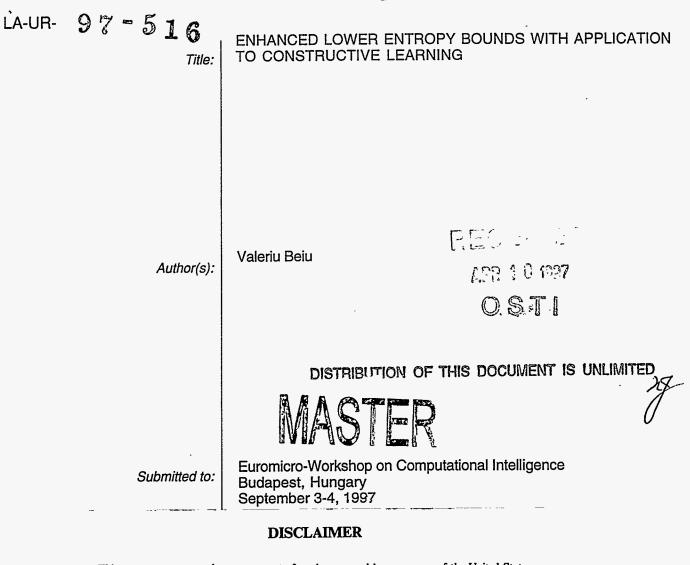
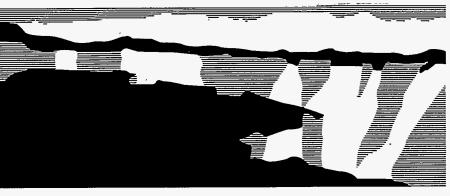
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Enhanced Lower Entropy Bounds with Application to Constructive Learning

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Abstract — In this paper we shall prove two new lower bounds for the number-of-bits required by neural networks for classification problems defined by *m* examples from \mathbb{R}^n . Because they are obtained in a constructive way, they can be used for designing a constructive algorithm. These results rely on techniques used for determining tight upper bounds [6], which start by upper bounding the space with an *n*-dimensional ball. Very recently, a better upper bound has been detailed [9] by showing that the volume of the ball can always be replaced by the volume of the intersection of two balls. A first lower bound for the case of integer weights in the range [-p, p] has been detailed in [14]: it is based on computing the logarithm of the quotient between the volume of the ball containing all the examples (rough approximation like in [6]) and the maximum volume of a polyhedron. A first improvement over that bound will come from a tighter upper bound of the maximum volume of the polyhedron by two *n*-dimensional cones (instead of a ball, as used in [14]). An even tighter bound will be obtained by upper bounding the space by the intersection of two balls (as has been done in [9] for obtaining a tight upper bound).

Keywords — neural networks, *size* complexity, entropy, classification problems, limited *weights*, constructive algorithms.

1. Introduction and Notations

Multilayer feedforward neural networks (NNs) have been experimentally shown to be quite effective in many different applications (see Applications of Neural Networks in [3], together with Part F: Applications of Neural Computation and Part G: Neural Networks in Practice: Case Studies from [15]), but cost effective solutions for large scale computational paradigms have to be hardware implementable — and NNs are by no means an exception. That is why a rigorous analysis of the mathematical properties that enable them to perform so well has generated two directions of research:

- one to find existence /constructive proofs for what is now known as the "universal approximation problem" (i.e., any continuous function can be approximated arbitrarily well by a NN);
- another one to find tight bounds on the number of neurons (*size*) needed by the approximation problem (or some particular cases).

The focus of this paper will be on the second aspect. Here we shall denote by *network* any acyclic graph having several input nodes (*inputs*) and some (at least one) output nodes (*outputs*). If with each edge a synaptic *weight* is associated and each node computes the weighted sum of its inputs to which a nonlinear activation function is then applied (*artificial neuron*):

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1. Introduction and Notations

$$f(\mathbf{z}) = f(z_1, \dots, z_{\Delta}) = \sigma\left(\sum_{i=1}^{\Delta} w_i z_i + \theta\right), \tag{1}$$

the network is a NN ($w_i \in \mathbb{R}$ are the synaptic weights, $\theta \in \mathbb{R}$ is the threshold, Δ is the number of inputs of one neuron, and σ is a non-linear activation function).

