Datasets for the Agnostic Learning vs. Prior Knowledge Competition

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This documents provides details about the five datasets used in the "Agnostic Learning vs. Prior Knowledge" competition organized for IJCNN 2007. We used the same 5 datasets already used for the WCCI 2006 performance prediction challenge. However, the data were reshuffled. We make available two data formats: (1) the raw data as provided from the original data source, (2) the preprocessed data representation of the WCCI 2006 challenge. All tasks are two-class classification problems. The goal of the challenge is to determine **how much can be gained in performance when prior/domain knowledge is available** compared to using a "black-box" method on the preprocessed data, or whether the "black box" agnostic methods match or outperform "Gnostic" methods.

This document provides guidance to the competitors interested in the "prior knowledge" track. **The competitors entering in the "agnostic learning" track should not exploit this document to reverse engineer the agnostic track data**. The rule of the game is that they should ignore the information made available in this document to make entries into the challenge.

The competitors have several months to build classifiers with provided (labeled) training data. A web server is provided to submit prediction results on additional unlabeled data. Two unlabeled datasets are used for evaluation: a small validation set used during the development period and a very large test set to do the final evaluation and the ranking of the participants. During a development period, the validation set performance is published immediately upon submission of prediction results. The test set performance remains undisclosed until the end of the competition. The labels of the validation set are published shortly before the end of the competition.

The data sets were chosen to span a variety of domains (drug discovery, ecology, handwritten digit recognition, text classification, and marketing.) We chose data sets that had sufficiently many examples to create a large enough test set to obtain statistically significant results. The input variables are continuous or binary, sparse or dense. All problems are two-class classification problems.

The data characteristics are summarized in Table 1.

Table 1: Datasets of the challenge. The columns "sparsity", "type", "Featnum" and "Tr/FN" refer to the feature representation used for the WCCI 2006 challenge and made available to the "agnostic learning" track.

Dataset	Domain	Sparsity (%)	Type	FracPos (%)	Tr/FN	FeatNum	Train	Valid	Test
ADA	Marketing	79.4	mixed	24.8	86.4	48	4147	415	41471
GINA	Handwriting	69.2	continuous	49.2	3.25	970	3153	315	31532
HIVA	Drug discovery	90.9	binary	3.5	2.38	1617	3845	384	38449
NOVA	Text mining	99.7	binary	28.5	0.1	16969	1754	175	17537
SYLVA	Ecology	77.9	mixed	6.2	60.58	216	13086	1308	130858

Method:

Preparing the feature representation used for the agnostic track included preprocessing data to obtain features in the same numerical range (0 to 999 for continuous data and 0/1 for binary data) and randomizing the order of the patterns and the features to homogenize the data.

For all data representations, the data were split into the same three training, validation and test sets. However, the data of the agnostic track and the prior knowledge track were reshuffled in a difference way within each set. The features of the agnostic track were shuffled differently than in the WCCI 2006 challenge. The proportions of the data split are the same as in the WCCI 2006 challenge: the validation set is 100 times smaller than the test set to make it 10 times less accurate to compute the performances on the basis of the validation set only. The training set is ten times larger than the validation set.

The classification performance is evaluated by the Balanced Error Rate (BER), that is the average error rate of the two classes. Both validation and test set truth-values (labels) are withheld during the benchmark. The validation set serves as development test set to give on-line performance feed-back to the participants. One month before the end of the challenge, the validation set labels are made available. At the end of the benchmark, the participants send their test set results. The scores on the test set results are disclosed simultaneously to all participants after the benchmark is over.

Data formats:

For both track, the following four files in text format are used for each dataset:
dataname.param: Parameters and statistics about the data
dataname_train.labels: Binary labels (truth values of the classes) for training examples.
dataname_valid.labels: Binary validation set labels (withheld during the benchmark).
dataname_test.labels: Binary test set labels (withheld during the benchmark).

For the prior knowledge track, multi-class labels are provided in addition to the binary labels:
dataname_train.mlabels: Training multiclass labels.
dataname_valid.mlabels: Validation multiclass labels (withheld during the benchmark).
dataname_test.mlabels: Test multiclass labels (withheld during the benchmark).
Note: the challenge is about binary classification. Multi-class labels are provided as additional hints/prior knowledge.

For the agnostic track, the data matrices are provided in text format:
dataname_train.data: Training set (a sparse or a regular matrix, patterns in lines, features in columns).
dataname_valid.data: Development test set or "validation" set.
dataname_test.data: Test set.
The matrix data formats used are:

- For regular matrices: a space delimited file with a new-line character at the end of each line.
- For sparse matrices with binary values: for each line of the matrix, a space delimited list of indices of the non-zero values. A new-line character at the end of each line. In this challenge there are no sparse matrices with non-binary values.

For the prior knowledge track, the datasets are provided in various formats specified in more details in the sections devoted to the specific datasets.

