Classification with Guaranteed Probability of Error

Marco C. Campi

Department of Electrical Engineering
University of Brescia
Via Branze 38, 25123 Brescia, Italy
E-mail: marco.campi@ing.unibs.it
webpage: http://www.ing.unibs.it/∼campi

Abstract

We introduce a general-purpose learning machine that we call the *Guaranteed Error Machine*, or GEM, and two learning algorithms, a *real GEM algorithm* and an *ideal GEM algorithm*. The real GEM algorithm is for use in real applications, while the ideal GEM algorithm is introduced as a theoretical tool; however, these two algorithms have identical behavior most of the time. Differently from most learning machines, GEM has a ternary-valued output, that is besides 0 and 1 it can return an *unknown* label, expressing doubt. Our central result is that, under general conditions, the statistics of the generalization error for the ideal GEM algorithm is universal, in the sense that *it remains the same, independently of the (unknown) mechanism that generates the data.* As a consequence, the user can select a desired level of generalization error and the learning machine is automatically adjusted so as to meet this desired level, and no knowledge of the data generation mechanism is required in this process; the adjustment is achieved by modulating the size of the region where the machine returns the *unknown* label. The key-point is that no conservatism is present in this process because the statistics of the generalization error is known. We further show that the generalization error of the real algorithm is always no larger than the generalization error of the ideal algorithm. Thus, the generalization error computed for the latter can be rigorously used as a bound for the former, and, moreover, it provably provides tight evaluations in normal cases.

Keywords: computational learning theory, guaranteed generalization error, convex optimization, invariant statistics, ternary-valued classifiers

1 Introduction

1.1 Preliminaries and notations

Machine learning studies the problem of predicting the *class label* of *instances*. An instance x, $x \in \mathbb{R}^d$, is a vector of measured attributes, and the class label y is a discrete quantity, belonging to a finite set, whose value is determined by x, that is there exists a function $y = y(x)$. We here consider binary classification, i.e. $y \in \{0, 1\}$. 0 and 1 represent two different classes, whose meaning varies depending on the application at hand and can e.g. be sick or healthy, right or wrong, male or female. To an x, there is associated a $y \in \{0, 1\}$, but we have no access to the map $y = y(x)$, so, given an x, we have to guess its class y by means of some *classifier* $\hat{y} = \hat{y}(x)$. A binary-valued classifier returns the value 0 or 1 and it errs on x if $y(x) \neq \hat{y}(x)$, and the goal of machine learning is that of constructing classifiers that err as rarely as possible. Later we shall generalize this point of view by introducing ternary-valued classifiers that can also provide an unknown answer, expressing doubt.

In *statistical* machine learning, it is assumed that x values occur according to a probability μ and the reliability of a classifier is measured by $\mu(y(x) \neq \hat{y}(x))$, the probability of the set in $\mathbb{R}^d$ where $y(x)$ and $\hat{y}(x)$ do not agree. $\mu(y(x) \neq \hat{y}(x))$ is called the *probability error* (or *generalization error*) and it will be indicated in this paper with $PE(\hat{y})$.

Given $\hat{y}(\cdot)$, $PE(\hat{y})$ cannot be computed, for its computation would require knowledge of μ and $y(\cdot)$. Hence, selecting a good classifier cannot rely on direct minimization of this probability. Instead, we assume that one has access to a database of past examples $\mathcal{E}_N := (x_1, y_1), \ldots, (x_N, y_N)$, where the x_i's are independently extracted according to μ and $y_i = y(x_i)$, and is asked to select a classifier $\hat{y}_N(\cdot)$ based on $\mathcal{E}_N$. An algorithm is a rule that makes this selection.

See e.g. [8, 19, 6] for general presentations of machine learning.

1.2 The stochastic nature of $\mathbf{PE(\hat{y}_N)}$

$PE(\hat{y}_N)$ is a random quantity since it depends on $\mathcal{E}_N$. This is to say that different sets of examples can be more or less effective to form an estimate of $y(\cdot)$ and, when an algorithm is fed with $\mathcal{E}_N$, it returns a classifier $\hat{y}_N(\cdot)$ that more or less closely match $y(\cdot)$ depending on the seen $\mathcal{E}_N$.

In more formal terms, let us consider a given fixed data generation mechanism, that is a pair $(\mu, y(\cdot))$. This assigns a probabilistic model according to which each single example $(x_i, y_i) = (x_i, y(x_i))$ is drawn. From this model, a probabilistic model for $\mathcal{E}_N$ can be obtained by the independence of examples: a multi-extraction of instances $x_1, x_2, \ldots, x_N$ is selected in $(\mathbb{R}^d)^N = \mathbb{R}^d \times \cdots \times \mathbb{R}^d$ according to the product probability $\mu^N := \mu \times \cdots \times \mu$, and this multi-extraction maps into $\mathcal{E}_N := (x_1, y(x_1)), \ldots, (x_N, y(x_N))$. Thus, $\mathcal{E}_N$ is a random variable defined over $((\mathbb{R}^d)^N, \mu^N)$. If we now choose an algorithm, to each $\mathcal{E}_N$ a classifier $\hat{y}_N(\cdot)$ is associated and in turn $PE(\hat{y}_N) = \mu(y(x) \neq \hat{y}_N(x))$ becomes a fixed number for any given

$\mathcal{E}_N$. Thus, through $\mathcal{E}_N$, $PE(\hat{y}_N)$ is a random variable defined over $((\mathbb{R}^d)^N, \mu^N)$.

One fact that is important to make explicit is that $PE(\hat{y}_N)$ is a random variable whose probabilistic characteristics, its distribution in particular, depend on the unknown data generation mechanism $(\mu, y(\cdot))$. Thus, the same algorithm can generate classifiers that are likely to be more or less reliable depending on the context in which the algorithm is applied.

1.3 The Guaranteed Error Machine

In this paper, we introduce $\{0, 1, unknown\}$-valued classifiers that have a guaranteed probability of error, also called Guaranteed Error Machines (GEM). The learning algorithm for the GEM has a tunable parameter k which may be used to enlarge the region where the classifier does provide a classification, that is it returns a value 0 or 1. A large value of k leads to classifiers that are more likely to return a 0 or 1 value, but these classifiers misclassify more frequently, whereas smaller values of k correspond to more risk-adverse classifiers paying emphasis on reducing the probability of misclassification, but also returning *unknown*'s with higher probability.

In more precise terms, let us start by generalizing to $\{0, 1, unknown\}$-valued classifiers the definition of probability of error: define $PE(\hat{y}_N) = \mu(\hat{y}_N(x) = 0 \text{ } or \text{ } 1, \text{ } and \text{ } y(x) \neq \hat{y}_N(x))$, that is $PE(\hat{y}_N)$ is now the probability that an answer is issued and this answer is incorrect. First, we introduce an *ideal* GEM *algorithm*. For each value of the tunable parameter k, we compute the *exact probability distribution* of $PE(\hat{y}_N)$, and show that, under mild conditions, this distribution *does not depend on the data generation mechanism* $(\mu, y(\cdot))$. This deep theoretical result bears important practical implications: when selecting the tunable parameter k, the user has full control on how $PE(\hat{y}_N)$ distributes since this distribution does not depend on the unknown element of the problem, the data generation mechanism $(\mu, y(\cdot))$. Thus, the user can choose a level of risk and select that k that meets the selected risk level, even without any knowledge of $(\mu, y(\cdot))$. For simple-to-estimate data generation mechanisms, the algorithm will construct classifiers that return a 0 or 1 answer most of the time, while an *unknown* will be more often issued in case of difficult-to-estimate data generation mechanisms. The very point is that no conservatism is present in this selection procedure since the algorithm pushes the classifier all way down to the desired level of risk, automatically and without prior knowledge on the data generation mechanism.

The ideal GEM algorithm selects the size of the unknown region to tune the level of risk. Like pulling down one end of a rope wrapped around a pulley lifts the other end, similarly in the ideal GEM algorithm pulling down the level of risk determines an increase in the size of the *unknown* region. This tuning mechanism, however, is effective until the *unknown* region is present, that is it does not shrink to the empty set so that the classifier classifies the whole x space. In the ideal GEM algorithm, when this happens an *unknown* region is artificially introduced to preserve the possibility to tune.

