC" <i>BGRS 2004</i> accepted
78	R Yu and E C Tan "Application of Time-Frequency Analysis in Exon
70	Classification". 10th International Symposium On Integrated Circuits. Devices
	& Systems (ISIC 2004), 8-10 Sep 2004, Singapore.
79	Bing Liu, Chunru Wan and Lipo Wang, "Unsupervised gene selection via
	spectral biclustering," International Joint Conference on Neural Networks,
	Budapest, July, 2004.
80	C. W. Ong and J. C. Tay, "A Robust Rule-based Event Management
	Architecture for Call-Data Records," accepted for publication in the Eighth
	International Conference on Knowledge-Based Intelligent Information and
	Engineering Systems 2004.

No.	Conference				
81	Ho Nhu Binh and Tay Joc Cing, "GENACE: An Efficient Cultural Algorithm				
	for solving the Flexible Job-Shop Problem", In Proceedings of the IEEE				
	Congress on Evolutionary Computation 2004, pp1759-1766.				
82	Tay Joc Cing and Djoko Wibowo, "An Effective Chromosome Representation				
	for Evolving Flexible Job Shop Schedules", In Proceedings of AAAI Genetic				
	and Evolutionary Computation 2004, pp210-221.				
83	Duch W, Blachnik M, "Fuzzy rule-based systems derived from similarity to				
	prototypes", Lecture Notes in Computer Science, ICONIP 2004, submitted				
	5/04, (in print).				

### Impact Factors

Impact factors for Years 2003-2004 (years with available data):

	2003 - 2004
Total impact	114.385
Number of papers	40
Number of Staff*	23
Number of Academic Staff	23
Impact factor per paper	2.86
Impact factor per Staff*	4.97
Impact factor per Academic Staff	4.97

\*Staff includes both academic and research staff except research students. Research staff includes RF, RA and PO, regardless of the funding source.

### VI. POSTGRADUATE STUDENTS COMPLETED

### PhD Students

No	Name	Supervisor	Previous	Year	Placement
			degree	Graduated	
1	Dr Tan Choong	A/P Jagath	PhD Eng,	2003	Research Fellow,
	Leong	Rajapakse	NTU		BioInformatics
					Research Center
					Nanyang
					Technological
					University, Singapore
2	Dr. R. G. N.	A/P Jagath	PhD Eng,	2004	Senior Lecturer,
	Meegama	Rajapakse	NTU		Department of
					Computer Science
					University of
					Sabaragamuwa, Sri
					Lanka

### **MSc** Students

No	Name	Supervisor	Previous	Year	Project Title
			degree	Graduated	
1	Yang Kanyan	A/P Jagath	MSc	2004	Brain connectivity
		Rajapakse			with ICA
2	Jia Yiyu	A/P Kwoh	MSc	2004	Statistical analysis
		Chee Keong			of intron phases at
					the splice sites of
					eukaryotic genes
3	Zhao Ying	A/P Kwoh	MSc	2004	Probalitistic based
		Chee Keong			algorithm to analyse
					gene expression
					data

### **VII. PRESTIGE**

### **Professional Activities**

No.	Title	Staff Name	Activity
1	Senior Member	A/P Jagath	Institute of Electrical and Electronic
		Rajapakse	Engineers (IEEE)
2	Governing Board	A/P Jagath	Asia-Pacific Neural Network Assembly
	Member	Rajapakse	(APNNA)
3	Governing Board	A/P Jagath	Asia Pacific Neural Network Assembly
	Member	Rajapakse	(APNNA): Promote research and organize
			activities in neural information
			processing; organization of International
			Conference on Neural Information
			Processing (ICONIP)
4	Member,	A/P Jagath	The International Association of Science
	Technical	Rajapakse	and Technology for Development
	Committee on		(IASTED) (2003 - 2006): Responsible for
	Neural Networks		advisement on the planning and the
			organization of IASTED activities such as
			conferences, meetings, and publications.
5	Member,	A/P Jagath	Knowledge Engineering and Discovery
	International	Rajapakse	Research Institute, Auckland University
	Advisory Board		of Technology, Sept 2002 - present: Make
			recommendations to the Institute and the
			Institutions in New Zealand in terms of
			directions of research, links with industry,
			integrating international research groups
			from different countries, sharing
			information and developing joint research
			projects.
6	Member, ICA	A/P Jagath	Organization of annual conference on
	Steering	кајаракѕе	Independent Component Analysis (ICA)
7	Committee	A/D Wong Lim	Ton Kah Kao DSTA Defense Science
/	Mombor	A/P wong Lini	Award Committee (2002)
8	Management	A/P Wong Lim	National University of Singapore Institute
0	Committee	Soon	of Engineering Science (2004-2005)
9	Board of	A/P Wong Lim	Association of Asian Societies for
_	Directors	Soon	Bioinformatics (2003)
10	Board of directors	A/P Wong Lim	Molecular Connections, Bangalore, India
		Soon	
11	SAB	A/P Wong Lim	geneticXchange inc, California, USA
		Soon	
12	Chairman	A/P Wong Lim	A*STAR Tech Scan Panel on Information
		Soon	Management
13	Member	Dr Salil K Bose	New York Academy of Sciences

