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Distributed learning with bagging-like performance

Nitesh V. Chawla^a, Thomas E. Moore^a, Lawrence O. Hall^{a,*}, Kevin W. Bowyer^b, Philip Kegelmeyer^c, Clayton Springer^c

^a Department of Computer Science and Engineering, University of South Florida, 4202 East Flower Avenue, Tampa, FL 33620 USA
 ^b Department of Computer Science and Engineering, University of Notre Dame, Notre Dame, IN 46556 USA
 ^c Sandia National Laboratories, Biosystems Research Department, P.O. Box 969, MS 9951, Livermore, CA 94551-0969, USA

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9 Abstract

10 Bagging forms a committee of classifiers by bootstrap aggregation of training sets from a pool of training data. A 11 simple alternative to bagging is to partition the data into disjoint subsets. Experiments with decision tree and neural 12 network classifiers on various datasets show that, given the same size partitions and bags, disjoint partitions result in 13 performance equivalent to, or better than, bootstrap aggregates (bags). Many applications (e.g., protein structure 14 prediction) involve use of datasets that are too large to handle in the memory of the typical computer. Hence, bagging with samples the size of the data is impractical. Our results indicate that, in such applications, the simple approach of 15 creating a committee of n classifiers from disjoint partitions each of size 1/n (which will be memory resident during 16 17 learning) in a distributed way results in a classifier which has a bagging-like performance gain. The use of distributed disjoint partitions in learning is significantly less complex and faster than bagging. 18

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20 Keywords: Distributed learning; Bagging; Large data sets; Ensembles; Multiple classifiers

21 1. Introduction

Many data mining applications use data sets that are too large to be handled in the memory of the typical computer (Shafer et al., 1996; Darlington et al., 1997; Chan and Stolfo, 1993; Provost et al., 1999; Moore and Lee, 1998; Bowyer et al., 2000; Hall et al., 1999, 2000; Oates and Jensen, 27 1998). One possible approach is to subsample the 28 data in some manner (Provost et al., 1999; Brei-29 man, 1999). However, it can be difficult a priori to 30 know how to subsample so that accuracy is not 31 affected. Also, recent work by Perlich et al. (in 32 press) has shown that classifier accuracy tends to 33 increase with more training data even for large 34 data sets. Another possible approach is to parti-35 tion the original data into smaller subsets, and 36 form a committee of classifiers (Chan and Stolfo, 37 1993; Provost and Hennessy, 1996). One advan-38 tage of this approach is that the partition size can - 39 simply be set at whatever amount of the original 40

^{*}Corresponding author. Tel.: +813-974-4195; fax: +813-974-5456.

E-mail addresses: chawla@csee.usf.edu (N.V. Chawla), tmoore4@csee.usf.edu (T.E. Moore), hall@csee.usf.edu (L.O. Hall), kwb@cse.nd.edu (K.W. Bowyer), wpk@ca.sandia.gov (P. Kegelmeyer), csprin@ca.sandia.gov (C. Springer).

No. of Pages 17, DTD = 4.3.1SPS, Chennai

98

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N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

41 data can be conveniently handled on the available
42 system. Another advantage is that the committee
43 potentially has better accuracy than a single classifier constructed on all the data.

45 In its typical form, bagging involves random 46 sampling with replacement from the original pool 47 of training data to create "bags" of data for a committee of thirty to one hundred classifiers. 48 49 Bagging has been shown to almost always result in equal or (usually) improved performance over a 50 single classifier created on all of the original data 51 52 (Breiman, 1996; Quinlan, 1996; Bauer and Kohavi, 53 1999). The success of bagging suggests that it might be a useful approach to create accurate 54 classifiers for large data sets. We define large data 55 sets as those which do not fit in the memory of a 56 57 typical scientific computer. However, experience with bagging has primarily been in the context of 58 small data sets. If the original data set will not fit in 59 60 the main memory of the typical computer, then none of the thirty or more bags one might create 61 62 will fit. This raises the question of which particu-63 lars of the bagging approach are essential in the 64 context of large data sets. We consider the question of whether simple partitioning of the training 65 data into tractable-size subsets can produce an 66 67 ensemble of classifiers with accuracy equal to that 68 of a single classifier built on all of the data. In this work, we show that simple partitioning of a large 69 70 original data set into disjoint subsets results in 71 better performance than creating bags of the same size. In other words, it is the committee of classi-72 73 fiers that is essential and bootstrap aggregation to 74 form the individual classifiers is not essential. Further, it is straightforward to create one or 75 76 several different disjoint partitions of data and the 77 process is rapid.