The results on each dataset should be formatted in 6 ASCII files:
dataname_train.resu: +-1 classifier outputs for training set examples (mandatory for all submission.).
dataname_valid.resu: +-1 classifier outputs for validation set examples (mandatory for all submission.).
dataname_test.resu: +-1 classifier outputs for final test set examples (mandatory for final submissions.)
dataname_train.conf: confidence values for training examples (optional.)
dataname_valid.conf: confidence values for validation examples (optional.)
dataname_test.conf: confidence values for test examples (optional.)
The confidence values can be the absolute discriminant values. They do not need to be normalized to look like probabilities. They will be used to compute ROC curves and Area Under such Curve (AUC).

Only entries containing results on the five datasets will qualify towards the final ranking. You can make mixed entries (using domain knowledge for some entries and preprocessed data for others). Mixed entries will be entered in the "prior knowledge" track.

Model formats:
There is also the possibility of submitting information about the models used. This is described in a separate document.

Result rating:
The scoring method retained is the test set balanced error rate (test_ber): the average of the class error rates (the class error rates are the error rates obtained with test examples of individual classes, using the predictions provided by the participants.)

In addition to test_ber, other statistics will be computed, but not used for scoring, including the AUC, i.e. the area under the ROC curve.

Dataset A: SYLVA

1) Topic

The task of SYLVA is to classify forest cover types. The forest cover type for 30 x 30 meter cells is obtained from US Forest Service (USFS) Region 2 Resource Information System (RIS) data. We brought it back to a two-class classification problem (classifying Ponderosa pine vs. everything else). The "agnostic data" consists in 216 input variables. Each pattern is composed of 4 records: 2 true records matching the target and 2 records picked at random. Thus ½ of the features are distracters. The "prior knowledge data" is identical to the "agnostic data", except that the distracters are removed and the identity of the features is revealed.

2) Sources

a. Original owners

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Acknowledgements, Copyright Information, and Availability

a. Donor of database

This version of the database was prepared for the WCCI 2006 performance prediction challenge and the IJCNN 2007 agnostic learning vs. prior knowledge challenge by Isabelle Guyon, 955 Creston Road, Berkeley, CA 94708, USA (isabelle@clopinet.com).

b. Date received: August 28, 1998, UCI Machine Learning Repository, under the name Forest Cover Type.

c. Date prepared for the challenges: June 2005 – September 2006.

3) Past usage

Blackard, Jock A. 1998. "Comparison of Neural Networks and Discriminant Analysis in Predicting Forest Cover Types." Ph.D. dissertation. Department of Forest Sciences. Colorado State University. Fort Collins, Colorado.

Classification performance with first 11,340 records used for training data, next 3,780 records used for validation data, and last 565,892 records used for testing data subset: -- 70% backpropagation -- 58% Linear Discriminant Analysis

4) Experimental design

The original data comprises a total of 581012 instances (observations) grouped in 7 classes (forest cover types) and having 54 attributes corresponding to 12 measures (10 quantitative variables, 4 binary wilderness areas and 40 binary soil type variables). The actual forest cover type for a given observation (30 x 30 meter cell) was determined from US Forest Service (USFS) Region 2 Resource Information System (RIS) data. Independent variables were derived from data originally obtained from US Geological Survey (USGS) and USFS data. Data is in raw form (not scaled) and contains binary (0 or 1) columns of data for qualitative independent variables (wilderness areas and soil types).

Variable Information

Given is the variable name, variable type, the measurement unit and a brief description. The forest cover type is the classification problem. The order of this listing corresponds to the order of numerals along the rows of the database.

Name	Data Type	Measurement	Description
Elevation	quantitative	meters	Elevation in meters
Aspect	quantitative	azimuth	Aspect in degrees azimuth
Slope	quantitative	degrees	Slope in degrees
Horizontal_Distance_To_Hydrology	quantitative	meters	Horz Dist to nearest surface water features
Vertical_Distance_To_Hydrology	quantitative	meters	Vert Dist to nearest surface water features
Horizontal_Distance_To_Roadways	quantitative	meters	Horz Dist to nearest roadway
Hillshade_9am	quantitative	0 to 255 index	Hillshade index at 9am, summer solstice
Hillshade_Noon	quantitative	0 to 255 index	Hillshade index at noon, summer soltice
Hillshade_3pm	quantitative	0 to 255 index	Hillshade index at 3pm, summer solstice
Horizontal_Distance_To_Fire_Points	quantitative	meters	Horz Dist to nearest wildfire ignition points
Wilderness_Area (4 binary columns)	qualitative	0 (absence) or 1 (presence)	Wilderness area designation
Soil_Type (40 binary columns)	qualitative	0 (absence) or 1 (presence)	Soil Type designation
Cover_Type (7 types)	integer	1 to 7	Forest Cover Type designation

Code Designations

Wilderness Areas:

1 -- Rawah Wilderness Area
2 -- Neota Wilderness Area
3 -- Comanche Peak Wilderness Area
4 -- Cache la Poudre Wilderness Area

Soil Types:

1 to 40 : based on the USFS Ecological Landtype Units for this study area.

