Activities report from August 2012 to April 2013

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 $\begin{array}{c} \mbox{Project "Reusable Deep Neural Networks: Applications to Biomedical Data"} \\ (\mbox{PDTC/EIA-EIA}/119004/2010) \end{array}$

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Contents

1	Introduction	3
2	Introduction to deep learning	3
3	Visit to LISA lab3.1Input from Prof. Bengio3.2Activities and notes	3 3 5
4	Notes on existing software	5
5	Introduction to convolutional neural networks	7
6	Notes on UCI biomedical datasets	7
7	Notes on relevant conferences	8
A	Slides: Introduction to deep learning	10
в	Slides: Introduction to convolutional neural networks	14
С	Spreadsheet: Notes on UCI biomedical data sets	17
Re	eferences	19

1 Introduction

This report describes several activities I have undertaken since the beginning of my contract in August 2012 until the end of the project's first year, at the start of May, 2013. Each of the following sections addresses an individual activity. Activities are ordered more or less chronologically.

Besides the tasks described here, work related with the training of restricted Boltzmann machines (RBMs) and stacked auto-encoders is described in detail in two separate technical reports [1, 2].

2 Introduction to deep learning

My work in the project started in August 2012, with a review of introductory materials about deep learning, which included the first three sections of the 2009 article/book "Learning deep architectures for AI" by Bengio [4], as well as the 2010 review paper "Deep machine learning – a new frontier in artificial intelligence research" by Arel et al. [3].

Those readings allowed me to become acquainted with the concepts of shallow versus deep architectures, the motivations for the use of deep architectures (such as their inspiration from nature and their theoretical advantages in terms of efficiency), and the limitations associated with deep architectures until the breakthrough led by Hinton et al. [8] in 2006.

I prepared an overview of these topics and presented it in the project meeting of October 12, 2012. This presentation included a first list of some publicly available software implementations of deep learning models. It is included in Appendix A of this report.

3 Visit to LISA lab

In January 2013, for a period of four weeks, I visited the LISA machine learning laboratory¹ at the University of Montreal, headed by Prof. Yoshua Bengio. LISA is one of the most important research groups worldwide in the area of deep learning, routinely producing state-of-the-art research.

3.1 Input from Prof. Bengio

Prof. Bengio offered some comments of particular relevance to our project, as well as some feedback on the work carried out to date within the project, regarding the training of RBMs, which I have demonstrated to him. His comments are summarised in the following paragraphs.

Machine learning models in general need large amounts of training data. Often, there is not a lot of data available in biomedical applications, especially

¹See https://www.iro.umontreal.ca/rubrique.php3?id_rubrique=27&lang=en.

data annotated by experts. In order to train deep learning models aimed at biomedical applications, it would be important to have at least a large amount of non-labelled data, for unsupervised pre-training.

Computer vision is where deep learning excels the most. A drop in object classification error rate from about 30% to less than 16% has been recently achieved using deep convolutional nets, as reported by Krizhevsky et al. [9].

The unsupervised training of auto-encoders could offer an opportunity for the use of alternative cost functions, given that auto-encoders are trained to reconstruct their own inputs. Moreover, auto-encoders are much simpler to train than RBMs. These remarks by Prof. Bengio prompted our own work with auto-encoders, started by Luís Alexandre and continued by myself and Chetak Kandaswamy, as described in a separate technical report [2].

Regarding the unsupervised training of RBMs, division of the training data into mini-batches is important not only to avoid operations with very large matrices, but also in terms of efficiency. Using all the available training data at each training epoch (iteration) would be excessive, because we don't need to update the model's parameters precisely in the right direction at each epoch; a smaller amount of data is sufficient to update the parameters in the right general direction, and much less time-consuming. An analogy can be drawn with a person going from a point A to a point B in a number of steps: the person doesn't need to worry about moving precisely in the direction of point B at each step taken; a number of roughly precise steps will lead to B just the same.