78 Classifiers can be built in a distributed way on 79 disjoint partitions. Each of n classifiers can be 80 learned on a separate processor in parallel. Further, for large enough partitions (bags) the per-81 82 formance of the resulting classifier will meet or exceed that of a classifier built on all the data. The 83 84 time required to build an ensemble of *n* classifiers 85 which are learned independently on n processors 86 without communication will be the longest time required to learn a single classifier on a processor. 87

In Section 2, we discuss related work. In Section 88 3, we describe our experimental setup for small 89 data sets from the UC Irvine repository (Blake and 90 Merz, 1998), as well as the setup for experiments 91 92 with a mid-size and large data set from our own research. We also describe the base classifiers and 93 computing systems used in the experiments. Sec-94 95 tion 4 contains the experimental results. Finally, Section 5 contains a discussion of the results and 96 conclusions that can be drawn. 97

2. Literature review

Bagging (Breiman, 1996) has been shown to 99 improve classifier accuracy. Bagging basically 100 combines models learned on different samplings of 101 a given dataset. According to Breiman, bagging 102 exploits the instability in the classifiers, since per-103 turbing the training set produces different classifi-104 ers using the same learning algorithm. Quinlan 105 (1996) experimented with bagging on various da-106 tasets and found that bagging substantially im-107 proved accuracy. However, the experiments were 108 performed on *small* datasets, the largest one being 109 20,000 examples. 110

Domingos (1997) empirically tested two alter-111 native theories supporting bagging: (1) bagging 112 works because it approximates Bayesian model 113 averaging or (2) it works because it shifts the 114 priors to a more appropriate region in the decision 115 space. The empirical results showed that bagging 116 worked possibly because it counter-acts the in-117 herent simplicity bias of the decision trees. That is, 118 with M different bags, M different classifiers are 119 learned, and together their output is more complex 120 than that of the single learner. 121

In (Street and Kim, 2001) an ensemble of clas-122 sifiers are built from training data which is treated 123 as a stream. Each classifier is trained on a fixed 124 amount of data from the stream. The size of the 125 ensemble is fixed at 25 classifiers. Classifiers 126 "compete" for entry into the ensemble based on 127 their accuracy and diversity. This approach allows 128 129 an ensemble classifier to be built from an unlimited amount of training data. It also facilitates building 130 an ensemble classifier which might be built on data 131 with temporal dependencies, where the concept to 132

133 be modeled may vary over time. In their experi134 ments, the ensemble classifier was usually slightly
135 less accurate than a classifier which was built with
136 as much data as the current ensemble had used. In
137 our work larger training sets are used.

138 In (Breiman, 1999) classifiers were built on 139 small randomly chosen subsets of an overall training set. This approach can deal with ex-140 141 tremely large training datasets, but requires many classifiers because it uses somewhere around 800 142 143 examples per classifier in the discussed experi-144 ments. Also, the process of continually selecting 145 small subsets can be computationally problematic 146 for very large datasets. This is different from the approach we are looking at, in which the number 147 of training samples may be as large as main 148 149 memory space available.

150 Chan and Stolfo (1995) compared arbiter and 151 combiner strategies by applying a learning algo-152 rithm to disjoint subsets of data. An arbiter 153 scheme uses a learned representation of which 154 classifier to choose given an example and a com-155 biner takes classifier outputs of a test example as 156 input and produces a classification. The described experiments showed that the arbiter strategy can 157 158 sometimes better sustain the accuracy compared to 159 the classifier learned on the entire data set. The 160 combiner strategy showed a drop in accuracy with the increase in the number of subsets, which can be 161 162 attributed to the lack of information content in the 163 small subsets. However, a few cases resulted in an 164 improvement in accuracy. We are interested in disjoint subsets of larger original data sets than in 165 (Chan and Stolfo, 1995) and so there is reason to 166 expect that accuracy can be maintained. 167