The ideal GEM algorithm is used in this paper merely as a theoretical tool, and it is not for use in real applications. We next introduce a *real* GEM *algorithm*, the algorithm used in practice. The machine obtained with the real GEM algorithm is identical to that constructed by the ideal GEM algorithm, except that the artificial *unknown* region is not introduced. As a consequence, most of the time the two algorithms work the same, while in simple-to-estimate classification problems the real GEM algorithm may reach the condition of total classification (no *unknown*'s) even before hitting the selected level of risk. Hence, we show that the probability of error of the real GEM algorithm is always no more than that of the ideal GEM algorithm and the results valid for the ideal GEM algorithm can therefore be rigorously used to establish reliability results for the real GEM algorithm.

Further discussion on the theoretical results and on their use is postponed to Section 3 after the GEM algorithms have been formally introduced in the next Section 2.

1.4 A bibliographical note

Classifiers that can choose not to classify (like our *unknown* here) have been previously introduced by other authors in contexts different from ours. A Bayesian classifier with rejection option was considered as early as in [4]. See [5, 10, 14, 9, 15] for other studies. However, although classifiers that can choose not to classify are valuable in practice, few theoretical results are to date available, a fact also recently noted in [11, 2],

2 The GEM algorithm

We first introduce the real GEM algorithm (henceforth also simply called the GEM algorithm), then followed by the ideal GEM algorithm obtained as a modification of the GEM algorithm. In the algorithms, k is an integer that has to be fixed in advance; depending on k, different probability distributions for $PE(\hat{y}_N)$ are obtained, as given in Theorem 1. We also recall that d is the size of x and N is the number of examples. Throughout, we assume $k \leq N - 1$.

THE GEM ALGORITHM

0. Let $x_B = x_1$, $j = 1$, $P = \{2, 3, \ldots, N\}$, and $Q = \emptyset$ (empty set).

1. **If** $|Q| \leq k - (d(d+1)/2 + d)$ ($|\cdot|$ means cardinality), go to point 2a;
elseif $k - (d(d+1)/2 + d) < |Q| \leq k - (d+1)$, go to point 2b;
else, go to point 2c.

2a. Solve the following convex optimization problem:

$$\min_{A=A^T \in \mathbb{R}^{d \times d}, b \in \mathbb{R}^d} \quad Trace(A)$$

$$\text{subject to:} \qquad (x_i - x_B)^T A (x_i - x_B) + b^T (x_i - x_B) \geq 1, \quad \text{for all } i \in P \text{ such that } y_i \neq y(x_B)$$
$$\text{and } A \succeq 0 \quad \text{(A semi-definite positive).}$$

If more than one pair (A, b) solves the problem, take the pair (A, b) with smallest norm of b, $\|b\| = \sqrt{\sum_{r=1}^{d} b_r^2}$. If a tie still occurs, break it according to a lexicographic rule on the elements of A and b. Let (A^*, b^*) be the optimal solution.
Go to point 3.

2b. Solve the following convex optimization problem:

$$\min_{a \geq 0} \quad a$$

$$\text{subject to:} \quad a \cdot \|x_i - x_B\|^2 + b^T (x_i - x_B) \geq 1, \quad \text{for all } i \in P \text{ such that } y_i \neq y(x_B).$$

If more than one pair (a, b) solves the problem, take the pair (a, b) with smallest norm of b. Let (a^*, b^*) be the optimal solution, and define $A^* = a^* I$ (I = identity matrix).
Go to point 3.

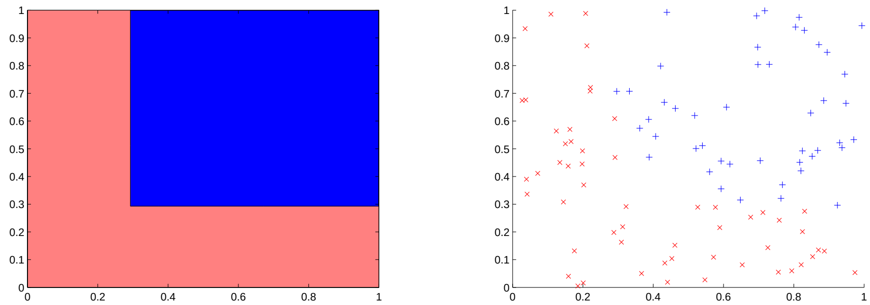
2c. Solve the following convex optimization problem:

$$\min_{a \geq 0} \quad a$$

$$\text{subject to:} \quad a \cdot \|x_i - x_B\|^2 \geq 1, \qquad \text{for all } i \in P \text{ such that } y_i \neq y(x_B).$$

Let a^* be the optimal solution, and define $A^* = a^* I$ and $b^* = 0$.
Go to point 3.

3. Form the region $\mathcal{R}_j = \{x : (x - x_B)^T A^* (x - x_B) + (b^*)^T (x - x_B) < 1\}$, and let $\ell_j = y(x_B)$.



(a) (b)

Figure 1: **(a)** function $y(x)$, upper square has label 1. **(b)** data set: x= 0, += 1.

Update P by removing the indexes of the instances in $\mathcal{R}_j$. If P is empty, go to point 4; update $Q = Q \cup \{\text{indexes of the active instances}\}$, where the "active" instances are those that fall on the boundary of $\mathcal{R}_j$;
if $|Q| < k$, search for the "active" instance furthest away from x_B (if there is more than 1 instance at the furthest distance from x_B take any one of them) and rename as x_B this instance; let $j = j + 1$, and go to point 1;
else, go to point 4.

4. Define the classifier

$$\hat{y}_N(x) = \begin{cases} \text{unknown}, & \text{if } x \notin \mathcal{R}_r, 1 \leq r \leq j \\ \ell_q, & \text{otherwise, with } q = \min r \text{ such that } x \in \mathcal{R}_r, 1 \leq r \leq j. \end{cases}$$

*

Points 2a, 2b, and 2c construct regions containing examples all having the same class label as the label $y(x_B)$ of the "base" instance x_B, and classify these regions according to $y(x_B)$. Point 2a constructs regions more complex than 2b, which are in turn more complex than those in 2c: 2a constructs (hyper)ellipsoids containing x_B, those in 2b are (hyper)spheres containing x_B, while those in 2c are (hyper)spheres having x_B at their center. If P does not become empty, the procedure is halted when the total number of the active instances $|Q|$ reaches the selected bound k, and re-directing the algorithm to simpler constructions when $|Q|$ gets close to k as done in point 1 serves the purpose of exactly reaching k upon termination of the algorithm. As we shall see, this is the key-property to make the generalization error of the algorithm guaranteed.

To help the reader understand the algorithm operation, a toy example is provided in Figures 1 and 2. Figure 1(a) represents the function $y(x)$; $N = 100$ examples were extracted

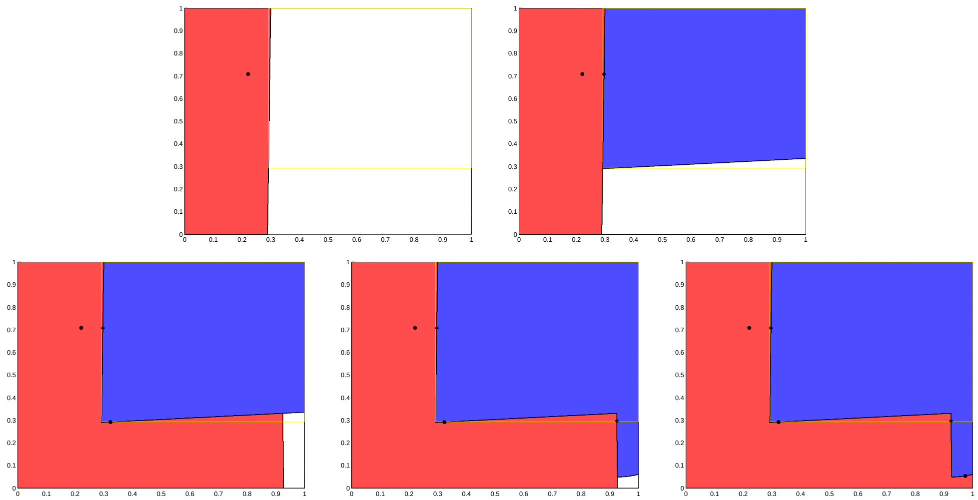


Figure 2: The regions constructed by the GEM algorithm.

according to a uniform distribution and they are shown in Figure 1(b). We set $k = 5$ and executed the GEM algorithm. The algorithm performed 1 construction according to point 2a, 2 constructions according to 2b, and 2 constructions according to 2c, determining each time $n = 1$ active instances. Figure 2 displays the regions constructed in succession by the algorithm. No unknown region was left at the end.