A clarification regarding the sampling mechanism used during the training of RBMs: what we're using is so-called *block* Gibbs sampling, as opposed to Gibbs sampling "one bit at at time". Block Gibbs sampling allows to more efficiently explore the modes of the multi-dimensional data distribution, since all bits are samples in parallel. This is possible in *restricted* Boltzmann machines, but not in unrestricted ones.

On the subject of sampling from a trained RBM, in theory, when starting from a random visible vector, it is necessary to perform a large number of Gibbs sampling steps to obtain a good sample, like we did in our implementation. However, once this "burn in" is achieved, each new step, if done without restarting from a random vector, is enough to yield a good sample. In practice, if we start not from a random vector but from a training vector, we can assume that the "burn in" is already done and start drawing samples right away. These techniques can greatly speed up the generation of samples.

The fact that the type of RBM we've implemented is meant for use with binary data doesn't preclude its use with real-valued data scaled between 0 and 1. Our discouraging results with real-valued data, in particular with the Iris data set, could be due to the choice of learning rate. In some cases it is important to adjust the learning rate throughout the training. (Later, in our work with auto-encoders, we have implemented adaptive learning rates.)

In case we pursue experiments with RBMs, we should now focus on using more efficient code, so that we may use data sets with large numbers of features and examples.

3.2 Activities and notes

During my visit, I did a more in-depth reading of some parts of Prof. Bengio's 2009 book [4], in particular the sections on neural networks for deep architectures (Section 4) and on energy-based models and Boltzmann machines (Section 5). Prof. Bengio's lecture notes "Introduction to Gradient-Based Learning"² proved to be very useful as an introduction to gradient descent learning methods. The material I read on convolutional neural networks later helped me to prepare the presentation described in Section 5.

I spent some time also with the previously mentioned paper by Krizhevsky et al. [9], which reports recent developments on the use of convolutional neural networks, as well as with the pre-print of a new review on deep learning by Bengio et al. [5], which is now publicly available. While not precluding the reading of the 2009 book, this article contains a lot of information on recent developments and research directions.

In order to demonstrate my Matlab implementation of RBM training algorithms to Prof. Bengio, I spent some time tidying up its experimental scripts and collecting results into a report. This ultimately became the technical report on experiments with RBMs being submitted separately [1].

I read some introductory materials on the Python programming language, the NumPy numerical library, as well as Theano, a Python library that facilitates the development of deep learning models, while giving the option of performing their training on one or more graphical processing units (GPUs). The LISA lab was the ideal place to become acquainted with these programming technologies, as Theano has been developed by researchers at LISA and is extensively used in their work.

Throughout the visit, I collected some notes on various software implementations of deep learning models that are publicly available. Those notes are presented in Section 4.

I had the chance to attend a seminar presented by a leading researcher of the Canadian company D-Wave Systems Inc.³, on the use of quantum computing for training deep learning models. This company specialises in the development and commercialisation of quantum computers, an emerging field with potential deep learning applications. I attended also a brief "tea talk" about a paper co-authored by Prof. Pedro Domingos, a Portuguese researcher based in the U.S. who works with deep architectures [6].

4 Notes on existing software

The following is a list of some software implementations of deep learning models that are publicly available, collected during my introductory readings and also during my visit the LISA lab. In each case, the group or researcher responsible for the software is given (with a link to the relevant web page), as well as the

²See http://www.iro.umontreal.ca/~bengioy/ift6266/H12/html/gradient_en.html.

³See http://www.dwavesys.com.

programming language and relevant libraries used, and the models that are implemented.