A classification problem is defined by a set of m examples (i.e., data-set) belonging to k different classes. For simplicity we shall limit the number of classes to two (k=2), known as a *dichotomy*, but all our results are valid in general. Now:

$$m = m_+ + m_- \tag{2}$$

and $x_1, x_2, ..., x_{m_+}$ are the positive examples, while $y_1, y_2, ..., y_{m_-}$ are the negative examples; they are taken from an *n*-dimensional space \mathbb{R}^n $(n \in \mathbb{N} \setminus \{1\})$:

$$x_{i} = (x_{i,1}, x_{i,2}, \dots, x_{i,n}) \in \mathbb{R}^{n}, \ i = 1, 2, \dots, m_{+}, \ m_{+} \in \mathbb{N} \text{ and}$$
$$y_{i} = (y_{i,1}, y_{i,2}, \dots, y_{i,n}) \in \mathbb{R}^{n}, \ j = 1, 2, \dots, m_{-}, \ m_{-} \in \mathbb{N}.$$
(3)

The distance between two vectors (examples) is the classical Euclidean distance:

$$dist_{\rm E}(a,b) = \sqrt{(a_1-b_1)^2 + (a_2-b_2)^2 + \ldots + (a_n-b_n)^2} = \left\{\sum_{i=1}^n (a_i-b_i)^2\right\}^{1/2}.$$
(4)

For characterising the data-set, we also define the *minimum* and the *maximum distance* between any positive and negative examples:

$$d = \min_{i=1,...,m_{\star}} [dist_{E}(x_{i}, y_{j})] \text{ and } D = \max_{i=1,...,m_{\star}} [dist_{E}(x_{i}, y_{j})]$$
(5)

A ball of radius r ($r \in \mathbb{R}^+ \setminus \{0\}$) centered at $c \in \mathbb{R}^n$ will be denoted by $B_n[c, r]$:

$$B_n[c, r] = \{ x \in |\mathbb{R}^n: dist_{\mathbb{R}}(c, x) \le r \};$$
(6)

if n=2 this is a round disc; if n=3 it is a round ball. We shall denote by μ_n the *n*-dimensional Lebesgue measure in \mathbb{R}^n . If $A \subseteq \mathbb{R}^2$, $\mu_2(A)$ is the 'area' of A; if $A \subseteq \mathbb{R}^3$, $\mu_3(A)$ is the 'volume' of A. Finally, $\alpha(n) = \mu_n(B_n[0, 1])$ is the volume of the unit ball in \mathbb{R}^n . In particular we have $\alpha(2) = \pi$, $\alpha(3) = 4\pi/3$, while in general $\alpha(2n) = \pi^n/n!$ [12, 17, 20] and $\alpha(2n-1) = 2^n \cdot \pi^{n-1}/[1\cdot 3\cdot 5\cdot \ldots\cdot (2n-1)]$, or in terms of the gamma function: $\alpha(n) = \pi^{n/2}/\Gamma(n/2+1)$.

This paper will prove two lower bounds — based on the entropy of the data-set — on the *number-of-bits* required for classification problems. In Section 2 we shall briefly go through some very recent results, while the proofs will be given in Section 3. They are based on computing the required *number-of-bits* for representing the data-set as the loga-rithm of the quotient between the volume of a ball containing all the examples (rough approximation like in [6]) and the maximum volume of a polyhedron [14]. The first improvement over the bound detailed in [14] is based on a tighter upper bound of the volume of the polyhedron by two *n*-dimensional cones instead of a ball (as used in [14]). An even tighter bound can be obtained because all the examples from one class always lie inside the intersection of two balls [9], thus the volume of a ball can be replaced by the volume of the intersection of two balls.