If the GEM algorithm terminates at point 3 with P empty, then it is easy to see that all the $\mathbb{R}^d$ space of x is classified. The ideal GEM algorithm is defined as a modification of the real GEM algorithm, where the modification is effective only when P becomes empty:

THE IDEAL GEM ALGORITHM

Add at the end of point 4 of the real GEM algorithm the following part:
"If P is empty, construct the largest open ball $\mathcal{B}$ centered in x_1 that contains other (besides x_1) $k - |Q| - 1$ of the instances x_i, $i \in \{2, 3, \ldots, N\} - Q$. So, if e.g. $k = 20$ and $|Q| = 18$, $\mathcal{B}$ contains just one instance and, by enlarging $\mathcal{B}$ as much as possible, it touches another instance at its boundary. Then, let $Q = Q \cup \{$indexes of the instances inside and on the boundary of $\mathcal{B}\}$, and redefine $\hat{y}_N(x) = 1 - y(x)$ for all x in $\mathcal{B}$ except for the instances x_i, $i \in \{2, 3, \ldots, N\} - Q$, for which we maintain a correct classification $\hat{y}_N(x_i) = y(x_i)$; thus, $\hat{y}_N(x)$ misclassifies all $x \neq x_i$ in $\mathcal{B}$." $*$

The ideal GEM algorithm cannot be used in practice since the redefinition of $\hat{y}_N(x)$ in the ball $\mathcal{B}$ requires knowledge of $y(x)$; and, moreover, it would not certainly make sense in practice to deliberately misclassify in $\mathcal{B}$! We show in Theorem 1 that, for the ideal GEM algorithm, $PE(\hat{y}_N)$ is exactly distributed as a Beta variable, independently of $(\mu, y(\cdot))$. We also show that this Beta can be used to bound the misclassification of the real GEM algorithm, which always misclassify no more than the ideal GEM algorithm. Since the modification in the ideal GEM algorithm is effective only in the special condition of total classification, for normally assumed risk levels the two algorithms behave the same and the Beta distribution provides tight risk evaluations for the real GEM algorithm as well.

Theorem 1 *Suppose that the probability μ according to which x values are extracted has density. Then, the probability distribution of $PE(\hat{y}_N)$ for the ideal GEM algorithm is given by*

$$F_{PE}(z) := \mu^N\{PE(\hat{y}_N) \leq z\} = \sum_{i=k}^{N-1} \binom{N-1}{i} z^i (1-z)^{N-1-i}. \tag{1}$$

Note that $F_{PE}(z)$ does not depend on the data generation mechanism $(\mu, y(\cdot))$.
Moreover, this $F_{PE}(z)$ "dominates" the probability distribution of $PE(\hat{y}_N)$ for the real GEM algorithm, in the sense that $\mu^N\{PE(\hat{y}_N) \leq z\} \geq \sum_{i=k}^{N-1} \binom{N-1}{i} z^i (1-z)^{N-i}$ for this algorithm.

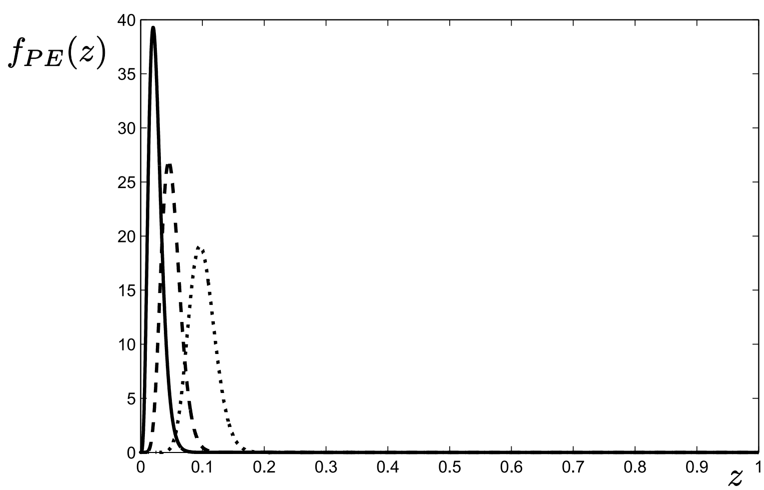


Figure 3: The $Beta(k, N-k)$ density. $N = 200$, $k = 5$ (solid), 10 (dashed), 20 (dotted).

In the theorem, $\mu^N = \mu \times \cdots \times \mu$ is the product probability according to which the examples $\mathcal{E}_N = (x_1, y_1), \ldots, (x_N, y_N)$ are extracted. The right-hand-side of (1) is a $Beta(k, N-k)$ distribution (see e.g. [17]), and in words the theorem says that the probability of error $PE(\hat{y}_N)$ of the ideal GEM algorithm distributes as a $Beta(k, N-k)$ variable, irrespective of the data generation mechanism $(\mu, y(\cdot))$. Moreover, for the real GEM algorithm, $PE(\hat{y}_N) \leq z$ holds with probability no less than that for the ideal GEM algorithm. To visualize the result, the density of a $Beta(k, N-k)$ is depicted in Figure 3 for a few values of N and k.

The proof of Theorem 1 is given in Section 5. In the next section, we discuss the practical use of the GEM algorithm, while Section 4 presents some empirical results with real data.

3 Practical use of the GEM algorithm

A number of remarks on the interpretation of the results, as well as on their practical use, are in order.

(i) The theoretical result

The fact that in the ideal GEM algorithm $PE(\hat{y}_N)$ has a $Beta(k, N-k)$ distribution that does not depend on how the examples are generated is, we believe, a deep theoretical result. It can be phrased by saying that the distribution of $PE(\hat{y}_N)$ is *universal*. The $Beta(k, N-k)$ distribution also tightly describes the behavior of the real GEM algorithm, as confirmed by the empirical results in Section 4, and, in any case, it provides theoretically guaranteed lower bounds for the probability that $PE(\hat{y}_N) \leq z$.

(ii) A Monte-Carlo test

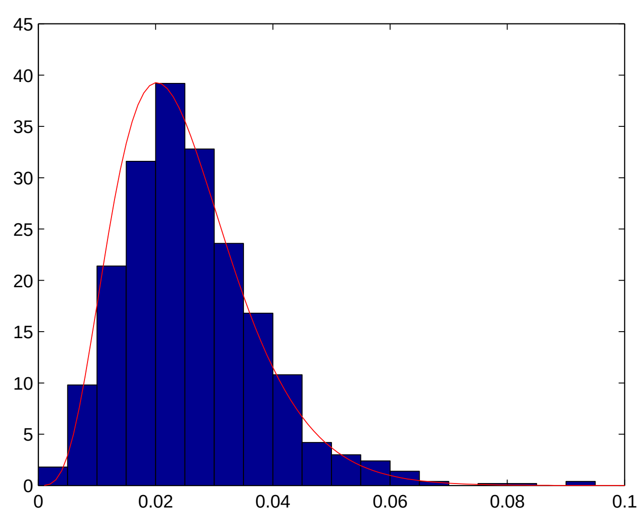


Figure 4: Histogram of $PE(\hat{y}_{200})$.

A Monte-Carlo test was performed for the $y(x)$ function represented in Figure 1(a).

$N = 200$ examples were extracted $M = 1000$ times. For each multi-extraction of 200 examples, we constructed the classifier $\hat{y}_{200}$ with the ideal GEM algorithm with $k = 5$ and then computed the associated $PE(\hat{y}_{200})$. Note that this computation is here possible due to the artificial nature of the example, i.e. $(\mu, y(\cdot))$ is known. The histogram obtained from the $M = 1000$ trials is shown in Figure 4 against the theoretical $Beta(5, 200-5)$ density. Should we have extracted x values according to a probability density different from the uniform one, or should the $y(x)$ function have been a different one, the density of $PE(\hat{y}_{200})$ would have remained the same.