168 Chan and Stolfo (1996) relaxed their definition 169 of strict disjoint subsets by allowing a small 170 amount of overlap across the subsets. On the da-171 tasets DNA Splice Junction with 3190 examples 172 and protein coding region with 20,000 examples, it 173 was found that overlapping did not bring any gain 174 to their meta-learning strategy. Each classifier 175 trained on a disjoint set is biased towards its own set, and when these classifiers are combined a 176 177 protocol of knowledge sharing is established, and 178 each individual classifier's bias is reduced. Again, 179 we are interested in large data sets relative to those considered in this work. 180

Domingos (1996) describes how a specific-to-181 general rule induction system (RISE) was sped up 182 by applying it to disjoint training sets. This al-183 lowed the time required for learning to become 184 linear in the number of examples. The resulting 185 rule based classifiers were voted (with some 186 weighting) in an approach very similar to bagging. 187 The major difference was that the size of each 188 training data set was much smaller than the orig-189 inal. On a set of seven data sets from the Irvine 190 repository using disjoint partitions of between 100 191 and 500 examples they found that the resulting 192 voting performance was generally as good as or 193 better than applying RISE to all the data. 194

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Dietterich (2000) describes how an ensemble of 195 decision trees was built from a single unmodified 196 training set. Diversity in the trees was obtained by 197 randomly choosing a test at each internal node 198 from among the top k tests (ranked by information 199 gain, with k typically 20). Each tree was generally 200 suboptimal, but when voted as an ensemble they 201 provided a bagging-like and sometimes better ac-202 curacy gain. This result seems to suggest that 203 bagging-like performance can be obtained from a 204 set of diverse classifiers (in the sense that they 205 make errors on different examples) which may 206 each be suboptimal (in the sense that they are not 207 as good as a classifier built on all the data without 208 any manipulation), but similar in accuracy. 209

Hall et al. (2000) learned decision trees using 210 disjoint partitions of data and then combined the 211 classifiers. It was found that when using a conflict 212 resolution strategy for combining rules, the accuracy usually did not decrease for a small number of 214 partitions, at least on the datasets tested. Our 215 current work is similar to this, but focuses on 216 comparison of bagging-like approaches to simple 217 partitioning of large datasets. 218

Provost et al. (1999) found that subsampling the 219 data gave the same accuracy as the entire dataset 220 at much lower computational cost. They analyzed 221 "progressive sampling" methods-progressively 222 increasing the sample size until the model accuracy 223 no longer improved. It was found that adding 224 more training instances did not help the accuracy 225 of the classifier, and after some number of in-226 stances the performance of the classifier plateaus. 227 As pointed out later in the discussion section, our 228

N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

results indicate that simple subsampling to pro-duce one smaller training set is not a profitablestrategy for the larger datasets that we consider.However, more complicated subsampling strate-

233 gies may be useful.

234 3. Experiments

235 Three sets of experiments were performed. The 236 first uses five small datasets, representative of 237 those commonly used in pattern recognition and machine learning research. It compares four ap-238 proaches to creating a committee of N classifiers. 239 240 with each classifier created using (1/N)th of the training data. The performance of the approaches 241 242 is also compared to that of *true bagging*—bags of the same size as the pool of training data, ran-243 domly sampled with replacement. The point of this 244 245 first set of experiments is to isolate the essential factor(s) leading to good performance in the 246 committee of classifiers. The second set of experi-247 248 ments uses a mid-size dataset of almost 230,000 249 examples. The same four approaches are evaluated 250 on this data set. The point is to verify that the pattern of performance results observed with 251 smaller data sets holds with a larger data set. 252

253 Based on the first two sets of experiments, the 254 disjoint partitioning approach is identified as of-255 fering equivalent performance for a given size of 256 partition/bag. It is also the simplest of the approaches considered. The last experiment uses a 257 258 large dataset of approximately 3.6 million exam-259 ples to investigate the degree of performance improvement that the disjoint partitioning approach 260 can achieve over a classifier built on all the original 261 262 data.