Forest Cover Types:

1 -- Spruce/Fir
2 -- Lodgepole Pine
3 -- Ponderosa Pine
4 -- Cottonwood/Willow
5 -- Aspen
6 -- Douglas-fir
7 – Krummholz

Class Distribution

Number of records of Spruce-Fir:	211840
Number of records of Lodgepole Pine:	283301
Number of records of Ponderosa Pine:	35754
Number of records of Cottonwood/Willow:	2747
Number of records of Aspen:	9493
Number of records of Douglas-fir:	17367
Number of records of Krummholz:	20510
Total records:	581012

Data preprocessing and data split

We carved a binary classification task out these data. We decided to separate Ponderosa pine from all others. To disguise the data and render the task more challenging for the "agnostic track", we created patterns containing the concatenation of 4 patterns: two of the target class and two randomly chosen from either class. In this way there are pairs of redundant features and ½ of the features are non-informative. The "prior knowledge data" does not contain the distracters. The multi-class label information is provided with the "prior knowledge data" as a 2-digit number representing for each pattern the combination of 2 records used. All the examples of the positive class have code "33" (two Ponderosa pine records), others have different 2-digit numbers.

5) Number of examples and class distribution

Prior knowledge data

	Positive ex.	Negative ex.	Total	Check sum
Training set	805	12281	13086	118996108
Validation set	81	1228	1309	11904801
Test set	8052	122805	130857	1191536355
All	8938	136314	145252	1322437264

Agnostic data

	Positive ex.	Negative ex.	Total	Check sum
Training set	805	12281	13086	238271607
Validation set	81	1228	1309	23817234
Test set	8052	122805	130857	2382779242
All	8938	136314	145252	2644868083

6) Type of input variables and variable statistics

Prior knowledge data

Real variables	Random probes	Total
108	0	108

Agnostic data

Real variables	Random probes	Total
108	108	216

All variables are **integer** quantized on 1000 levels. There are **no missing values**. The data is not very sparse, but for data compression reasons, we thresholded the values. Approximately 78% of the variable values are zero. The data was saved as a **dense** matrix.

7) Baseline results

The best entry in the "Performance prediction challenge" had e test_ber=0.53%.

Dataset B: GINA

1) Topic

The task of GINA is handwritten digit recognition. We chose the problem of separating the odd numbers from even numbers. We use 2-digit numbers. Only the unit digit is informative for that task, therefore at least ½ of the features are distracters. This is a two-class classification problem with sparse continuous input variables, in which each class is composed of several clusters. It is a problems with heterogeneous classes.

2) Sources

a. Original owners

The data set was constructed from the MNIST data that is made available by Yann LeCun of the NEC Research Institute at http://yann.lecun.com/exdb/mnist/.

The digits have been size-normalized and centered in a fixed-size image of dimension 28x28. We show examples of digits in Figure B1.

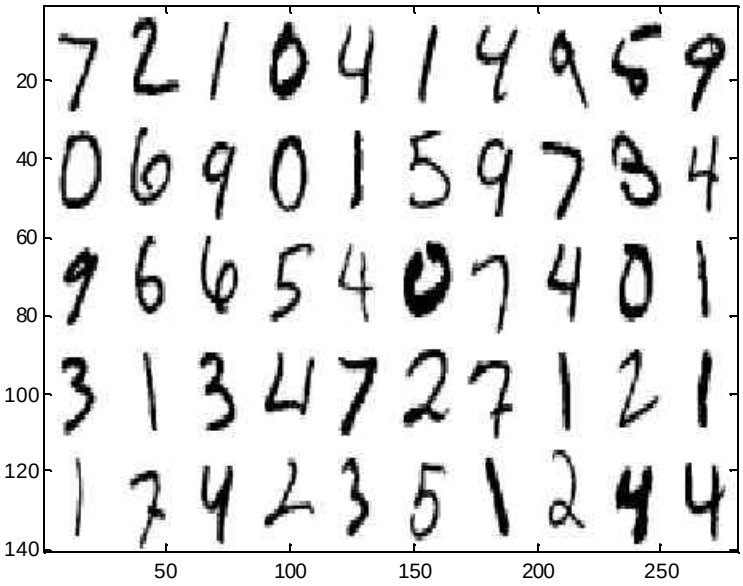

Figure B1: Examples of digits from the MNIST database.