2. Previous Results

The problem to find the smallest *size* NN which can realise an arbitrary function given a set of *m* vectors (examples, or points) in *n* dimensions is not new. Many results have been obtained for NNs having a *threshold* activation function (see references in [7, 8]). Probably the first lower bound on the *size* of a threshold gate circuit for "almost all" *n*-ary Boolean functions (BFs) was given by Neciporuk in 1964: $size \ge 2 (2^{n}/n)^{1/2}$ [23]. Later, Lupanov has proven a very tight upper bound: $size \le 2 (2^{n}/n)^{1/2} \times \{1 + \Omega [(2^{n}/n)^{1/2}]\}$ for the case when depth = 4 [22]. Similar existence exponential bounds can be found in [123], while in [27] a $\Omega (2^{n/3})$ existence lower bound for arbitrary BFs has been presented.

For classification problems, one of the first result was that a NN with only one hidden layer having m-1 nodes could compute an arbitrary dichotomy (sufficient condition). The main improvements have been as follows:

- Baum [4] presented a NN with one hidden layer having $\lceil m/n \rceil$ neurons¹ capable of realising an arbitrary dichotomy on a set of *m* points in general position in $|\mathbb{R}^n$; if the points are on the corners of the *n*-dimensional hypercube (i.e., binary vectors), m-1 nodes are still needed;
- a slightly tighter bound was proven in [18]: only [1 + (m-2)/n] neurons are needed in the hidden layer for realising an arbitrary dichotomy on a set of *m* points which satisfy a more relaxed topological assumption (only the points from a sequence from some subsets are required to be *in general position*); also, the m-1 nodes condition was shown to be the least upper bound needed;
- Arai [2] showed that m-1 hidden neurons are necessary for arbitrary separability (any mapping between input and output for the case of binary-valued units), but improved the bound for the two-category classification problem to m/3 (without any condition on the inputs).

These results show that for binary inputs the size grows exponentially (as $m \le 2^n$). Some existence lower bounds for the arbitrary dichotomy problem are (see [16]): (i) a depth-2 NN requires at least $m/[n \log(m/n)]$ hidden neurons (if $m \ge 3n$); (ii) a depth-3 NN requires at least $2(m/\log m)^{1/2}$ neurons in each of the two hidden layer (if $m \gg n^2$); this bound is identical to the one presented in [23] for $m = 2^n$; (iii) an arbitrarily interconnected NN without feedback needs $(2m/\log m)^{1/2}$ neurons (if $m \gg n^2$). Several other bounds for arbitrary BFs can be found in [25]. All of these are: (i) revealing a gap between the upper and the lower bounds, thus encouraging research efforts to reduce (or even close) these gaps; (ii) suggesting that NNs with more hidden layers might have a smaller size.

A different approach to classification problems has been presented in [6, 9, 14]; it is based on computing the entropy (see also [1] and [28]) of the data-set.

Proposition 1 (from [6]). The dichotomy of m examples from \mathbb{R}^n can be solved with:

$$\#bits < mn \cdot \{ [\log(D/d)] + 5/2 \}.$$

Sketch of proof. Find the examples (from the different classes) which are the closest to one another: $x_d, y_{d'}$ (the distance between them is d). Translate the origin of the axes into

¹ [x] is the ceiling of x, i.e., the smallest integer greater than or equal to x, and [x] is the floor of x, i.e., the largest integer less than or equal to x, and all the logarithms are taken to base 2.

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 x_d and rotate the axes such as the origin (i.e., x_d) and y_d . represent the opposite corners of a hypercube of side length is $l = d/\sqrt{n}$. Quantize the whole space; as there are no examples situated at a distance closer than d, there will be no hypercube containing examples from the two different classes. Because the largest distance is D, there is a ball in $|\mathbb{R}^n$ of radius D which contains all the *m* examples. The *number-of-bits* for one example can be computed as $\lceil \log (V_{ball}/v_{hc}) \rceil$ where the volume of the ball is $V_{ball}(D, n) = \alpha(n) \cdot D^n$, and the volume of the hypercube is $v_{hc}(d, n) = (d/\sqrt{n})^n$. By multiplying with *m* the result follows:

$$\#bits = \left\lceil \log\left\{\frac{V_{ball}(D,n)}{v_{hc}(d,n)}\right\}\right\rceil = \left\lceil \log\left\{\frac{\pi^{n/2}D^n}{\Gamma(n/2+1)} \cdot \frac{n^{n/2}}{d^n}\right\}\right\rceil < n \{\lceil \log(D/d) \rceil + 5/2\}.$$