(iii) Practical use of the result

The $Beta(k, N-k)$ distribution can be used in different ways.

A first use is that one selects a risk level $\bar{z}$ and requires that $PE(\hat{y}_N) \leq \bar{z}$ holds with high probability. Since the $Beta(k, N-k)$ tail is very thin, $PE(\hat{y}_N) \leq \bar{z}$ can be enforced with such a high level of probability that the complement event that $PE(\hat{y}_N) > \bar{z}$ looses any practical relevance. To appreciate this behavior, in Table 1 we give the probability that $PE(\hat{y}_N) > \bar{z}$ for $\bar{z} = 5\%$ and $N = 1000$ for different values of k.

k	1	2	3	4	5
pr	$5.5\ 10^{-23}$	$2.9\ 10^{-21}$	$7.9\ 10^{-20}$	$1.4\ 10^{-18}$	$1.9\ 10^{-17}$

k	10	15	20	25	30
pr	$5.4\ 10^{-13}$	$9.7\ 10^{-10}$	$2.9\ 10^{-7}$	$2.4\ 10^{-5}$	$7.3\ 10^{-4}$

Table 1: $pr := \mu^N\{PE(\hat{y}_N) > 5\%\}$ for different values of k, $N = 1000$.

For a quick evaluation of the largest k such that $\mu^N\{PE(\hat{y}_N) > \bar{z}\}$ is a rare event with probability no more than a given $\bar{pr}$, one can resort to the Chernoff bound for the $Beta$ tail, see [3] for the original reference or e.g. [20], yielding

$$k \leq \frac{1}{2}(N-1)\bar{z} + \ln \bar{pr}. \tag{2}$$

To see this, note that this last inequality implies

$$\ln \bar{pr} \geq k - \frac{1}{2}(N-1)\bar{z} \geq k - \frac{1}{2}(N-1)\bar{z} - 1 - \frac{(1-k)^2}{2(N-1)\bar{z}} = -\frac{[(N-1)\bar{z} + (1-k)]^2}{2(N-1)\bar{z}}, \tag{3}$$

so that $\bar{pr} \geq exp\left(-\frac{[(N-1)\bar{z}+(1-k)]^2}{2(N-1)\bar{z}}\right)$. On the other hand, the Chernoff bound says that the tail for $z > \bar{z}$ of a $Beta(k, N-k)$ distribution is no more than $exp\left(-\frac{[(N-1)\bar{z}+(1-k)]^2}{2(N-1)\bar{z}}\right)$, so leading to the conclusion that

$$\bar{pr} \geq \text{"tail for } z > \bar{z} \text{ of a } Beta(k, N-k)\text{"} \geq \mu^N\{PE(\hat{y}_N) > \bar{z}\}.$$

For e.g. $N = 1000$, $\bar{z} = 5\%$ and $\bar{pr} = 2.4\ 10^{-5}$, (2) gives $k = 14$ (compare with Table 1 where the real k is 25).

A second use of the $Beta(k, N-k)$ distribution is to tune k so that the total probability of seeing N examples and that the next $(N+1)$-th example is misclassified is below a fixed threshold. This probability is given by the mean of $PE(\hat{y}_N)$. It can be computed by observing that the $Beta$ density is $f_{PE}(z) := \frac{d}{dz}F_{PE}(z) = \binom{N-1}{k} k z^{k-1}(1-z)^{N-1-k}$, so that, by integration by parts, one obtains:

$$E[PE(\hat{y}_N)] = \int_0^1 z f_{PE}(z) dz = \frac{k}{N}. \tag{4}$$

Thus, with e.g. $N = 1000$ examples one can be 5% confident that the 1001-st example will not be misclassified provided that $k = 50$.

(iv) An impossibility result

Obtaining a result similar to Theorem 1 for $\{0,1\}$-valued classifiers is impossible. Theorem 1 says that $PE(\hat{y}_N)$ distributes as a $Beta(k, N-k)$ variable and, therefore, the probability of the event $\{PE(\hat{y}_N) > z\}$ can be tuned to be small at will by suitably selecting k and N. Instead, for $\{0,1\}$-valued classifiers the following FACT holds:

FACT: *Let $\rho > 0$ be any small number. For any N and for any algorithm generating $\{0,1\}$-valued classifiers, there exist a data generation mechanism $(\mu, y(\cdot))$ such that*

$$\mu^N\{PE(\hat{y}_N) > \bar{z}\} \geq 0.5 - \bar{z} - \rho.$$

*

This FACT immediately follows from Theorem 7.1 in [8], a theorem originally proven in [7]. Thus, with e.g. $\rho = 0.1$ we see that $\mu^N\{PE(\hat{y}_N) > \bar{z} = 5\%\} \geq 0.5 - 0.05 - 0.1 = 0.35$ and no algorithm exists guaranteeing that the probability of error is below 5% with high probability close to 1, no matter how large N is. This is not a surprising fact: for any large N, there are difficult-to-estimate data generation mechanisms $(\mu, y(\cdot))$ where the algorithm fails to behave satisfactorily, if the algorithm is not allowed to issue an *unknown*.

(v) More general algorithms

An inspection of the proof of Theorem 1 reveals that the key-property of the ideal GEM algorithm to make the result valid is that, upon termination, the algorithm has stored k active instances in Q. Other constructions than those in points 2a, 2b, and 2c of the algorithm permits to obtain this result. For example, one can introduce one more construction where the elements of A and b are constrained in such a way that the total number of degrees of freedom of the corresponding optimization problem is, say, p and enter this point only if $|Q| \leq k - p$. Theorem 1 easily extends to cover this case. More in general, along extensions similar to that just traced, the analysis of this paper carries over to a whole family of variants of the GEM algorithm.

(vi) The case of stochastic $\mathbf{y}(\mathbf{x})$

So far we have assumed that, given an x, $y(x)$ is univocally determined. Generalizing this situation, we can now consider the possibility that $y(x)$ is not totally determined by x and that it can take value 0 or 1 according to a random scheme. To formalize this situation, introduce the space $\mathbb{R}^d \times \{0,1\}$ for the examples (x, y) and let now μ be a probability defined over $\mathbb{R}^d \times \{0,1\}$ according to which the examples are extracted. In this context, $\hat{y}(x)$ is still a classifier constructed according to the GEM algorithms that associates just one value to each x, and we let $PE(\hat{y}) = \mu((x,y) : y \neq \hat{y}(x))$. The proof of Theorem 1 remains substantially unchanged in this case, and one can easily prove that the theorem results carry over to quantify the probability of error for a stochastic $y(x)$ as well.

4 Empirical results

We present empirical results obtained by applying GEM to some publicly available data sets, Glass, Iris, BreastW, Haberman, Pima, Bupa, Credit. The first data set has been obtained from `http://www.cs.utsa.edu/~bylander/cs4793/`, while the other six have been downloaded from the UCI machine learning repository, [1].