263 3.1. Variations of partitioning and bagging

We investigated four different approaches to creating a committee of classifiers from an original data set (see Fig. 1 for an illustration). One approach is to simply randomly partition the original data into N disjoint partitions of size (1/N)th of the original data. Thus the union of the N training sets is identical to the original data. Results of this

original data set:	
ABCDEFGHIJKLMN	ΟΡ
Disjoint partitions (random order of d	ata)
ABCD EFGH IJKL MN	OP D
Small Bags (replication within and acr	oss):
ACHL BPLP DIOH KC	FK SB
No Replication Small Bags:	
ACHL OPLN DIOH KC	FP NRSB
Disjoint Bags (no replication across, la	rger):
ABCDC EFGHE IJKLJ MN	OPO DB

Fig. 1. Four approaches to a committee of classifiers.

approach are labeled with 'D' (for "disjoint") on 271 the graphs. 272

The second approach is to create N bags of size 273 (1/N)th of the data. Each bag is created inde-274 pendently, by random sampling is done with re-275 placement, so the union of the training sets is 276 generally not the same as the original data. This 277 approach is labeled 'SB' (for "small bags") on the 278 graphs. Comparison of the SB performance versus 279 that of disjoint partitions shows whether the ran-280 dom replication of data elements results in any 281 inherent advantage. 282

The third approach is like small bags, but 283 sampling without replacement for each individual 284 bag. When sampling the individual bags without 285 replacement, elements of the original data do not 286 repeat within a bag, but may repeat across bags. 287 This approach is labeled 'NRSB' (for "no-repli-288 cation small bags") on the graphs. 289

The fourth approach begins with the disjoint 290 partitions. Then, independently for each partition, 291 a number of its elements are randomly selected 292 with replacement to be added to the partition to 293 form a "disjoint bagged" training set. Thus the 294 union of the training sets is a superset of the 295 original data; all elements of the original data 296 appear, plus some random replications. The 297 number of added elements is equal to the average 298 number of repeated elements in a bag in the "small 299 bags." Thus a bag used in this approach is slightly 300 larger than (1/N)th of the original data. The 301 amount of "extra" data included decreases as the 302

303 bag size decreases. Results of this approach are
304 labeled 'DB' (for "disjoint bagged") on the graphs.
305 Comparison of the results of this approach to the
306 results of disjoint partitions looks again at whether
307 the random replication of data elements results in
308 any inherent advantage, but through the effect of
309 allowing larger bag size.

In addition to the above four approaches, we 310 also ran "true bagging" on each of the five small 311 datasets. By "true bagging" we mean creating M312 bags, each of the size of the original data, inde-313 314 pendently using random sampling with replacement. True bagging is expected to out-perform 315 316 committees of classifiers formed using smaller bags, but the point is to provide a baseline per-317 formance comparison for the other approaches. 318

For each experiment in which voting is used,
ties are broken by assigning the example to the
largest class (in the training set) participating in
the tie.

323 3.2. Datasets

324 Three of the small data sets are from the UCI 325 repository (Blake and Merz, 1998), one is from the ELENA project, ¹ and one is from our own re-326 search. The mid-size dataset comes from the 327 328 problem of predicting the secondary structure of proteins. It is part of the training data set used 329 330 with a neural network that won the CASP-3 sec-331 ondary structure prediction contest (Jones, 1999). We concatenated his train set one and test set one 332 333 as our overall training set. This dataset contains 334 almost 230,000 elements. Each amino acid in a protein can have its structure labeled as helix (H), 335 336 coil (C), or sheet (E). The features for a given amino acid are twenty values in the range -17 to 337 338 17, representing the log likelihood of the amino acid being any one of twenty basic amino acids. 339 340 Using a window of size 15 centered around the 341 target amino acid and an extra bit for each window to indicate an N or C terminus (beginning or 342 end of chain) gives a feature vector of size 315. 343

Our large dataset also comes from the protein 344 database (PDB) (Berman et al., 2000) used in the 345 CASP contests (Lawrence Livermore National 346 Laboratories, 2001). For 18,098 protein chains 347 taken from the PDB, there are a total of 3,679,152 348 amino acids for structure prediction. Using a 349 window of size seventeen centered around the 350 target amino acid (without an extra N/C terminus 351 bit), we have a feature vector of size 340. This 352 training data takes from 1.3 to 30 GB to store, 353 depending on how feature values are encoded (e.g. 354 signed char, integer, or float). The test data for the 355 experiments with the large dataset consists of a 356 separate set of data. It is all protein chains entered 357 into the PDB from July 11 2000 to July 28 2000, 358 that are based on X-ray crystal structures with 359 resolution of three angstroms or finer. There were 360 146 chains entered in this time frame, made up of 361 38,423 amino acids. All results are reported on a 362 per amino acid basis. 363