1. LISA lab

Deep Learning Tutorials http://deeplearning.net/tutorial/ Python / Numpy / Theano

- logistic regression
- multilayer perceptrons
- deep convolutional networks
- autoencoders, denoising autoencoders
- stacked denoising autoencoders
- restricted boltzmann machines
- deep belief networks
- 2. LISA lab

```
Wiki, "fundamental research projects"
http://www.iro.umontreal.ca/~lisa/twiki/bin/view.cgi/Public/
C++ / PLearn
```

- deep belief networks
- stacked autoassociators
- 3. Rasmusberg Palm

DeepLearnToolbox https://github.com/rasmusbergpalm/DeepLearnToolbox Matlab

- deep belief networks
- stacked autoencoders
- convolutional neural networks
- convolutional autoencoders
- vanilla neural networks
- 4. Ruslan Salakhutdinov, Geoff Hinton

Training a deep autoencoder or a classifier on MNIST digits [7] http://www.cs.toronto.edu/~hinton/MatlabForSciencePaper.html Matlab

- restricted boltzmann machines
 - binary hidden and binary visible
 - Gaussian hidden and binary visible
- deep autoencoders
- deep belief networks ?

5. Ruslan Salakhutdinov

```
Learning Deep Boltzmann Machines
http://www.utstat.toronto.edu/~rsalakhu/DBM.html
Matlab
```

• deep boltzmann machines

```
6. Hugo Larochelle
Efficient Learning of Deep Boltzmann Machines [10]
an enhancement of 5
http://www.dmi.usherb.ca/~larocheh/code/dbm_recnet.tar.gz
Matlab
```

• deep boltzmann machines

```
7. Andrej Karpathy
matrbm
a simplified version of 4
http://code.google.com/p/matrbm/
Matlab
```

- restricted boltzmann machines
- deep belief networks (of stacked RBMs)

5 Introduction to convolutional neural networks

Following up on my visit to the LISA lab, I prepared an introduction to convolutional neural networks, focusing on the motivation for their use, the main differences from traditional networks, the concepts of shared weights and multiple feature maps, down-sampling layers, and a description of the LeNet-5 model. This introduction was presented in the project meeting of February 22, 1013 and is included in Appendix **B** of this report.

6 Notes on UCI biomedical datasets

In order to form an idea of the type of biomedical data that we could use in our experiments while relying only on CPU power (as opposed to using GPUs), I searched the Machine Learning Repository maintained by the University of California - Irvine (UCI)⁴ for data sets that fulfilled a number of characteristics, namely: being life sciences related; being frequently and recently used; being appropriate for classification learning; and being neither too small (less than 1000 examples) nor too big (say below 10000 examples).

A spreadsheet gathering the collected information on 62 available life sciences data sets is included in Appendix C. The data sets are ordered by decreasing number of papers citing them. This number of citations, as well as the range of

⁴See http://archive.ics.uci.edu/ml/index.html.

dates of those citations, provides a measure of how popular and recently used each data set is.

Taking into account the characteristics we desired, the five data sets highlighted in yellow seemed to be the most interesting ones, namely: Mushroom data; Splice-junction gene sequence data; Abalone data; Thyroid disease data; and Yeast data. These findings were discussed in the project meeting of March 15, 2013. We have subsequently used two of these data sets in our experiments with auto-encoders.

7 Notes on relevant conferences

I gathered in the table shown below information on conferences that are potentially interesting for publication of our work. Conferences are categorised into machine learning (ML), computer vision (CV), and biomedical engineering (BME). This list was discussed in the project meeting of April 19, 2013, but it should be kept up to date.

Deadline	Conference			ML	CV	BME	Notes
2012-11-10	ISBI	2013				x	
2012-11-15	AISTATS	2013		x			(1)
2012-11-15	CVPR	2013		x	x		IEEE conference.
2012-12-07	ESANN	2013		x			
2013-01-15	ICLR	2013		x			(1)
2013-02-04	EMBC	2013				x	
2012-10-01 2012-12-15 2013-02-15	ICML	2013		23 - x			(2)
2013-03-01	<u>IJCNN</u>	2013		1 - x			
2013-04-07	ICANN	2013		6 - x			
2013-04-12	ICCV	2013			x		
2013-04-19	GCPR	2013	Germany	8 - x			
2013-04-22	ECML/PKDD	2013	Czech Republic	7 - x			(3)
2013-04-24	<u>BMVC</u>	2013	UK		x		
2013-04-30	PReMI	2013	India	2 - x			
2013-05-11	ALT	2013	Singapore	x			
2013-05-13	<u>UKCI</u>	2013	UK	x			
2013-05-16	<u>ICNC</u>	2013	China	4 - x			IEEE conference.
2013-05-24	IDEAL	2013	China	x			
2013-05-31	<u>AI*IA</u>	2013	Italy	x			
2013-05-31	<u>NIPS</u>	2013	USA	17 - x			
2013-06-01	<u>ICETET</u>	2013	India	7 - x			
2013-06-15	CIARP	2013	Cuba	4 - x			
2013-06-15	ICONIP	2013	South Korea	5 - x			Bengio as plenary speaker.
2013-06-15	PRIA	2013	Russia	x	x		
2013-09-25	<u>ICPRAM</u>	2014	France	x			
2013-12-20	ICPR	2014	Sweden	11 - x			