Tables 2 - 4 display the results obtained with Glass and Iris, where with Iris we have classified in Table 3 Iris Setosa vs other Iris types (Versicolor and Virginica) and in Table 4 we have eliminated the examples of Iris Setosa from the data set and have classified Iris Versicolor vs Iris Virginica. k is the tunable parameter in the GEM algorithm; $\#\ of\ errors$ is the total number of errors in a 10-fold cross validation. Precisely, we left out each time a number of examples equal to the integer part of the total number of examples divided by 10, and these examples were used as a test set. $\#\ of\ errors$ was then computed as the sum of the errors found in the test set at each trial. In parentheses, we have reported the ratio $\frac{\#\ of\ errors}{total\ \#\ of\ test\ examples}$, an estimate of the expected probability of error; $\#\ of\ unknowns$ and $\#\ of\ correct$ is obtained similarly to $\#\ of\ errors$ summing the number of unknowns and of correctly classified examples in the 10 test sets; the last row gives the theoretical value of $E[PE(\hat{y}_N)]$, computed using (4). This theoretical value should be compared with the empirical ratio $\frac{\#\ of\ errors}{total\ \#\ of\ test\ examples}$, and we notice a tight adherence between the two. The theoretical value is guaranteed and when the empirical ratio exceeds the theoretical value we have to think that this is imputable to the stochastic fluctuation of the former. In a real application, the user selects a reliability level and tunes k accordingly, guided by the theory. The algorithm adjusts the learning machine automatically to hit the desired reliability level, and the user can a-posteriori inspect the number of unknowns. A large number of unknowns indicates that the classification problem was a difficult one and the user can select his/her favorite compromise between reliability and number of unknowns.

k	3	9	10	20	30	40	44
$\#\ of\ errors$	3 (1.88%)	8 (5.00%)	10 (6.25%)	16 (10.00%)	26 (16.25%)	47 (29.38%)	48 (30.00%)
$\#\ of\ unknowns$	127	103	113	75	35	1	0
$\#\ of\ correct$	30	49	37	69	99	112	112
$E[PE(\hat{y}_N)]$	2.04%	6.12%	6.80%	13.61%	20.41%	27.21%	29.93%

Table 2: Glass, # of examples = 163.

k	2	3	4
$\#\ of\ errors$	2 (1.43%)	3 (2.14%)	3 (2.14%)
$\#\ of\ unknowns$	5	4	0
$\#\ of\ correct$	133	133	137
$E[PE(\hat{y}_N)]$	1.48%	2.22%	2.96%

Table 3: Iris Setosa, # of examples = 149.

In Tables 5 through 9 we have similar results for BreastW, Haberman, Pima, Bupa, Credit. Strictly speaking, for these data sets Theorem 1 is not applicable because some attributes are discrete and therefore μ has no density. However, an inspection of the theorem proof reveals that the existence of the density serves only to prevent degenerate situations from occurring where some instances fall exactly on the boundary of the region generated by other instances, a fact that generally does not happen even when μ has no density. Again we notice a good

k	3	4	5	6	10
# *of errors*	1 (1.11%)	3 (3.33%)	5 (5.56%)	6 (6.67%)	8 (8.89%)
# *of unknowns*	73	64	7	4	0
# *of correct*	16	23	78	80	82
$E[PE(\hat{y}_N)]$	3.33%	4.44%	5.56%	6.67%	11.11%

Table 4: Iris Versicolor vs Iris Virginica, # of examples = 99.

adherence between the theoretical value and the practical behavior, showing the robustness of the theoretical result.

k	5	10	15	20	25	30	35
# *of errors*	5 (0.74%)	12 (1.76%)	20 (2.94%)	25 (3.68%)	26 (3.82%)	29 (4.26%)	31 (4.56%)
# *of unknowns*	378	347	148	106	49	16	0
# *of correct*	297	321	512	549	605	635	649
$E[PE(\hat{y}_N)]$	0.81%	1.63%	2.44%	3.25%	4.07%	4.88%	5.69%

Table 5: BreastW, # of examples = 683.

k	10	20	40	60	80	90	100
# *of errors*	12 (4.14%)	24 (8.28%)	41 (14.14%)	59 (20.34%)	85 (29.31%)	95 (32.76%)	101 (34.83%)
# *of unknowns*	252	217	159	105	39	15	0
# *of correct*	26	49	90	126	166	180	189
$E[PE(\hat{y}_N)]$	3.77%	7.55%	15.09%	22.64%	30.19%	33.96%	37.74%

Table 6: Haberman, # of examples = 294.

k	10	30	50	100	150	200	250
# *of errors*	9 (1.18%)	28 (3.68%)	49 (6.45%)	114 (15.00%)	158 (20.79%)	209 (27.50%)	241 (31.71%)
# *of unknowns*	724	657	601	402	244	92	0
# *of correct*	27	75	110	244	358	459	519
$E[PE(\hat{y}_N)]$	1.45%	4.34%	7.23%	14.45%	21.68%	28.90%	36.13%

Table 7: Pima, # of examples = 768.

We further compared GEM with other methods, the nearest-neighbor classifier (NNC, [8]), the support vector machine (SVM, [19, 6]) with $C = \infty$ and with finite C, and the simple

k	10	15	30	50	90	120	135
$\# \; of \; errors$	11 (3.24%)	16 (4.71%)	31 (9.12%)	50 (14.71%)	89 (26.18%)	122 (35.88%)	129 (37.94%)
$\# \; of \; unknowns$	308	303	255	203	104	15	0
$\# \; of \; correct$	21	21	54	87	147	203	211
$E[PE(\hat{y}_N)]$	3.22%	4.82%	9.65%	16.08%	28.94%	38.59%	43.41%

Table 8: Bupa, # of examples = 345.

k	10	30	50	80	100	135	150
$\# \; of \; errors$	12 (1.85%)	39 (6.00%)	66 (10.15%)	100 (15.38%)	117 (18.00%)	153 (23.54%)	153 (23.54%)
$\# \; of \; unknowns$	597	445	339	199	138	13	0
$\# \; of \; correct$	35	166	245	351	395	484	497
$E[PE(\hat{y}_N)]$	1.70%	5.10%	8.50%	13.61%	17.01%	22.96%	25.51%

Table 9: Credit, # of examples = 653.

set covering machine (SCM, [13, 12]) of type c (conjunction) and d (disjunction) and with finite p and s (which provide better performance that the SCM with infinite p and s). Since all these methods do not use unknowns, to perform a comparison we chose the k value in GEM to be the first k giving 0 unknowns. Moreover, as explained above, with GEM each trial we left out as test examples a number of examples equal to the integer part of one tenth of the total number of the examples, so that summing up all the test examples we do not reach exactly the total size of the data set. Thus, to provide a fair comparison with the other methods, we have multiplied the number of errors observed with GEM by the ratio between the total number of examples divided by the total number of test examples. Table 10 gives the results, where the figures for NNC, SVM and SCM have been taken from [13]. It may seem that GEM does not compare favorably with the other methods in most of the cases. However, it is important to remark that the reported figures for SVM and SCM are those that achieved the smallest 10-fold cross validation error among an exhaustive scan of many values of the free parameters (the kernel parameter γ and the soft margin parameter C for SVM, and parameters p and s for SCM). Thus, these parameters are "tuned" to the data set and the figures in Table 10 are underestimates of the real generalization error. On the contrary, with GEM *we displayed the results obtained in one single algorithmic run* and the obtained figures are reliable estimates of the generalization error, as confirmed by their adherence to the theoretical value of $E[PE(\hat{y}_N)]$.

	GEM	NNC	SVM ($C = \infty$)	SVM (finite C)	SCM type c	SCM type d
Glass	48.2	36	42	34	35	36
BreastW	31.1	29	27	19	18	16
Haberman	103.6	107	111	71	71	93
Pima	243.5	247	243	203	189	206
Bupa	130.9	124	121	107	109	106
Credit	153.7	214	205	190	198	195

Table 10: # of errors, comparison of different methods.

5 Proof of Theorem 1

We start with some set-theory results.

Consider a set Z and two maps m and t as follows.
Let k be a fixed integer. Given a finite set of at least k points of Z, say $\{z_1, z_2, \dots, z_p\}$ with $p \geq k$, $m\{z_1, z_2, \dots, z_p\}$ extracts k of these points and returns the set that contains the extracted points. However, we do not require that m is always defined, that is there can be sets $\{z_1, z_2, \dots, z_p\}$ for which $m\{z_1, z_2, \dots, z_p\}$ is not defined (this will help us in the construction of m for the classification problem, see later on). What we instead require is that m is always defined when $p = k$, in which case $m\{z_1, z_2, \dots, z_k\} = \{z_1, z_2, \dots, z_k\}$ since m extracts a k-dimensional subset.
As for map t, t maps any finite set of exactly k points of Z into a (possibly infinite) subset $A \subseteq Z$.