The exact value detailed is $\#bits_{example} < \lceil n \log (D/d) + 2.0471n - (\log n)/2 - 0.8257 \rceil$. A non constructive bound has also been presented.

Proposition 2 (from [6]). The entropy of a dichotomy of m examples from \mathbb{R}^n is bounded by $2^{m \lceil \log m \rceil}$.

A better bound has been obtained by replacing the volume V_{ball} with the volume of the intersection of two balls V(D, n).

Proposition 3 (from [9]). The volume of the intersection of two balls in \mathbb{R}^n of the same radius $r \in \mathbb{R}^+ \setminus \{0\}$, placed such that the center of each one is on the boundary of the other one, is $V(r, n) = 2 \alpha (n-1) r^n \cdot a(n)$ with:

$$a(n) = \int_{\pi/6}^{\pi/2} (\cos\theta)^n d\theta = \frac{n-1}{n} \cdot a(n-2) - \frac{3^{(n-1)/2}}{n \cdot 2^n}$$

Proposition 4 (from [9]). The dichotomy of $m = m_+ + m_-$ examples from \mathbb{IR}^n can always be solved with:

$$\#bits < m_{max} n \cdot \{ \lceil \log (D/d) \rceil + 2 \}$$

where $m_{max} = \max(m_{+}, m_{-}) > m/2$.

The exact value detailed is $\#bits_{example} < \lceil n \log (D/d) + 1.8396n - 1.0800 \rceil$.

These bounds are valid for NNs having integer $|weights| < 2^{\#bits_{example}/n}$ (see [10, 11]), but the bound on weights is a result of bounding the number-of-bits. The problem can be tackled the other way around, i.e. by taking the weights from $\{-p, -p+1, ..., p\}$ (see [19] and Fig.1a), and proving lower bounds on the number-of-bits [14].

Proposition 5 (from [14]). Using integer weights in the range [-p, p], one can correctly classify any set of patterns for which the minimum distance between two patterns of opposite classes is $d_{min} = 1/p$.

Proposition 6 (from [14]). The number-of-bits necessary for the separation of the patterns in general position using weights in the set $\{-p, -p+1, ..., 0, ..., p\}$ is:

 $\#bits > m n \cdot \lceil \log (2pD) \rceil = m n \cdot \lceil \log (D/d) \rceil$

Proposition 7. The volume of an n-dimensional cone of height h and having as basis an (n-1)-dimensional ball of radius $r \in \mathbb{R}^+ \setminus \{0\}$ is:

$$V_{cone}(r, n, h) = \frac{h \cdot V_{ball}(r, n-1)}{n}$$

Proof. The volume of an *n*-dimensional cone can be computed by summing the 'volume' of very thin cylinders, or, at the limit, by summing the 'area' of the thin discs. This gives:

$$V_{cone}(r, n, h) = \int_{0}^{h} \mu_{n-1} (B_{n-1}[(x, 0, ..., 0), r]) dx$$

$$= \int_{0}^{h} \alpha (n-1) \cdot \left(\frac{rx}{h}\right)^{n-1} dx$$

$$= \alpha (n-1) \cdot \frac{r^{n-1}}{h^{n-1}} \cdot \int_{0}^{h} x^{n-1} dx$$

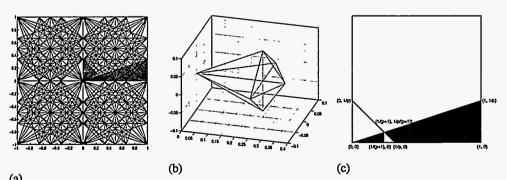
$$= \alpha (n-1) \cdot \frac{r^{n-1}}{h^{n-1}} \cdot \left[\frac{x^{n}}{n}\right]_{x=0}^{x=h}$$

$$= \alpha (n-1) \cdot \frac{r^{n-1}}{h^{n-1}} \cdot \frac{h^{n}}{n}$$

$$= V_{ball}(r, n-1) \cdot \frac{h}{n}$$

and concludes the proof.