Notes:

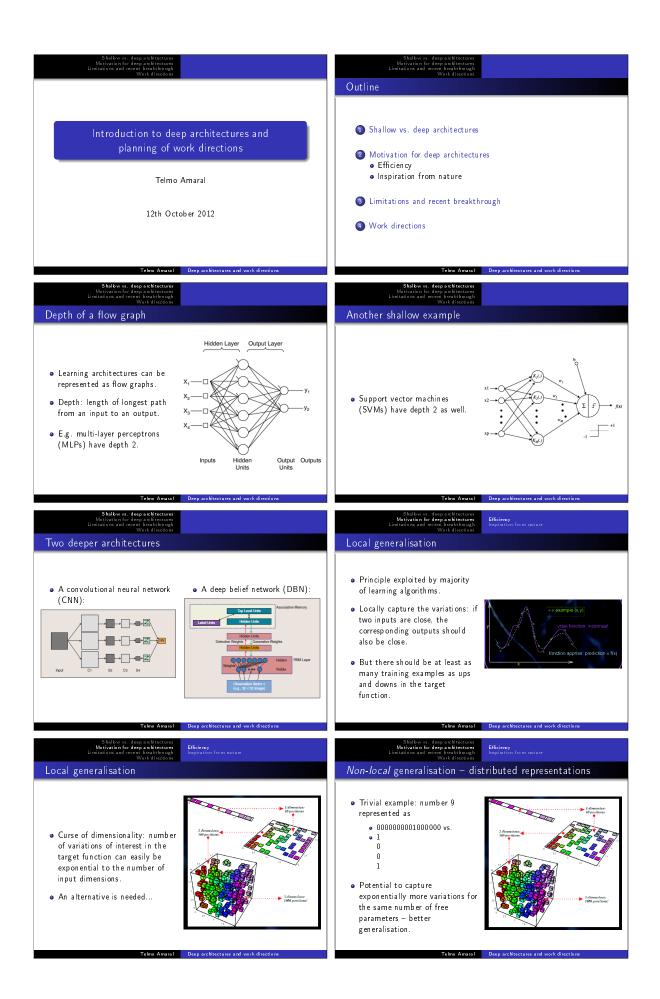
Numbers next to x's are $% \left({{{\rm{Field}}}} \right)$ Field Ratings from Microsoft Academic Search