Table 1: Number of examples in the original data

Digit	0	1	2	3	4	5	6	7	8	9	Total
Training	5923	6742	5958	6131	5842	5421	5918	6265	5851	5949	60000
Test	980	1135	1032	1010	982	892	958	1028	974	1009	10000
Total	6903	7877	6990	7141	6824	6313	6876	7293	6825	6958	70000

b. Donor of database

This version of the database was prepared for the WCCI 2006 performance prediction challenge and the IJCNN 2007 agnostic learning vs. prior knowledge challenge by Isabelle Guyon, 955 Creston Road, Berkeley, CA 94708, USA (isabelle@clopinet.com).

c. Date prepared for the challenges: June 2005 – September 2006.

3) Past usage

Many methods have been tried on the MNIST database, in its original data split (60,000 training examples, 10,000 test examples, 10 classes.) Here is an abbreviated list from http://yann.lecun.com/exdb/mnist/:

METHOD	TEST ERROR RATE (%)
linear classifier (1-layer NN)	12.0
linear classifier (1-layer NN) [deskewing]	8.4
pairwise linear classifier	7.6
K-nearest-neighbors, Euclidean	5.0
K-nearest-neighbors, Euclidean, deskewed	2.4

40 PCA + quadratic classifier	3.3
1000 RBF + linear classifier	3.6
K-NN, Tangent Distance, 16x16	1.1
SVM deg 4 polynomial	1.1
Reduced Set SVM deg 5 polynomial	1.0
Virtual SVM deg 9 poly [distortions]	0.8
2-layer NN, 300 hidden units	4.7
2-layer NN, 300 HU, [distortions]	3.6
2-layer NN, 300 HU, [deskewing]	1.6
2-layer NN, 1000 hidden units	4.5
2-layer NN, 1000 HU, [distortions]	3.8
3-layer NN, 300+100 hidden units	3.05
3-layer NN, 300+100 HU [distortions]	2.5
3-layer NN, 500+150 hidden units	2.95
3-layer NN, 500+150 HU [distortions]	2.45
LeNet-1 [with 16x16 input]	1.7
LeNet-4	1.1
LeNet-4 with K-NN instead of last layer	1.1
LeNet-4 with local learning instead of ll	1.1
LeNet-5, [no distortions]	0.95
LeNet-5, [huge distortions]	0.85
LeNet-5, [distortions]	0.8
Boosted LeNet-4, [distortions]	0.7
K-NN, shape context matching	0.67

Reference:
Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. "Gradient-based learning applied to document recognition." Proceedings of the IEEE, 86(11):2278-2324, November 1998.
http://yann.lecun.com/exdb/publis/index.html#lecun-98

The dataset restricted to a selection of digits “4” and “9” was used in the NIPS 2003 feature selection challenge http://clopinet.com/isabelle/Projects/NIPS2003/ and http://www.nipsfsc.ecs.soton.ac.uk/, under the name GISETTE.

4) Experimental design

To construct the “agnostic” dataset, we performed the following steps:

- We removed the pixels that were 99% of the time white. This reduced the original feature set of 784 pixels to 485.

- The original resolution (256 gray levels) was kept.
- In spite of the fact that the data are rather sparse (about 30% of the values are non-zero), we saved the data as a dense matrix because we found that it can be compressed better in this way (to 19 MB.)
- The feature names are the (i,j) matrix coordinates of the pixels (in a 28x28 matrix.)
- We created 2 digit numbers by dividing the datasets into to parts and pairing the digits at random.
- The task is to separate odd from even numbers. The digit of the tens being not informative, the features of that digit act as distracters.

To construct the "prior" dataset, we went back to the original data and fetched the "informative" digit in its original representation. Therefore, this data representation consists in a vector of concatenating the lines of a 28x28 pixel map.

5) Number of examples and class distribution

Prior knowledge data

	Positive ex.	**Negative ex.**	**Total**	**Check sum**
Training set	1550	1603	3153	82735983
Validation set	155	160	315	8243382
Test set	15504	16028	31532	825458881
All	17209	17791	35000	916438246

Agnostic data

	Positive ex.	**Negative ex.**	**Total**	**Check sum**
Training set	1550	1603	3153	164947945
Validation set	155	160	315	16688946
Test set	15504	16028	31532	1646492864
All	17209	17791	35000	1828129755

6) Type of input variables and variable statistics

Prior knowledge data

Real variables	**Random probes**	**Total**
784	0	784

Agnostic data

Real variables	**Random probes**	**Total**
485	485	970

All variables are **integer** quantized on 256 levels. There are **no missing values**. The data is rather **sparse**. Approximately 69% of the entries are zero for the agnostic data. The data was saved as a **dense** matrix, because it compresses better in that format.

7) Baseline results

The best entry of the "performance prediction challenge" obtained a test_ber=2.88%.