The size and class distribution of the datasets 364 are summarized in Table 1. Note that the experi-365 ments include both two-class (Mammography, 366 Phoneme) and multi-class (Letter, PenDigits, Sat-367 Image) datasets. They also include datasets that 368 are approximately balanced (Letter, PenDigits) 369 and those that are skewed (Mammography, Pho-370 neme, SatImage). 371

The four approaches to creating a committee of 372 classifiers, plus true bagging, were applied to each 373 of the small datasets. The number of bags/parti-374 tions was varied from one to eight. Given the 375 modest size of the datasets, creating bags/parti-376 tions of less than (1/8)th the original size appears 377 to begin to starve the classifiers for training data. 378 For the experiments on the small and mid-size 379 datasets, the reported results are calculated from 380 10-fold cross-validation. 381

3.3. Base classifiers and computing systems 382

For the experiments on the small and mid-size 383 datasets, release eight of the C4.5 decision tree 384 system (Quinlan, 1992) and the cascade correlation 385 neural network learning code (Fahlman and 386 Lebiere, 1990) were run on standard SUN work-387 stations and a 24-node Beowulf cluster computer 388 (Mimir). Mimir consists of 900 Mhz Athlon pro-389

N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

¹ ftp.dice.ucl.ac.be in the directory pub/neural-nets/ELENA/ databases.

N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

Table 1				
Data sets	sizes	and	class	distributions

Letter dataset	(UCI)-20,000 sampl	es in 26 classes			
A:789	B:766	C:736	D:805	E:768	F:775
G:773	H:734	I:755	J:747	K:739	L:761
M:792	N:783	O:753	P:803	Q:783	R :758
S:748	T:796	U:813	V:764	W:752	X:787
Y:786	Z:734				
Phoneme datas	set (ELENA)—5404 s	amples in two classes			
0:3818	1:1586				
PenDigits data	set (UCI)—10,992 sa	mples in ten classes			
0:1143	1:1143	2:1141	3:1055	4:1144	5:1055
6:1056	7:1142	8:1055	9:1055		
SatImage data	set (UCI)—6435 sam	ples in six classes			
1:1533	2:703	3:1358	4:626	5:707	7:1508
Mammography	y dataset—11,183 san	ples in two classes			
1:10,923	2:260				
Jones' PDB da	taset—227,260 sampl	es in three classes			
H:75,455		C:100,909		E:50,896	
PDB dataset—	-3,619,461 samples in	three classes			
H:1,254,335	•	C:1,537,261		E:827,865	

390 cessors each with 512 Mb of memory and pro391 cessors are connected with 100 Bt Ethernet. The
392 neural network was only applied to the small data
393 sets due to its extremely long training times and
394 larger memory requirements.

The one run of the large dataset to produce a single classifier was done on a single node of a 64processor SGI IRIX64 with 32 GB of main memory at Sandia National Labs, also using the standard C4.5 release eight. Creating the one decision tree on the large dataset took approximately *thirty days* on the SGI and was not attempted with the much slower neural network learning code.

403 The experiments using partitions of the large 404 dataset were run on the DOE's "ASCI Red" parallel supercomputer (Sandia National Labs, 1998). 405 406 The ASCI Red has 4640 compute nodes, each 407 containing two Pentium III processors sharing 256 MB of memory. The processors run a version of 408 409 the UNIX operating system. The system is based on a distributed-memory mesh architecture, and is 410 capable of 3.15 TeraFLOPS. These experiments 411 412 used a version of C4.5 modified with MPI calls for 413 parallel execution. The parallel structure of this 414 version of C4.5 is quite simple. The disjoint partitions are loaded into the different compute node 415 memories and each compute node independently 416 grows a decision tree. The parallel computation to 417 create eight decision trees on one-eighths of the 418 large dataset takes approximately 8 h; that is, eight 419 processors running in parallel for 8 h. It is possible 420 to create 32 distributed trees built on 1/8 size 421 partitions of the data in approximately 10 h. 422

4.1. C4.5 on small data sets 424

423

Figs. 2–6 summarize the experimental compar-425 ison of the different approaches on the small da-426 tasets detailed in Table 1 for C4.5. The plots 427 compare the performance of two, four, six, and 428 eight disjoint partitions (D) to that of C4.5 on the 429 complete data set, and to classifier committees 430 formed using the other three approaches (DB, SB, 431 NRSB). Results are shown as the average paired 432 difference across the 10 folds in the 10-fold cross-433 validation, with standard error indicated. Note the 434 zero mean accuracy mid-line; if a point is above 435







Fig. 3. Comparison on PenDigits dataset with C4.5.