Example 1 *Let $Z = \mathbb{R}$. Given a set of reals $\{z_1, z_2, \dots, z_p\}$, we can take $m\{z_1, z_2, \dots, z_p\} = \{z_{min}, z_{max}\}$, where z_{min} and z_{max} are the* min *and* max *numbers in the set. So, $k = 2$ here. Also, we define $t\{z_1, z_2\} = [z_1, z_2]$, the interval connecting the two points.* $*$

Example 2 (sketched) *In the classification problem of this paper, Z is the instance space, m is the map that selects the "active" instances and t returns the region in Z where the classifier provides a correct classification. Details are provided later on in this section.* $*$

In what follows, R and S indicate two finite sets, both containing at least k points of Z. We consider three classes of pairs (R, S):

$$\begin{aligned}
\mathcal{A} &= \{(R,S) \text{ such that: } m(R) \text{ and } m(S) \text{ are defined, } R \subseteq S, \text{ and } S \subseteq t(m(R))\} \\
\mathcal{B} &= \{(R,S) \text{ such that: } m(R) \text{ and } m(S) \text{ are defined, } R \subseteq S, \text{ and } m(S) = m(R)\} \\
\mathcal{C} &= \{(R,S) \text{ such that: } m(R) \text{ and } m(S) \text{ are defined, } R \subseteq S, \text{ and } m(S) \subseteq R\}.
\end{aligned}$$

The following proposition establishes a link among $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$.

Proposition 1 *$\mathcal{A} = \mathcal{B}$ if and only if $\mathcal{A} = \mathcal{C}$.*

Example 3 (Example 1 continued) *The reader may want to verify that $\mathcal{A} = \mathcal{B}$ and also $\mathcal{A} = \mathcal{C}$ in Example 1.* $*$

Proof of Proposition 1.
(a) Suppose $\mathcal{A} = \mathcal{B}$.
To prove that $\mathcal{A} = \mathcal{B} \Rightarrow \mathcal{A} = \mathcal{C}$, we show in (a.1) that $\mathcal{A} \subseteq \mathcal{C}$ and in (a.2) that $\mathcal{C} \subseteq \mathcal{A}$.
(a.1) If $(R, S) \in \mathcal{A}$, then: $m(S) = [\text{since } \mathcal{A} = \mathcal{B}] = m(R) \subseteq R$, i.e. $(R, S) \in \mathcal{C}$.
(a.2) If $(R, S) \in \mathcal{C}$, then

$$m(S) \subseteq R. \tag{5}$$

Moreover,

$$S \subseteq t(m(S)), \tag{6}$$

as it follows from observing that $(S, S) \in \mathcal{B}$ so that, being $\mathcal{B} = \mathcal{A}$, $(S, S) \in \mathcal{A}$ and (6) follows. Thus,

$$R \subseteq S \subseteq [\text{use (6)}] \subseteq t(m(S)) = t(m(m(S))), \tag{7}$$

where the last equality is true since m extracts a subset of k points, so that $m(m(S))$ is the extraction of a subset of k points from $m(S)$ which is already a set of k points, and, hence, $m(m(S)) = m(S)$.
(5) and (7) together implies that $(m(S), R) \in \mathcal{A}$ and, owing to that $\mathcal{A} = \mathcal{B}$, we obtain $(m(S), R) \in \mathcal{B}$, i.e.

$$m(m(S)) = m(R),$$

which in turn gives $m(S) = m(R)$, that is $(R, S) \in \mathcal{B}$. Since $\mathcal{B} = \mathcal{A}$, the thesis that $(R, S) \in \mathcal{A}$ is proven.
(b) Suppose now that $\mathcal{A} = \mathcal{C}$.
To prove that $\mathcal{A} = \mathcal{C} \Rightarrow \mathcal{A} = \mathcal{B}$, we show in (b.1) that $\mathcal{A} \subseteq \mathcal{B}$ and in (b.2) that $\mathcal{B} \subseteq \mathcal{A}$.
(b.1) If $(R, S) \in \mathcal{A}$, then $S \subseteq t(m(R)) = t(m(m(R)))$, so that $(m(R), S) \in \mathcal{A}$. But $\mathcal{A} = \mathcal{C}$ and, therefore, $(m(R), S) \in \mathcal{C}$ yielding $m(S) \subseteq m(R)$, from which $m(S) = m(R)$ since both sets contain k points. Whence, $(R, S) \in \mathcal{B}$.
(b.2) If $(R, S) \in \mathcal{B}$, then $m(S) = m(R) \subseteq R$ and we have that $(R, S) \in \mathcal{C} = \mathcal{A}$.
Summarizing, in (a) we have proven that $\mathcal{A} = \mathcal{B} \Rightarrow \mathcal{A} = \mathcal{C}$ and in (b) the opposite implication that $\mathcal{A} = \mathcal{C} \Rightarrow \mathcal{A} = \mathcal{B}$, so that the proposition statement that $\mathcal{A} = \mathcal{B}$ and $\mathcal{A} = \mathcal{C}$ are equivalent is established. $*$

We are now in a position to state the following fundamental result.

Theorem 2 *Consider a set Z and two maps m and t as above. Introduce a probability measure μ on Z according to which z_i points are independently extracted and suppose that:*
(i) μ has no concentrated mass, i.e. $\mu(z) = 0$, $\forall z \in Z$;
(ii) for any fixed p, $m\{z_1, z_2, \ldots, z_p\}$ is defined except for at most an exceptional set with zero probability μ^p;
(iii) $\mathcal{A} = \mathcal{B}$.
Given an integer $M \geq k$, consider the function $\xi : Z^M \to [0, 1]$ defined through: $\xi(z_1, z_2, \ldots, z_M) = \mu(t(m\{z_1, z_2, \ldots, z_M\}))$. Then, ξ has a $Beta(M+1-k, k)$ distribution, independently of the probability μ.

Example 4 (Example 3 continued) *In the situation of Example 3, the theorem simply says that if points are extracted in $\mathbb{R}$ through a probability with no concentrated mass, then $\mu(t(m\{z_1, z_2, \ldots, z_M\})) = \mu(t\{z_{min}, z_{max}\}) = \mu[z_{min}, z_{max}]$, i.e. the mass inside the interval $[z_{min}, z_{max}]$, is a random variable (it is random through the random extractions of $z_1, z_2, \ldots, z_M$) that distributes according to a $Beta(M-1, 2)$.* $*$

Proof of Theorem 2.
A $Beta(M+1-k, k)$ distribution writes $F_{Beta}(z) = \sum_{i=0}^{k-1} \binom{M}{i} z^{M-i}(1-z)^i$ and has density $f_{Beta}(z) = \binom{M}{k-1}(M-k+1)z^{M-k}(1-z)^{k-1}$. Its moments are

$$\int_0^1 z^j \, \mathrm{d}F_{Beta}(z) = \int_0^1 z^j \cdot \binom{M}{k-1}(M-k+1)z^{M-k}(1-z)^{k-1} \, \mathrm{d}z = \frac{\binom{M+j-k}{j}}{\binom{M+j}{M}}, \qquad (8)$$

as it can be verified by integration by parts. We want to establish the result that the moments of ξ are indeed given by the right-hand-side of (8), viz.

$$E[\xi^j] = \frac{\binom{M+j-k}{j}}{\binom{M+j}{M}}, \quad j = 1, 2, \ldots, \qquad (9)$$

which is enough to prove that ξ is distributed as a $Beta(M+1-k, k)$ since the distribution of a random variable with compact support (the support of ξ is $[0, 1]$) is completely determined by its moments (see e.g. Corollary 1, §12.9, Chapter II of [18]).
To prove (9), argue as follows: $\xi = \mu(t(m\{z_1, z_2, \ldots, z_M\}))$ is the probability that one more point z extracted according to probability μ falls in $t(m\{z_1, z_2, \ldots, z_M\})$, so that ξ^j is the probability that j more points independently extracted all fall in $t(m\{z_1, z_2, \ldots, z_M\})$, i.e.