Dataset C: NOVA

1) Topic

The task of NOVA is text classification from the 20-Newsgroup data. We selected the separation of politics and religion topics from all the other topics. This is a two-class classification problem. The raw data comes as text files for the "prior knowledge" track. The preprocessed data for the "agnostic" track is a sparse binary representation using a bag-of-word representation with a vocabulary of approximately 17000 words.

2) Sources

a. Original owners

Tom Mitchell
School of Computer Science
Carnegie Mellon University
tom.mitchell@cmu.edu

Available from the UCI machine learning repository. The version we are using for the agnostic track was preprocessed by Ron Bekkerman http://www.cs.technion.ac.il/~ronb/thesis.html into the "bag-of-words" representation.

b. Donor of database

This version of the database was prepared for the WCCI 2006 performance prediction challenge and the IJCNN 2007 agnostic learning vs. prior knowledge challenge by Isabelle Guyon, 955 Creston Road, Berkeley, CA 94708, USA (isabelle@clopinet.com).

c. Date prepared for the challenges: June 2005 – September 2006.

3) Past usage

T. Mitchell. Machine Learning, McGraw Hill, 1997.

T. Joachims (1996). A probabilistic analysis of the Rocchio algorithm with TFIDF for text categorization, Computer Science Technical Report CMU-CS-96-118. Carnegie Mellon University.

Ron Bekkerman, Ran El-Yaniv, Naftali Tishby, and Yoad Winter. Distributional Word Clusters vs. Words for Text Categorization. JMLR 3(Mar):1183-1208, 2003.

4) Experimental design

We selected 8 newsgroups relating to politics or religion topics as our positive class (Table C.1.)
For the "prior knowledge"data, we kept the original text, but we removed the header. The format of the data files is as follows. Each entry corresponding to a newsgroup message is encoded as:

- 1st line: Subject: xxx
- 2nd line: Lines: yyy
- 3rd line: Blank
- The message with yyy lines.
- $$$$

Each entry corresponds to an example.

For the "agnostic" data, the vocabulary selection includes the following filters:
- remove words containing digits and convert to lowercase
- remove words appearing less than twice in the whole dataset.
- remove short words with less than 3 letters.
- exclude ~2000 words found frequenly in all documents.
- truncate the words at a max of 7 letters.

Table C.1: Twenty newsgroup database.

Newsgroup	Number of examples
alt.atheism	1114
comp.graphics	1002
comp.os.ms-windows.misc	1000
comp.sys.ibm.pc.hardware	1028
comp.sys.mac.hardware	1002
comp.windows.x	1000
misc.forsale	1005
rec.autos	1004
rec.motorcycles	1000
rec.sport.baseball	1000
rec.sport.hockey	1000
sci.crypt	1000
sci.electronics	1000
sci.med	1001
sci.space	1000
soc.religion.christian	997
talk.politics.guns	1008
talk.politics.mideast	1000
talk.politics.misc	1163
talk.religion.misc	1023

5) Number of examples and class distribution

Prior knowledge data

	Positive ex.	Negative ex.	Total
Training set	499	1255	1754
Validation set	50	125	175
Test set	4990	12547	17537
All	5539	13927	19466

Agnostic data

	Positive ex.	Negative ex.	Total	Check sum
Training set	499	1255	1754	103583
Validation set	50	125	175	9660
Test set	4990	12547	17537	984667
All	5539	13927	19466	1097910

6) Type of input variables and variable statistics (agnostic data only)

Real variables	Random probes	Total
16969	0	16969

All variables are **binary**. There are **no missing values**. The data is very **sparse**. Over 99% of the entries are zero. The data was saved as a **sparse-binary** matrix.

7) Baseline results

The best performance of the "Performance prediction challenge" was test_ber=4.44%.

Dataset D: HIVA

1) Topic

The task of HIVA is to predict which compounds are active against the AIDS HIV infection. The original data has 3 classes (active, moderately active, and inactive). We brought it back to a two-class classification problem (active vs. inactive). The problem is therefore to relate structure to activity (a QSAR=quantitative structure-activity relationship problem) to screen new compounds before actually testing them (a HTS=high-throughput screening problem.)
The molecules in the original data are described by their chemical formula. We provide additionally the 3d structure for the "prior knowledge" track. For the "agnostic track" we represented the data as 2000 sparse binary input variables. The variables represent properties of the molecule inferred from its structure.

2) Sources

a. Original owners

The data is made available by the National Cancer Institute (NCI), via the DTP AIDS Antiviral Screen program at: http://dtp.nci.nih.gov/docs/aids/aids_data.html.

The DTP AIDS Antiviral Screen has checked tens of thousands of compounds for evidence of anti-HIV activity. Available are screening results and chemical structural data on compounds that are not covered by a confidentiality agreement.

b. Donor of database

This version of the database was prepared for the WCCI 2006 performance prediction challenge and the IJCNN 2007 agnostic learning vs. prior knowledge challenge by Isabelle Guyon, 955 Creston Road, Berkeley, CA 94708, USA (isabelle@clopinet.com).

c. Date prepared for the challenges: June 2005 – September 2006.