# **Conference** Activities

No.	Title	Staff Name	Activity
1	Member,	A/P Jagath	First IEEE Symposium on Computational
	Technical	Rajapakse	Intelligence in Bioinformatics and
	Program		Computational Biology, San Diego,
	Committee		October, 2004
2	Member,	A/P Jagath	4th Symposium of Independent
	International	Rajapakse	Component Analysis and Blind Signal
	Program		Separation (ICA2004), Granada, Spain,
	Committee		2004.
3	Member,	A/P Jagath	3 <sup>rd</sup> Symposium of Independent Component
	International	Rajapakse	Analysis and Blind Signal Separation
	Program		(ICA2003), Japan, 2003.
	Committee		
4	Member, Program	A/P Jagath	7 <sup>th</sup> IASTED International Conference on
	Committee	Rajapakse	Computers, Graphics, and Imaging,
	Member		CGIM 2004, August 2004, Hawaii, USA.
5	Member, Program	A/P Jagath	6 <sup>th</sup> IASTED International Conference on
	Committee	Rajapakse	Computers, Graphics, and Imaging,
	Member		CGIM 2003, August 2003, Hawaii.
6	Program	Asst/P	5th International Conference on Web-Age
	Committee	Vivekanand	Information Management (WAIM'2004)
		Gopalkrishnan	

### Journal Activities

No.	Title	Staff Name	Activity		
1	Guest Editor	A/P Jagath Rajapakse	Special Issue on "Softcomputing in		
			Bioinformatics", Softcomputing,		
			March 2004 issue		
2	Editorial Board	A/P Jagath Rajapakse	International Journal of Computational		
	Member		Intelligence		
3	Editorial Board	A/P Jagath Rajapakse	Neural Information Processing -		
	Member		Letters and Reviews: Review at least		
			four letters and reviews per year and		
			advise Editor-in-Chief on their		
			publication in the journal		
4	Guest Editor	Ast/P Sourav	Special Issue, Data and Knowledge		
		Bhowmick	Engineering Journal, Elsevier Science		
5	Associate Editor	A/P Wang Lipo	IEEE Transactions on Neural		
			Networks, 2002 -		
6	Associate Editor	A/P Wang Lipo	IEEE Transactions on Evolutionary		
			Computation, 2003		
7	Editorial Board	A/P Wang Lipo	Soft Computing, 2002		
	Member				
8	Editorial Board	A/P Wang Lipo	Neural Information Processing –		
	Member		Letters and Reviews, 2003		

### Editorial Services

No.	Title	Staff Name	Activity	
1	Series Editor	A/P Wong Lim Soon	Advances in Bioinformatics &	
			Computational Biology (book series)	
			(2004)	
2	Editor	A/P Wong Lim Soon	International Journal of Information	
		-	Technology	
3	Managing Editor	A/P Wong Lim Soon	Journal of Bioinformatics &	
			Computational Biology	
4	Advisor	Dr Salil K. Bose	Editorial Board of Journal of Biology	
			Education, UK	

# Staff Awards

No.	Staff	Awards
1	A/P Wong Lim Soon	2003 FEER Asian Innovation Gold Award

### Student Awards

No.	Student / Supervisor	Awards
1	Ho Sy Loi /	50,000 yen by Japanese Bioinformatics Society for the work
	A/P Jagath Rajapakse	presented at GIW2003 Splice site detection with a higher-
		order Markov model implemented on a neural network.
2	Minh Nguyen Ngoc /	50,000 yen by Japanese Bioinformatics Society for the work
	A/P Jagath Rajapakse	presented at GIW2003: Multi-class Support Vector
	- • •	Machines for Protein Secondary Structure Prediction.

### VIII. PATENTS AND COMMERCIAL PRODUCTS

No.	Staff Name	Patents
1	Ast/P Fong Cheuk Ming	International patents filed by the Motorola IP Law
		Department in 1999-2000 for innovations
		incorporated into our Mobilepad <sup>TM</sup> range of
		handheld wireless communication products.
2	A/P Prasanna Kolatkar	The use of a fungal immunomodulatory protein, Fve,
		for immunotherapy, against allergy, virus infection
		and cancer.

No.	Staff Name	Commercial Products
1	Ast/P Sourav Bhowmick	Research in biological data integration has been
		adopted and implemented in the commercial product
		gRNA now marketed by Genvea BioSciences,
		Singapore (previously marketed by HeliXense Pte
		Ltd, Singapore)

### IX. COLLABORATORS

The centre brings together scientists and engineers, who are interested in bioinformatics modeling and computation, and fosters cross-disciplinary interactions among different schools at NTU to perform advanced research in bioinformatics. It also makes the necessary partnerships with other research and educational institutions, locally and abroad, to achieve its objectives.

No.	International Collaborators	
1	Brain Science Institute, RIKEN, Japan	
2	Knowledge Engineering and Discovery Research Institute (KEDRI),	
	Auckland University of Technology	
3	Bioimaging Centre, Whitehead Institute, Massachusets Institute of	
	Technology (MIT), USA	
4	Signal & Image Processing Group, Max-Planck-Institute of Cognitive	
	Neuroscience, Germany	
5	RMIT University, Melbourne, Australia	
6	Stockholm University, Sweden	
7	The Children's Hospital Research Foundation, Cincinnati Children's Hospital	
	Medical Centre, USA	
8	Department of Neurology, University of Freiburg, Germany	

No.	Local Collaborators	
1	BioInformatics Institute (BII)	
2	Genomic Institute of Singapore (GIS)	
3	Institute for Infocomm Research (I2R)	
4	National Neuroscience Institute (NNI)	
5	Singapore General Hospital (SGH)	
6	National Cancer Centre (NCC)	