$$\xi^j = \mu^j(z_{M+1}, \ldots, z_{M+j} \in t(m\{z_1, z_2, \ldots, z_M\})),$$

or, more compactly with the notation $z_m^n = \{z_m, z_{m+1}, \dots, z_n\}$,

$$\xi^j = \mu^j \left(z_{M+1}^{M+j} \subseteq t(m(z_1^M)) \right).$$

$E[\xi^j]$ is the mean of ξ^j when z_1^M is let vary according to the probability μ^M. Hence, using notation Z_m^n for the domain $Z \times \cdots \times Z$ in which z_m^n vary, we have

$$\begin{aligned} E[\xi^j] &= \int_{Z_1^M} \xi^j \, \mathrm{d}\mu^M \\ &= \int_{Z_1^M} \mu^j \left(z_{M+1}^{M+j} \subseteq t(m(z_1^M)) \right) \, \mathrm{d}\mu^M \\ &= [\mathbb{I}(A) = \text{indicator function of set } A] \\ &= \int_{Z_1^M} \left[\int_{Z_{M+1}^{M+j}} \mathbb{I} \left(z_{M+1}^{M+j} \subseteq t(m(z_1^M)) \right) \, \mathrm{d}\mu^j \right] \, \mathrm{d}\mu^M \\ &= \int_{Z_1^{M+j}} \mathbb{I} \left(z_{M+1}^{M+j} \subseteq t(m(z_1^M)) \right) \, \mathrm{d}\mu^{M+j}. \end{aligned}$$

Now, let $I = \{i_1, \dots, i_M\}$ be a generic subset of M indexes from $\{1, 2, \dots, M+j\}$ and let $\mathcal{I}$ be the family of all possible choices of I ($\mathcal{I}$ contains $\binom{M+j}{M}$ elements). Moreover, let $\bar{I} = \{1, 2, \dots, M+j\} - I$. Since all z_i are extracted independently and with the same distribution, each group of M points z_i has identical statistical properties as any other group; therefore, if we indicate with z^I the set of points $z_i, i \in I$, we have that

$$\int_{Z_1^{M+j}} \mathbb{I} \left(z_{M+1}^{M+j} \subseteq t(m(z_1^M)) \right) \, \mathrm{d}\mu^{M+j} = \int_{Z_1^{M+j}} \mathbb{I} \left(z^{\bar{I}} \subseteq t(m(z^I)) \right) \, \mathrm{d}\mu^{M+j}, \quad \forall I \in \mathcal{I}.$$

Whence,

$$\begin{aligned} E[\xi^j] &= \int_{Z_1^{M+j}} \mathbb{I} \left(z_{M+1}^{M+j} \subseteq t(m(z_1^M)) \right) \, \mathrm{d}\mu^{M+j} \\ &= \frac{1}{\binom{M+j}{M}} \sum_{I \in \mathcal{I}} \int_{Z_1^{M+j}} \mathbb{I} \left(z^{\bar{I}} \subseteq t(m(z^I)) \right) \, \mathrm{d}\mu^{M+j} \\ &= \frac{1}{\binom{M+j}{M}} \int_{Z_1^{M+j}} \sum_{I \in \mathcal{I}} \mathbb{I} \left(z^{\bar{I}} \subseteq t(m(z^I)) \right) \, \mathrm{d}\mu^{M+j}. \end{aligned} \tag{10}$$

The indicator function in the integrand requires that $z^{\bar{I}} \subseteq t(m(z^I))$. On the other hand, $(z^I, z^I) \in \mathcal{B}$ which, by the fact that $\mathcal{B} = \mathcal{A}$, yields $z^I \subseteq t(m(z^I))$. Therefore, we can add the indexes $i \in I$ in the indicator function without any change of the result and write

$$\mathbb{I} \left(z^{\bar{I}} \subseteq t(m(z^I)) \right) = \mathbb{I} \left(z_1^{M+j} \subseteq t(m(z^I)) \right).$$

Further invoking Proposition 1, we see that $\mathcal{A} = \mathcal{B} \Rightarrow \mathcal{A} = \mathcal{C}$, so that, with $R = z^I$ and $S = z_1^{M+j}$, we have

$$\mathbb{I} \left(z_1^{M+j} \subseteq t(m(z^I)) \right) = \mathbb{I} \left(m(z_1^{M+j}) \subseteq z^I \right).$$

Substituting in turn the last two equations in (10), we come to the result that

$$E[\xi^j] = \frac{1}{\binom{M+j}{M}} \int_{Z_1^{M+j}} \sum_{I \in \mathcal{I}} \mathbb{I}\left(m(z_1^{M+j}) \subseteq z^I \right) \, \mathrm{d}\mu^{M+j}. \tag{11}$$

To complete the computation of $E[\xi^j]$, observe now that points $z_1, z_2, \ldots, z_{M+j}$ are with probability 1 all distinct since $\mu(z) = 0$, $\forall z \in Z$ (assumption (i)), and therefore the sum under the integral amounts to compute the number of times that a subset z^I of M points from a set z_1^{M+j} of $M+j$ distinct points contains a fixed set $m(z_1^{M+j})$ of k points in the set z_1^{M+j}. Since these k points are fixed, we have to decide which j points among the remaining $M+j-k$ in z_1^{M+j} have to be left out of z^I, and the number of possible different choices is $\binom{M+j-k}{j}$. Substituting in (11) yields (9), and this completes the proof. $*$

We shall now prove Theorem 1 as an application of Theorem 2.

We start by considering the ideal GEM algorithm.
Throughout, (x_1, y_1) is regarded as a given initial example which we suppose fixed, and derive the distribution of $PE(\hat{y}_N)$ as a function of the remaining $N-1$ examples $(x_2, y_2), \ldots, (x_N, y_N)$. In more technical terms, we derive the conditional distribution of $PE(\hat{y}_N)$ given (x_1, y_1). This distribution turns out to be a $Beta(k, N-k)$ regardless of (x_1, y_1), so that, by integration with respect to (x_1, y_1), the distribution of $PE(\hat{y}_N)$ is proven to be a $Beta(k, N-k)$.

The data generation mechanism $(\mu, y(\cdot))$ has to be thought of as given and fixed throughout (even though it is unknown). Therefore an example $(x_i, y_i) = (x_i, y(x_i))$ is determined once x_i has been assigned.

For easy reference, Theorem 2 will be applied to establish Theorem 1 with the following positions:

– $Z = \mathbb{R}^d$, the instance space;
– the probability μ of Theorem 2 is the probability μ with which x_i instances are observed. Note that condition (i) of Theorem 2 is satisfied because μ in Theorem 1 has density;
– $z_i = x_{i+1}$, $i = 1, 2, \ldots$ (remember that x_1 plays a special role of "initial" instance);
– for any $p \geq k$, suppose we apply the ideal GEM algorithm with $N = p + 1$. Then, upon termination, the algorithm has stored in Q at least k indexes taken from $\{2, 3, \ldots, p+1\}$ and, whenever they are exactly k, we define m through relation $m\{x_2, x_3, \ldots, x_{p+1}\} = \{x_i, i \in Q\}$. Later down, we shall prove that Q contains exactly k indexes with probability 1, that is

condition (ii) in Theorem 2 is fulfilled;
– given k examples (besides the initial example (x_1, y_1)), t by definition returns the set in $\mathbb{R}^d$ that is correctly classified or classified as *unknown* by the classifier constructed by the ideal GEM algorithm applied to the k given examples;
– $M = N - 1$.

By these positions, we have that $PE(\hat{y}_N) = 1 - \mu(t(m\{x_2, x_3, \ldots, x_N\}))$. If we prove the applicability of Theorem 2, then $\mu(t(m\{x_2, x_3, \ldots, x_N\}))$ distributes as a $Beta(N-k, k)$ so that the complementary variable $PE(\hat{y}_N)$ distributes as a $Beta(k, N-k)$ and the proof for the ideal GEM algorithm is complete. We therefore see that all that remains to be proven is that conditions (ii) and (iii) of Theorem 2 hold in our present context of application.

To prove (ii), we start off by showing the validity of the following property

(P) the optimization program in point 2a of the GEM algorithm returns the same solution if we remove all the constraints $(x_i - x_B)^T A(x_i - x_B) + b^T(x_i - x_B) \geq 1, i \in P$ such that $y_i \neq y(x_B)$, but at most $(d(d+1)/2 + d)$ of them, suitably selected.