3) Past usage

An earlier release of the database was uses in an Equbits case study:
http://www.limsfinder.com/community/articles_comments.php?id=1553_0_2_0_C75.
The feature set was obtained by a different method.

4) Experimental design

The screening results of the May 2004 release containing the screening results for 43,850 compounds were used. The results of the screening tests are evaluated and placed in one of three categories:

- **CA** - Confirmed active
- **CM** - Confirmed moderately active
- **CI** - Confirmed inactive

We converted this into a two-class classification problem: Inactive (CI) vs. Active (CA or CM.)
Chemical structural data for 42,390 compounds was obtained from the web page. It was converted to structural features by the program ChemTK version 4.1.1, Sage Informatics LLC. Four compounds failed parsing.
The 1617 features selected include:

- unbranched_fragments: 750 features
- pharmacophores: 495 features
- branched_fragments: 219 features
- internal_fingerprints: 132 features
- ring_systems: 21 features

Only binary features having a total number of ones larger than 100 (>400 for unbranched fragments) and at least 2% of ones in the positive class were retained. In all cases, the default program settings were used to generate keys (except for the pharmacophores for which "max number of pharmacophore points" was set to 4 instead of 3; the pharmacophore keys for Hacc, Hdon, ExtRing, ExtArom, ExtAliph were generated, as well as those for Hacc, Hdon, Neg, Pos.) The keys were then converted to attributes.

We briefly describe the attributes/features:
Branched fragments: each fragment is constructed through an "assembly" of shortest-path unbranched fragments, where each of the latter is required to be bounded by two atoms belonging to one or more pre-defined "terminal-atom".
Unbranched fragments: unique non-branching fragments contained in the set of input molecules.
Ring systems: A ring system is defined as any number of single or fused rings connected by an unbroken chain of atoms. The simplest example would be either a single ring (e.g., benzene) or a single fused system (e.g., naphthalene).
Pharmacophores: ChemTK uses a type of pharmacophore that measures distance via bond connectivity rather than a typical three-dimensional distance. For instance, to describe a hydrogen-bond acceptor and hydrogen-bond donor separated by five connecting bonds, the corresponding key string would be "HAcc.HDon.5". The pharmacophores were generated from the following features:
Neg. Explicit negative charge.
Pos. Explicit positive charge.
HAcc. Hydrogen-bond acceptor.
HDon. Hydrogen-bond donor.
ExtRing. Ring atom having a neighbor atom external to the ring.
ExtArom. Aromatic ring atom having a neighbor atom external to the ring.
ExtAliph. Aliphatic ring atom having a neighbor atom external to the ring.
Internal fingerprints: small, fixed catalog of pre-defined queries roughly similar to the

MACCS key set developed by MDL.
We matched the compounds in the structural description files and those in the compound activity file, using the NSC id number. We ended up with 42678 examples.

5) Data format, number of examples and class distribution

Prior knowledge data

	Positive ex.	Negative ex.	Total
Training set	135	3710	3845
Validation set	14	370	384
Test set	1354	37095	38449
All	1503	41175	42678

The raw data is formatted in the MDL-SD format (hiva_train.sd, hiva_valid.sd, hiva_test.sd). It represents the 3-dimensional structure of the molecule. It was produced from the chemical formulas byt the program Corina (http://www.molecular-networks.de/software/corina/index.html). Each record is separated by $$$$. One record contains:

- **Header block** -- line 1: molecule name; line 2: molecule header; line 3: comment line.
- **Connection Table** -- count line in Fortran format 2I3; **atom block**: One line per atom, including the atomic co-ordinates (X, Y, Z), symbol (SYM), mass difference for the isotope (MASS), formal charge (CHARGE), and stereo parity indicator (STEREO); **bond block:** One line per bond specifying the two atoms connected by the bond (ATOM1, ATOM2), the bond type (TYPE), stereochemistry (BONDST), and topology (TOPOL).
- **Data Block --** data header: Indicated by the greater than symbol >; data: may extend over multiple lines, up to a maximum of 200 characters in total (up to 80 characters per line); black line.

Agnostic data

	Positive ex.	Negative ex.	Total	Check sum
Training set	135	3710	3845	564954
Validation set	14	370	384	56056
Test set	1354	37095	38449	5674217
All	1503	41175	42678	6295227

6) Type of input variables and variable statistics (agnostic data only)

Real variables	Random probes	Total
1617	0	1617

All variables are binary. The data was saved as a **non-spase** matrix, even though it is 91% sparse because dense matrices load faster in Matlab and the ASCII format compresses well.

7) Baseline results

The best entry of the “Performance Prediction Challenge” ha a test_ber=27.56%.