Fig. 5. Comparison on SatImage dataset with C4.5.

No. of Pages 17, DTD = 4.3.1

SPS, Chennai



Fig. 6. Comparison on Mammography dataset with C4.5.

436 the line, then the first of the alternatives examined437 is superior. If the point is below, then the second438 was best. And the extent to which the error bar439 spans the mid-line is the extent to which the results440 are inconclusive.

441 As an example, the first cluster of four data points on the plot in Fig. 2 represents the results 442 for a committee of two classifiers on the Letter 443 444 data set. The first point is the difference between a committee of two disjoint partitions and C4.5 445 trained on all of the data; note that the committee 446 447 of two classifiers performs significantly worse. The second point is the difference between a committee 448 449 formed using two disjoint partitions versus a committee using two disjoint bags (DB), the third 450 point is two disjoint partitions versus two small 451 bags (SB), and the fourth point is two disjoint 452 partitions versus no-replication small bags 453 454 (NRSB).

From examining the sequence of plots it is clear
that disjoint partitions in a number of instances
beat small bags. It appears to make little difference
whether the small bags are created by sampling

with or without replacement. The ensembles cre-459 ated from "bagged disjoints" appear to generally 460 perform slightly better than those created from 461 simple disjoint partitions, but then the training sets 462 for the individual decision trees have repeated examples which give some examples greater 464 "weight". 465

Because it uses constant-size bags as the number of classifiers in the committee grows larger, 467 "true bagging" should naturally outperform any 468 of the four approaches. Data points for "true 469 bagging" performance are given in Table 2. Tables 470 3 and 4 show the accuracy results obtained by 471 learning four classifiers each built from 1/4 of a 472

Table	2				
Data	points	for	"true	bagging"	results

Dataset	C4.5	50 bags	75 bags	100 bags
Phoneme	86.50	89.15	89.02	88.15
SatImage	86.30	90.89	90.86	90.84
PenDigits	96.57	98.42	98.43	98.36
Mammography	98.50	98.76	98.79	98.79
Letter	88.10	93.54	93.65	93.80

N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

Table 3	
Four partitions/bags	accuracy

	F			
Dataset	D	SB	DB	NRSB
Phoneme	83.25	82.66	83.36	83.22
SatImage	87.24	86.31	87.00	85.95
PenDigits	96.15	95.65	96.33	96.12
Mammography	98.37	98.51	98.38	98.32
Letter	85.44	84.19	85.525	84.83

in percentage using C4.5

Table 4

Four partitions/bags accuracy in percentage using CC

Dataset	D	SB	DB	NRSB
Phoneme	83.75	84.06	83.92	83.59
SatImage	89.43	88.97	89	89.26
PenDigits	90.89	91.01	91.73	90.86
Mammography	97.78	98.19	98.43	98.02
Letter	82.15	81.88	81.96	82.17

473 disjoint four partition utilizing decision trees and

474 neural networks, respectively. Each value in the

475 table is an average over a 10-fold cross-validation.

476 The results from a four partition are representa-

tive, as more partitions cause greater "data star-477 vation" in some of the small domains. Bagging 478 with 50-100 bags clearly outperforms the small 479 ensembles. However, the point is that true bagging 480 is simply not a practical option for large datasets. 481 For the example large dataset here, true bagging 482 would require creating about 50 classifiers, each 483 training on a data set of the same size as the 484 original data. Recall that creating one classifier on 485 all the data took 30 days on a substantial SGI 486 system. When the dataset is too large to handle 487 conveniently in the memory of the typical com-488 puter, the dataset must be broken into some 489 number of practically sized, though not "small," 490 chunks. The question addressed here is whether 491 there is any advantage in creating the practically 492 sized chunks using some bagging-like approach, or 493 whether simple partitioning is sufficient. 494

4.2. Cascade correlation on small datasets 495

Figs. 7–11 summarize the experimental com- 496 parison of the different approaches on the small 497



Fig. 7. Comparison on Letter dataset with cascade correlation.



Fig. 8. Comparison on PenDigits dataset with cascade correlation.



Fig. 9. Comparison on Phoneme dataset with cascade correlation.





Fig. 11. Comparison on Mammography dataset with cascade correlation.