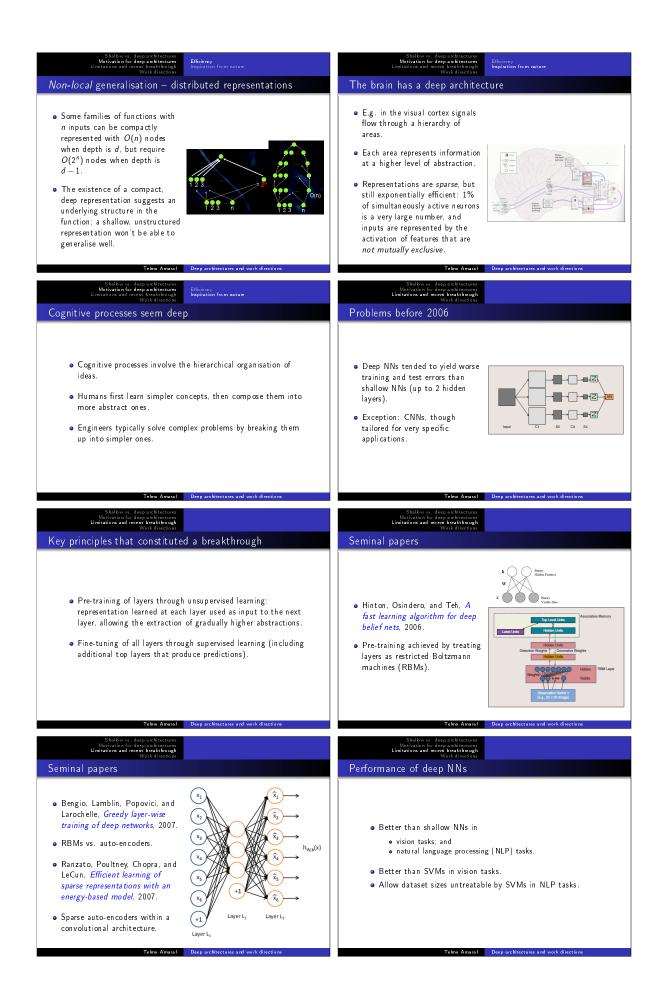
(1) AISTATS may not be very relevant, because its former Learning Workshop now became a separate conference, ICLR.

(2) ICML 2013 had three submission / reviewing cycles. Next year there may be even more. The idea seems to be to make the conference work also a journal.

(3) ECML/PKDD 2013 accepted submissions also for a new "journal track": papers could be submitted to one of two journals and, if accepted, would receive a presentation slot at the conference.

A Slides: Introduction to deep learning





Shallow vs. deep architectures Motivation for deep architectures Limitations and recent breakthrough Work directions

Some available software

- Rasmus Berg Palm's DeepLearn Toolbox, a Matlab deep learning toolbox, including DBNs; stacked and convolutional auto-encoders; CNNs and vanilla NNs.
 Hugo Larochelle's MLPython, a Python machine learning
- Hugo Larochelle's MLPython, a Python machine learning library, which can be used for deep learning research, featuring RBMs and auto-encoders.
- Ruslan Salakhutdinov's and Geoff Hinton's Matlab code for training a deep auto-encoder made of stacked RBMs. Andrej Karpathy's matrbm, simpler Matlab code for the same purpose.
- Ruslan Salakhutdinov's Matlab code for learning Deep Boltzmann Machines (DBMs, an alternative to DBNs). Hugo Larochelle's Matlab code for efficient learning of DBMs (apparently a continuation of the same work).

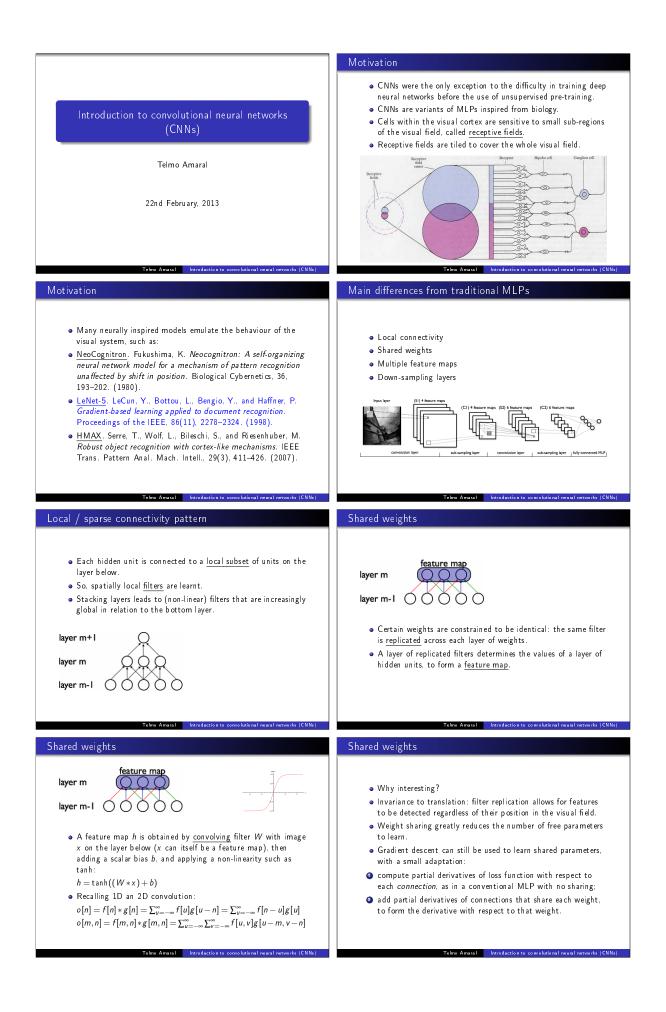
Snahow vs. otespanet Motivation for deep architectures Limitations and recent breakthrough Work directions