Dataset E: ADA

1) **Topic**

The task of ADA is to discover high revenue people from census data. This is a two-class classification problem. The raw data from the census bureau is known as the Adult database in the UCI machine-learning repository. It contains continuous, binary and categorical variables. The "prior knowledge track" has access to the original features and their identity. The agnostic track has access to a preprocessed numeric representation eliminating categorical variables.

2) **Sources**

a. Original owners

This data was extracted from the census bureau database found at
http://www.census.gov/ftp/pub/DES/www/welcome.html
Donor: Ronny Kohavi and Barry Becker,
Data Mining and Visualization
Silicon Graphics.
e-mail: ronnyk@sgi.com for questions.

The information below is exerpted from the UCI machine learning repository:

```
  Extraction was done by Barry Becker from the 1994 Census database. The prediction task
is to determine whether a person makes over 50K a year. The attributes are:
age: continuous.
workclass: Private, Self-emp-not-inc, Self-emp-inc, Federal-gov, Local-gov, State-gov,
Without-pay, Never-worked.
fnlwgt: continuous.
education: Bachelors, Some-college, 11th, HS-grad, Prof-school, Assoc-acdm, Assoc-voc,
9th, 7th-8th, 12th, Masters, 1st-4th, 10th, Doctorate, 5th-6th, Preschool.
education-num: continuous.
marital-status: Married-civ-spouse, Divorced, Never-married, Separated, Widowed, Married-
spouse-absent, Married-AF-spouse.
occupation: Tech-support, Craft-repair, Other-service, Sales, Exec-managerial, Prof-
specialty, Handlers-cleaners, Machine-op-inspct, Adm-clerical, Farming-fishing,
Transport-moving, Priv-house-serv, Protective-serv, Armed-Forces.
relationship: Wife, Own-child, Husband, Not-in-family, Other-relative, Unmarried.
race: White, Asian-Pac-Islander, Amer-Indian-Eskimo, Other, Black.
sex: Female, Male.
capital-gain: continuous.
capital-loss: continuous.
hours-per-week: continuous.
native-country: United-States, Cambodia, England, Puerto-Rico, Canada, Germany, Outlying-
US(Guam-USVI-etc), India, Japan, Greece, South, China, Cuba, Iran, Honduras, Philippines,
Italy, Poland, Jamaica, Vietnam, Mexico, Portugal, Ireland, France, Dominican-Republic,
Laos, Ecuador, Taiwan, Haiti, Columbia, Hungary, Guatemala, Nicaragua, Scotland,
Thailand, Yugoslavia, El-Salvador, Trinadad&Tobago, Peru, Hong, Holand-Netherlands.
income: >50K, <=50K.

Split into train-test using MLC++ GenCVFiles (2/3, 1/3 random).
 48842 instances, mix of continuous and discrete    (train=32561, test=16281)
 45222 if instances with unknown values are removed (train=30162, test=15060)
 Duplicate or conflicting instances : 6
 Class probabilities for adult.all file
 Probability for the label '>50K'  : 23.93% / 24.78% (without unknowns)
 Probability for the label '<=50K' : 76.07% / 75.22% (without unknowns)

 Description of fnlwgt (final weight)
 The weights on the CPS files are controlled to independent estimates of the
 civilian noninstitutional population of the US.  These are prepared monthly
```

```
for us by Population Division here at the Census Bureau.  We use 3 sets of
controls. People with similar demographic characteristics should have
similar weights.
```

b. Donor of database

This version of the database was prepared for the WCCI 2006 performance prediction challenge and the IJCNN 2007 agnostic learning vs. prior knowledge challenge by Isabelle Guyon, 955 Creston Road, Berkeley, CA 94708, USA (isabelle@clopinet.com).

c. Date prepared for the challenges: June 2005 – September 2006.

3) Past usage

```
First cited in:
@inproceedings{kohavi-nbtree,
   author={Ron Kohavi},
   title={Scaling Up the Accuracy of Naive-Bayes Classifiers: a
          Decision-Tree Hybrid},
   booktitle={Proceedings of the Second International Conference on
             Knowledge Discovery and Data Mining},
   year = 1996}
Error Accuracy reported as follows, after removal of unknowns from
   train/test sets):
   C4.5       : 84.46+-0.30
   Naive-Bayes: 83.88+-0.30
   NBTree     : 85.90+-0.28
The following algorithms were later run with the following error rates,
   all after removal of unknowns and using the original train/test split.
   All these numbers are straight runs using MLC++ with default values.

   Algorithm              Error
-- ----------------       -----
1  C4.5                   15.54
2  C4.5-auto              14.46
3  C4.5 rules             14.94
4  Voted ID3 (0.6)        15.64
5  Voted ID3 (0.8)        16.47
6  T2                     16.84
7  1R                     19.54
8  NBTree                 14.10
9  CN2                    16.00
10 HOODG                  14.82
11 FSS Naive Bayes        14.05
12 IDTM (Decision table)  14.46
13 Naive-Bayes            16.12
14 Nearest-neighbor (1)   21.42
15 Nearest-neighbor (3)   20.35
16 OC1                    15.04
17 Pebls                  Crashed.  Unknown why (bounds WERE increased)
```

Note: The performances reported are error rates, not BER. We tried to reproduce these performances and obtained 15.62% error with a linear ridge regression classifier. The performances slightly degraded when we tried to group features (15.67% when we replace the country code by a binary US/nonUS value and 16.40% with further reduction to 33 features.)