This property is a consequence of the fact that this program is a convex program in $(d(d+1)/2 + d)$ variables, where $d(d+1)/2$ are the free parameters of A (remember that A is symmetric) and d are the free parameters of b. To formally show property (P), assume for the sake of contradiction that no choice of at most $(d(d+1)/2 + d)$ constraints exists that maintains the solution unaltered. For any given $i \in P$ such that $y_i \neq y(x_B)$, consider the set H_i of (A, b), $A \succeq 0$, pairs that satisfy the associated constraint:

$$H_i = \left\{(A, b) \text{ such that } (x_i - x_B)^T A(x_i - x_B) + b^T(x_i - x_B) \geq 1\right\}.$$

Also consider one more set H_0 of (A, b), $A \succeq 0$, pairs defined as

$$H_0 = \{(A, b) \text{ that outperforms the solution of the program in point 2a}\}.$$

In this latter definition "outperforms" means that the $Trace(A)$ is lower than $Trace(A^*)$, or, for equal $Trace$, b has lower norm than b^*, or, for equal b norm, the lexicographic rule favors (A, b) over (A^*, b^*). An easy inspection shows that all these sets are convex, i.e. if (A_1, b_1) and (A_2, b_2) belong to one set, also $\alpha(A_1, b_1) + (1 - \alpha)(A_2, b_2)$, $\alpha \in [0, 1]$, belong to the same set. Moreover, the intersection of any $(d(d+1)/2 + d) + 1$ of these sets is always non-empty. Indeed, the intersection of $(d(d+1)/2+d)+1$ sets H_i, $i \neq 0$, is clearly non-empty since to the intersection belongs an (A, b) with $b = 0$ and $A = aI$ with a large enough. If instead H_0 is in the group of $(d(d+1)/2+d)+1$ sets, then there are only $(d(d+1)/2+d)$ sets of the type H_i, $i \neq 0$, but then, by the assumption made for the sake of contradiction, the solution of the program with only the constraints associated with these $(d(d+1)/2+d)$ sets will be different from the solution of the whole program, and therefore this solution will outperform the solution of the whole program. This means that this solution is also in H_0, proving that the intersection of all the $(d(d+1)/2+d)+1$ sets is non-empty in this case too. Now, resorting to Helly's theorem (see e.g. [16]) yields that the intersection of all the sets, viz. $\cap_{i \in P, y_i \neq y(x_B)} H_i \cap H_0$, is non-empty. This last relation means that we can find a pair (A^{**}, b^{**}) which is simultaneously in all the sets H_i, $i \in P, y_i \neq y(x_B)$, and therefore it satisfies all constraints $(x_i - x_B)^T A (x_i - x_B) + b^T (x_i - x_B) \geq 1$, and that is also in H_0, and therefore it outperforms (A^*, b^*). But (A^*, b^*) is the optimal solution, and this is a contradiction. Hence, we have proven (P).

Based on **(P)**, we prove now that the algorithm terminates after executing point 2a with $|Q| > k$ with probability 0 only, so that m is defined with probability 1.

Since point 2a is entered only when $|Q| \leq k - (d(d+1)/2+d)$, having $|Q| > k$ after executing point 2a implies that the algorithm has found more than $(d(d+1)/2+d)$ active instances while executing point 2a. But we have shown in **(P)** that at most $(d(d+1)/2+d)$ constraints determine the solution and, to have more than $(d(d+1)/2+d)$ active instances, at least one of the other instances must fall exactly on the boundary of the region generated by the at most $(d(d+1)/2+d)$ instances that determine the solution, a fact that happens only with probability 0 since μ has density.

A similar rationale permits one to conclude that $|Q| > k$ only happens with probability 0 even when the algorithm last executes points 2b or 2c. We have therefore proven that $|Q| = k$ with probability 1 upon termination of the algorithm and condition (ii) is established.

We finally prove condition (iii), i.e. that $\mathcal{A} = \mathcal{B}$.

Suppose that a set of instances S has a subset R, that $m(S)$ and $m(R)$ are defined, and that S is in $t(m(R))$, i.e. $(R, S) \in \mathcal{A}$. This means that the examples whose instances are in $S - R$ are correctly classified, or classified as *unknown*, by the classifier constructed with the examples with instances in R. If so, an easy inspection of the GEM algorithm reveals that $m(S) = m(R)$, so that $(R, S) \in \mathcal{B}$. Viceversa, suppose $(R, S) \in \mathcal{B}$. The region of correct classification, or classified as *unknown*, for the classifier generated by the examples with instances in S contains S itself since the ideal GEM algorithm does not misclassify any example. Thus,

$$
\begin{aligned}
S \quad &\subseteq \quad \text{region of correct classification, or classified as } \textit{unknown}, \text{ for the classifier} \\
&\qquad \text{generated by the examples with instances in } S \\
&= \quad t(m(S)) \\
&= \quad [\text{since } (R,S) \in \mathcal{B} \text{ implies } m(S) = m(R)] \\
&= \quad t(m(R)),
\end{aligned}
$$

and it remains proven that $(R, S) \in \mathcal{A}$. We have therefore proven condition (iii) that $\mathcal{A} = \mathcal{B}$, and this completes the proof for the ideal GEM algorithm.

The result that the probability distribution of $PE(\hat{y}_N)$ for the real GEM algorithm is dominated by that of the ideal GEM algorithm immediately follows from observing that $PE(\hat{y}_N)$ is, by construction, always no bigger for the former than for the latter. $*$

References

[1] A. Asuncion and D.J. Newman. UCI machine learning repository, URL: http://www.ics.uci.edu/∼mlearn/MLRepository.html, University of California, Irvine, School of Information and Computer Sciences, 2007.

[2] P.L. Bartlett and M.H. Wegkamp. Classification with a reject option using a hinge loss. *Journal of Machine Learning Research*, 9:1823–1840, 2008.

[3] H. Chernoff. A measure of asymptotic efficiency for tests of a hypothesis based on the sum of observations. *Annals of Mathematical Statistics*, 23:493–507, 1952.

[4] C.K. Chow. An optimum character recognition system using decision functions. *IRE Trans. Electronic Computers*, 6:247–254, 1957.

[5] C.K. Chow. On optimum recognition error and reject tradeoff. *IEEE Trans. on Information Theory*, 16:41–46, 1970.

[6] N. Cristianini and J. Shawe-Taylor. *An introduction to sypport vector machines and other kernel-based learning methods.* Cambridge University Press, 2000.

[7] L. Devroye. Necessary and sufficient conditions for the almost everywhere convergence of nearst neighbor regression function estimates. *Zeitschrift fur Wahrscheinlichkeitstheorie und verwandtegebiete*, 61:467–481, 1982.

[8] L. Devroye, L. Gyorfi, and G. Lugosi. *A probabilistic theory of pattern recognition*. Springer-Verlag, New York, 1996.

[9] C. Ferri, J. Hernandez-Orallo, and M.A. Salido. Volume under the roc surface for multi-class problems. *14th European Conference on Machine Learning*, pages 108–120, 2003.

[10] L. Gyorfi, Z. Gyorfi, and I. Vajda. Bayesian decision with rejection. *Problems of control and information theory*, 8:445–452, 1978.

[11] R. Herbei and M.H. Wegkamp. Classifcation with reject option. *Canadian Journal of Statistics*, 34(4):709–721, 2006.

[12] Z. Hussain, F. Laviolette, M. Marchand, J. Shawe-Taylor, S.C. Brubaker, and M.D. Mullin. Revised loss bounds for the set covering machine and sample-compression loss bounds for imbalanced data. *Journal of Machine Learning Research*, 8:2533–2549, 2007.

[13] M. Marchand and J. Shawe-Taylor. The set covering machine. *Journal of Machine Learning Research*, 3:723–746, 2002.

[14] R. Muzzolini, Y.H. Yang, and R. Pierson. Classifier design with incomplete knowledge. *Journal of American Statistical Association*, 31:345–369, 1998.

[15] T. Pietraszek. Optimizing abstaining classifiers using roc analysis. *22nd European Conference on Machine Learning*, pages 665–672, 2005.

[16] R.T. Rockafellar. *Convex Analysis*. Princeton University Press, Princeton, NJ, 1970.

[17] M.J. Schervish. *Theory of Statistics*. Springer, New York, 1995.

[18] A.N. Shiryaev. *Probability*. Springer, New York, NY, USA, 1996.

[19] V.N. Vapnik. *Statistical Learning Theory*. Wiley, New York, NY, 1998.

[20] M. Vidyasagar. *Theory of learning and generalization: with applications to neural networks and control systems*. Springer-Verlag, London, 1997.