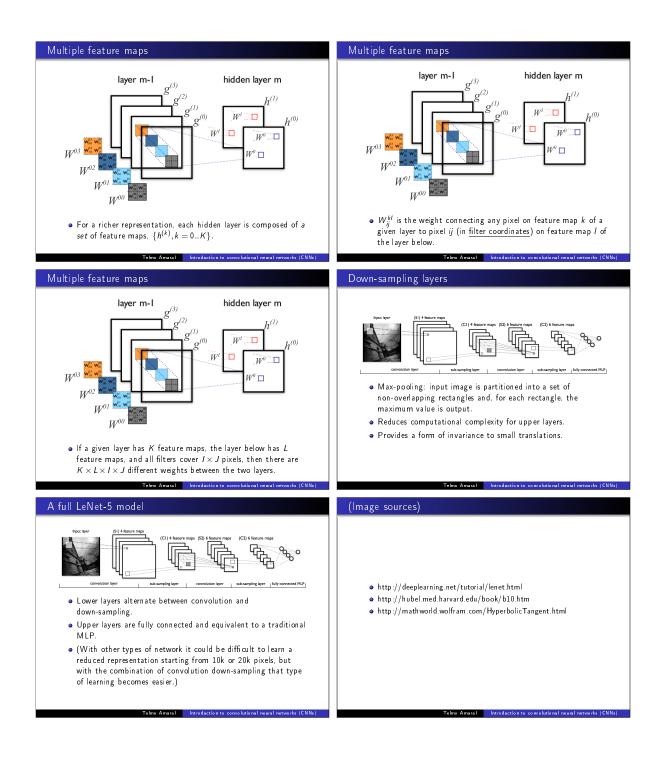
Main directions of work

- Use existing toolboxes such as MLPython and DeepLearn Toolbox to test DNNs with different types of building blocks (e.g. RBMs and auto-associators) and the more traditional risk functionals (e.g. MSE and cross-entropy).
- Develop our own implementation of DNNs, in order to experiment with risk functionals based on more sophisticated principles (e.g. error density, MEE, Z-EDM, and EXP).