4) Experimental design

To generate the "agnostic track" data, we performed the following steps:

- Convert the features to 14 numeric values $a \in 1 \ldots n$.
- Convert the numeric values to binary codes (a vector of n zeros with value one at the a^{th} position. This results in 88 features. The missing values get an all zero vector.

- Downsize the number of features to 48 by replacing the country code by a binary US/nonUS feature.
- Randomize the feature and pattern order.
- Remove the entries with missing values for workclass.

Table E.1. Features of the ADA datasets.

Feature name	**min**	**max**	**numval**	**comments**
age	0.19	1	continuous	No missing value.
workclass_Private	0	1	2	2799 missing values (corresponding entries removed.)
workclass_Self_emp_not_inc	0	1	2	
workclass_Self_emp_inc	0	1	2	
workclass_Federal_gov	0	1	2	
workclass_Local_gov	0	1	2	
workclass_State_gov	0	1	2	
workclass_Without_pay	0	1	2	
workclass_Never_worked	0	1	2	
fnlwgt	0.008	1	continuous	No missing value.
educationNum	0.06	1	16	Number corresponding to 16 discrete levels of education
maritalStatus_Married_civ_spouse	0	1	2	No missing value.
maritalStatus_Divorced	0	1	2	
maritalStatus_Never_married	0	1	2	
maritalStatus_Separated	0	1	2	
maritalStatus_Widowed	0	1	2	
maritalStatus_Married_spouse_absent	0	1	2	
maritalStatus_Married_AF_spouse	0	1	2	
occupation_Tech_support	0	1	2	2809 missing values (corresponding entries removed.)
occupation_Craft_repair	0	1	2	
occupation_Other_service	0	1	2	
occupation_Sales	0	1	2	
occupation_Exec_managerial	0	1	2	
occupation_Prof_specialty	0	1	2	
occupation_Handlers_cleaners	0	1	2	
occupation_Machine_op_inspct	0	1	2	
occupation_Adm_clerical	0	1	2	
occupation_Farming_fishing	0	1	2	
occupation_Transport_moving	0	1	2	
occupation_Priv_house_serv	0	1	2	
occupation_Protective_serv	0	1	2	
occupation_Armed_Forces	0	1	2	
relationship_Wife	0	1	2	No missing value.
relationship_Own_child	0	1	2	
relationship_Husband	0	1	2	
relationship_Not_in_family	0	1	2	
relationship_Other_relative	0	1	2	
relationship_Unmarried	0	1	2	

race_White	0	1	2	No missing value.
race_Asian_Pac_Islander	0	1	2	
race_Amer_Indian_Eskimo	0	1	2	
race_Other	0	1	2	
race_Black	0	1	2	
sex	0	1	2	0=female, 1=male. No missing value.
capitalGain	0	1	continuous	No missing value.
capitalLoss	0	1	continuous	No missing value.
hoursPerWeek	0.01	1	continuous	No missing value.
nativeCountry	0	1	2	0=US, 1=non-US. 857 missing values replaced by 1.

5) Data format, number of examples and class distribution

Prior knowledge dataset

	Positive ex.	**Negative ex.**	**Total**
Training set	1029	3118	4147
Validation set	103	312	415
Test set	10290	31181	41471
All	11422	34611	46033

The data are stored in coma-separated files (ada_train.csv, ada_valid.csv, and ada_est.csv).

Agnostic dataset

	Positive ex.	**Negative ex.**	**Total**	**Check sum**
Training set	1029	3118	4147	6798109
Validation set	103	312	415	681151
Test set	10290	31181	41471	67937286
All	11422	34611	46033	75416546

6) Type of input variables and variable statistics

Prior knowledge dataset

Real variables	**Random probes**	**Total**
14	0	14

Six variables are continuous, two are binary, the others are categorical. The missing values were eliminated.

Agnostic dataset

Real variables	**Random probes**	**Total**
48	0	48

Six variables are continuous, the others are binary. There are **no missing values**. The data is 80% **sparse**. The data was saved as a **dense** matrix because once compressed it makes almost no difference and it loads much faster.

7) Baseline results

The best entry in the Performance Prediction Challenge had a test_ber=16.96%.