498 datasets detailed in Table 1 using cascade correlation. The data was not normalized. The results 499 500 are similar to those obtained with C4.5. The disjoint partitions are generally as good or better than 501 small bags. The exception is that they lose to small 502 503 bags for a four partition on the Mammography 504 dataset and to DB at every partition in the Mammography data set. The Mammography da-505 taset is highly skewed with a small minority class 506 and the repeated examples in the disjoint bag data 507 508 sets seemed to make an important, if minor, dif-509 ference in accuracy. The other exception is on the PenDigits dataset where the DB approach is better 510 511 for a four partition.

It is interesting that the ensemble of neural 512 513 networks is generally no worse than learning from 514 all the data even when partitioning up the small data into eight subsets. In fact, the ensemble is 515 always better than a single neural network for the 516 Letter data set. In general, the ensembles built 517 from disjoint partitions are no worse than those 518 519 built from bags of the same size for cascade cor-520 relation neural networks.

4.3. Results on mid-size data set

The comparison of the four approaches on the 522 mid-size dataset are shown with C4.5 in Fig. 12. 523 The results are the means of paired differences and 524 the standard error from a 10-fold cross-validation 525 from 4 to 16 disjoint partitions. In all cases the 526 ensemble classifier learned from disjoint partitions 527 resulted in a significantly better classifier than ap-528 plying C4.5 to all of the data. 529

Again, we see that simple disjoint partitioning 530 offers excellent performance in comparison to the 531 other options. In particular, the "small bags" ap-532 proach performs poorly. Only the "bagged dis-533 joints," with its slightly larger number of examples 534 in each bag, offers any hint of performance im-535 provement over disjoint partitions. The "bagged 536 disjoints" have the same number of distinct ex-537 amples with a few repeat examples which essen-538 tially gives the repeat examples greater weight. 539



Fig. 12. Results on (Jones') "medium" PDB dataset.

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N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

14

N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

540 4.3.1. Timing

541 We did a detailed comparison of the time re-542 quired to create an ensemble on the Beowulf cluster for the Jones data set. Table 5 shows the 543 544 average and standard deviation over 10 trials. For 545 disjoint partitioning for a four partition, there is 546 an average of a 9.4 times speed up over learning a decision tree on all the data, which increases to 547 548 26.6 times for an eight partition, 46.1 times for a 16 partition and 71.3 times for a 24 partition. 549 550 While the speed gain is impressive, it is actually 551 true that for very large data sets that do not fit in main memory all the data cannot be practically 552 553 used unless a distributed approach is pursued.

554 4.4. Partitioning results on large dataset

Fig. 13 compares the results of creating one decision tree on all of the large dataset versus using a committee of *N* classifiers, for N = 8, 16, 24, and 32. All of the committees were formed using disjoint partitions of size (1/8)th of the large PDB dataset. This size partition just fills the memory of the compute nodes on the ASCI Red. The N = 8

Га	ble	5

Jones dataset: average and standard deviation of CPU time
longest time taken to learn a decision tree on a partition/bag by
a processor) in seconds for 10-folds

Approach	Average time	Standard deviation
C4.5	9094.38	137.11
4-D	963.61	14.42
4-SB	990.61	17.04
4-NRSB	967.96	21.22
8-D	342.172	8.46
8-SB	352.04	8.98
8-NRSB	339.51	5.45
12-D	197.19	5.52
12-SB	202.55	3.89
12-NRSB	196.98	4.72
16-D	127.48	3.6
16-SB	130.62	1.32
16-NRSB	128.50	2.7

Convention = D: disjoint; SB: small bag; NRSB: no-replication small bag. For instance, four-dimensional means four disjoint partitions.

point represents a straightforward disjoint partitioning, as was used with the smaller datasets. For 563



Fig. 13. Partitioning results for large PDB dataset.

564 the committees of 16, 24, 32, and 40 classifiers, we varied the earlier methodology to make use of 565 multiple different partitions of the dataset. For the 566 committees of 16, 24, 32, and 40 classifiers, mul-567 tiple different partitions of the dataset were used. 568 569 For example, to create a set of sixteen classifiers, 570 eight classifiers trained on a different eight partition of the data were added to those created on the 571 572 original eight-partition. We report an average and standard deviation over five trials of different en-573 574 sembles of trees of the appropriate size.