Telmo Amaral Deep architectures and work dir

B Slides: Introduction to convolutional neural networks





C Spreadsheet: Notes on UCI biomedical data sets

			Sheet1				
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Iris	Multivariate			150	- 00	+	14
Breast Cancer	Multivariate		Categorical	286	9 1988	52 +	1995 2005
Heart Disease	Multivariate Multivariate	Classification	Categorical, Integer, Real	303	75 1988	+ + 90 30	1989 2004 1003 2004
Soybean (Small)	Multivariate		Categorical	47		- + 00 00	1993 2004
Breast Cancer Wisconsin (Diagnostic)	Multivariate		Real	569		25 +	1995 2004
Breast Cancer Wisconsin (Original)	Multivariate		Integer	669 1 0 0	10 1992	25 +	1995 2004
Mushroom	Multivariate	Classification	Categorical	8124			
Molecular Biology (Promoter Gene Segu	Sequential. Domain-Theory	Classification	Categorical	106	1	22 +	1995 2005
Molecular Biology (Splice-iunction Gene		Classification	Categorical	3190		22 +	1993 2003
Abalone	Multivariate	Classification	Categorical, Integer, Real	4177		18 +	1997 2004 58.00% [Fouad, 2013]; 51.38% [Fathi, 2013]
Hepatitis	Multivariate	Classification	Categorical, Integer, Real	155	19 1988	17 +	1989 2004
Liver Disorders	Multivariate		Categorical, Integer, Real	345		16 +	1989 2004
Pima Indians Diabetes			Integer, Real	768		16 +	2004
Thyroid Disease	Multivariate, Domain-Theory	Classification	Categorical, Real	7200	21 1987	15 +	1994 2005 99.08% [Kabir, 2013] 97.50% [Dai, 2012]
Zoo	Multivariate	Classification	Categorical, Integer	101		12 +	1995 2004
Audiology (Original)	Multivariate		Categorical	226		+ -	1995 2004
Audiology (Standardized)	Multivariate		Categorical	977		+ -	1995 2004
Lympnograpny	MultiVariate		Lategorical Bool	148 226	1006 o	+ +	1007 2004
Ecoli Horse Colic	Multivariate	Classification	real Categorical Integer Real	368		+ + n o	
Yeast	Multivariate		Real	1484	1.		
Primary Tumor	Multivariate		Categorical	339	1	+	
Molecular Biology (Protein Secondary StSeguential	t Sequential		Categorical	128			1996 2003
Arrhythmia	Multivariate		Categorical, Integer, Real	452	279 1998	m	2002 2005
SPECT Heart	Multivariate		Categorical	267		+ M	
Dermatology	Multivariate	Classification	Categorical, Integer	366	33 1998	2 +	
Echocardiogram	Multivariate	Classification	Categorical, Integer, Real	132	12 1989	2 +	
Haberman's Survival	Multivariate		Integer	306	3 1999	+ -	
Lung Cancer	Multivariate		Integer	32	56 1992 0 1002	+ -	1998 2003
Post-Operative Patient	Multivariate		Categorical, Integer	06	5993 13	+ + > r	1002 Z001
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Demospongiae	Multivariate		Integer	503		0	
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ILPD (Indian Liver Patient Dataset)	Multivariate		Integer, Real	583		0	
KEGG Metabolic Reaction Network (Und Multivariate, Univariate, Text	d Multivariate, Univariate, Text	, Regression, Clustering	Integer, Real	65554	29 2011	0	
KEGG Metabolic Relation Network (Dire	Multivariate, Univariate, Text	, Regression, Clustering	Integer, Real	53414		0	
Mammographic Mass	Multivariate		Integer	1961		0 0	
One-hundred plant species leaves data			Real	1600		0 0	
pb3 Mutants	Multivariate		Keal	7//0T		5 0	
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PubChem Bioassay Data	Multivariate	ion	categorical Integer, Real	70077		00	
Ouadruped Mammals	Multivariate, Data-Generator		Real		72 1992	0	
seeds	Multivariate	. Clustering	Real	210		0 0	
Sponge	Multivariate		Categorical, Integer	76	45	0	
Abscisic Acid Signaling Network	Multivariate	very	Integer	300			
Covertype	Multivariate	Classification	Categorical, Integer	581012	54 1998		
Diabetes	Multivariate, Time-Series		Categorical, Integer		20		
E. Coli Genes	Relational						
EEG Database	Multivariate, Time-Series		Categorical, Integer, Real	122	4 1999		
ILCU I ocalization Data for Barcon Activity	Multivariate, IIIIle-Series Ilbivariate Sequential Time-Series	Classification	Deal	164860	0106 8		
Autorization data for reison Autoria. M. Tuberculosis Genes	Relational		Neal	00040T			
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