575 The average accuracy per amino acid of a single 576 classifier trained on (1/8)th of the large dataset is 577 71.21%. A single decision tree created using all the data performs substantially better than this, 578 75.72% versus 71.21%. At the same time, an av-579 580 erage committee of eight classifiers created on (1/8)ths of the data performs substantially better 581 582 than a single tree created on all the data, 79.1%583 versus 75.72%.

584 It took approximately 30 days to create a single 585 tree from all the data and an average of 10 h to 586 create an ensemble of from 8 to 32 trees. We did 587 some experiments to determine the relative speeds of the SGI machine vs. an ASCI Red processor 588 589 and found the ratio to be 1.92 for the same size 590 decision tree learning problem. So, the Red pro-591 cessor is significantly faster. Normalizing for pro-592 cessor speed, the distributed learner can be created 593 approximately 37 times faster than learning from 594 all the data.

595 5. Conclusions and discussion

596 The results support several important conclu-597 sions. The overall conclusion is that datasets too 598 large to handle practically in the memory of the 599 typical computer are appropriately handled by 600 simple partitioning to form a committee of classifiers. More specifically, a committee created using 601 602 disjoint partitions can be expected to perform at 603 least as well as a committee created using the same number and size of bootstrap aggregates ("bags"). 604 605 Also, the performance of the committee of classi-606 fiers can be expected to exceed that of a single 607 classifier built from all the data.

The following considerations may provide in-608 sight into the pattern of results. Practical factors 609 aside, one generally wants (a) each classifier in a 610 committee to be formed using as much data as 611 possible, and (b) the size of the committee to be as 612 large as possible. Practical considerations typically 613 (a) limit the amount of data that can be used in 614 training a single classifier, and (b) limit the size of a 615 classifier committee. If the data set is large enough, 616 or the memory limit small enough, then parti-617 tioning into N disjoint subsets gives a reasonable 618 size committee and this approach should suffice. If 619 the N disjoint partitions result in too small of a 620 committee, then the data set may be partitioned 621 multiple times to increase committee size, as we 622 did in Section 4.4. A typical result from parti-623 tioning the data multiple times is shown in Table 6 624 for the "small" Letter data set. The data set is 625 broken into a two partition five different ways. A 626 10-fold cross-validation is done, meaning that the 627 test set is left out and then the training set parti-628 tioned into halves (eight different ways). From the 629 table, it is clear that accuracy continues to increase 630 and with 16 partitions we are approaching the 631 accuracy of pure bagging (93.8% for 100 bags), 632 considerably outperforming a C4.5 generated de-633 cision tree from the whole data set. 634

Results obtained here seem to support the po-635 sition that bagging results depend simply on ob-636 taining a diverse set of classifiers (Breiman, 1996; 637 Chawla et al., 2001; Dietterich, 2000; Domingos, 638 1996). Building classifiers on disjoint partitions of 639 the data provides a set of classifiers that meet this 640 requirement. Each individual classifier performs 641 similarly, but correctly classifies a (partially) dif-642 ferent set of examples. 643

Table 6								
Multiple two	partitions on	the	Letter	data	set	for	а	10-fold
cross-validatio	on using C4 5							

8									
	Number of two partitions	Accuracy	Standard deviation						
	1	83.645	1.078						
	2	89.225	0.522						
	3	91.21	0.589						
	4	91.885	0.461						
	5	92.26	0.427						

C4.5 is 88.1% accurate in a 10-fold CV.

N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

16

N.V. Chawla et al. | Pattern Recognition Letters xxx (2002) xxx-xxx

644 Some researchers have suggested that many 645 large-data-set problems can be solved using only a 646 fraction of the data, perhaps by simple subsampling. However, recent work has suggested that all 647 the data (even for very large training data sets) 648 649 may result in the maximal accuracy classifier 650 (Perlich et al., in press). Classical pattern recog-651 nition would suggest that this question is more 652 appropriately viewed in terms of the density of 653 training sample population in the feature space, 654 rather than simply the size of the dataset. There is 655 excess data only when (parts of) feature space are densely populated. The fact that the average 656 657 (1/8)th partition of our large dataset had perfor-658 mance of 71.21%, whereas a single classifier 659 trained on all the data gave 75.72%, indicates that 660 the original data could not be profitably subsampled in a simple way. Given that the problem has a 661 662 340-dimension feature space, this is perhaps not 663 surprising, as even 3.6 million examples can result 664 in a sparse population of such a space.

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