(a) Fig. 1. (a) The hyperplanes implemented with integer weights in [-3, 3] (adapted from [19]); (b) the largest resulting polythope in 3D (adapted from [14]); (c) the largest polythope in the plane (used for computing h_1 , h_2 and r in Proposition 8).

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We can now prove a tighter bound for the largest polyhedron (than that with a ball which has been used in [14] — see Fig.1b).

Proposition 8. The volume of the two n-dimensional cones bounding the largest polyhedron obtained by using weights in the set $\{-p, -p+1, ..., 0, ..., p\}$ is:

$$V_{2_cones}(p,n) = \frac{\alpha (n-1)}{n \cdot p^n \cdot (p+1)^{n-1}}.$$

Proof. We shall first determine the height of each of the two cones h_1 and h_2 and the radius of the (n-1)-dimensional ball r (see Fig.1c). From one triangle we have $r = h_1/p$, while from another triangle we have $r = h_2$; we also know that $h_1 + h_2 = 1/p$. By solving this system of three equations with three unknowns we get:

$$h_1 = \frac{1}{p+1}$$
, $h_2 = \frac{1}{p(p+1)}$ and $r = \frac{1}{p(p+1)}$.

The volume of the two *n*-dimensional cones bounding the largest polyhedron can now be easily computed using *Proposition 7*:

$$V_{2_cones}(p, n) = \alpha (n-1) \cdot r^{n-1} \cdot \frac{n_1 + n_2}{n}$$

= $\alpha (n-1) \cdot \frac{1}{p^{n-1} (p+1)^{n-1}} \cdot \frac{1/p}{n}$
= $\frac{\alpha (n-1)}{n \cdot p^n \cdot (p+1)^{n-1}}$

which concludes the proof.

Proposition 9. For solving a dichotomy of $m = m_+ + m_-$ examples in general position in \mathbb{R}^n , more than:

$$\#bits = m \cdot \lceil n \log(D/d) + 0.6515 n + 0.6515 \rceil / 2$$

are needed.

Proof. The number-of-bits for one example can be computed as $\lceil \log (V_{ball} / V_{2_cones}) \rceil$, where the volume of the ball of radius D is $V_{ball}(D, n) = \alpha(n) \cdot D^n$, and the volume of the largest polyhedron has been upper bounded by the volume of the two cones (given by *Proposition* 8):

$$\#bits_{example} = \left\lceil \log\left\{\frac{V_{ball}(D,n)}{V_{2_cones}(p,n)}\right\} \right\rceil = \left\lceil \log\left\{\frac{\alpha(n) \cdot D^n}{\alpha(n-1)/n/p^n/(p+1)^{n-1}}\right\} \right\rceil$$
$$= \left\lceil \log\left\{\frac{\alpha(n)}{\alpha(n-1)}\right\} + n\log D + n\log p + (n-1)\log(p+1) + \log n\right\rceil$$

We shall first compute a bound for:

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$$\log\left\{\frac{\alpha(n)}{\alpha(n-1)}\right\} = \log\left\{\frac{\pi^{n/2}/\Gamma(n/2+1)}{\pi^{(n-1)/2}/\Gamma[(n-1)/2+1]}\right\}$$
$$= \log\left\{\frac{\pi^{n/2}}{\pi^{n/2-1/2}} \cdot \frac{\Gamma(n/2-1/2+1)}{\Gamma(n/2+1)}\right\}$$
$$= \log\left\{\pi^{1/2} \cdot \frac{\Gamma(n/2+1/2)}{\Gamma(n/2+1)}\right\}$$
$$= \log\left\{\frac{\Gamma(1/2) \cdot \Gamma(n/2+1/2)}{\Gamma(n/2+1)}\right\}$$
$$= \log\left\{\frac{\Gamma(n/2+1/2)}{\Gamma(n/2+1)}\right\}$$

where

$$B(m,n) = \int_{0}^{1} x^{m-1} (1-x)^{n-1} dx = 2 \cdot \int_{0}^{\pi/2} (\sin\theta)^{2m-1} (\cos\theta)^{2n-1} d\theta.$$

In our particular case 2m-1 is in fact 2(n/2+1/2)-1=n, while 2n-1 becomes 2(1/2)-1=0, and by substitution we obtain:

$$\log\left\{\frac{\alpha(n)}{\alpha(n-1)}\right\} = \log\left\{2 \cdot \int_{0}^{\pi/2} (\sin\theta)^{n} d\theta\right\}.$$

Because θ belongs to $[0, \pi/2]$, we also have $\theta/(\pi/2) \le \sin\theta \le \theta$, which gives us the following bound (here we do need an upper bound as this term is negative):

$$\log\left\{\frac{\alpha(n)}{\alpha(n-1)}\right\} < \log\left(2 \cdot \int_{0}^{\pi/2} \theta^{n} d\theta\right)$$
$$= \log\left\{2 \cdot \left[\frac{\theta^{n+1}}{n+1}\right]_{\theta=0}^{\theta=\pi/2}\right\}$$
$$= \log\left\{2 \cdot \frac{\pi^{n+1}}{2^{n+1}} \cdot \frac{1}{n+1}\right\}$$
$$= 1 + (n+1)\log(\pi/2) - \log(n+1)$$
$$= 0.6515 n - \log(n+1) + 1.6515$$

For the interested reader we mention that a slightly tighter bound for $\log\{\alpha(n)/\alpha(n-1)\}$ could be obtained by using Stirling's formula, but we are anyhow going to prove a tighter bound in *Proposition 10*.

Using this result and taking d = 1/(2p), which is the minimum value, we have:

$$\#bits_{avanue} > [0.6515 n - \log (n + 1) + 1.6515 + n \log D + n \log p + (n - 1) \log(p + 1) + \log n]$$

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$$= \left[0.6515 \, n + \log\left(\frac{n}{n+1}\right) + n \log D + n \log\left(\frac{1}{2d}\right) + (n-1) \log\left(1 + \frac{1}{2d}\right) + 1.6515 \right]$$
$$= \left[0.6515 \, n + \log\left(\frac{n}{n+1}\right) + n \log(D/d) - n + (n-1) \log\left(\frac{2d+1}{2d}\right) + 1.6515 \right]$$

In the worst case $\log\left(\frac{2d+1}{2d}\right)$ can be $\log 2 = 1$ (for p = 1, d = 1/2), thus:

$$#bits_{example} > \left[0.6515 \, n + n \log(D/d) - n + \log\left(\frac{n}{n+1}\right) + (n-1) + 1.6515 \right] \\> \left[n \log(D/d) + 0.6515 \, n + 0.6515 \right].$$

By multiplying with min $(m_+, m_-) \le m/2$ the proof is concluded.

A tighter lower bound can be obtained if instead of the volume V_{ball} used in *Proposition* 9, we use the volume of the intersection of two balls V(D, n) as detailed in [9].

Proposition 10. For solving a dichotomy of $m = m_+ + m_-$ examples in general position in \mathbb{R}^n , more than:

$$\#bits = \max(m_{+}, m_{-}) \cdot \lceil n \log(D/d) - 0.2075 n + \log n + 0.0665 \rceil$$

are needed.

Proof. The number-of-bits for one example can be computed as $\lceil \log (V(D, n) / V_{2_cones}) \rceil$, where the volume of the intersection of two balls is $V(D, n) = 2 \cdot \alpha (n-1) \cdot D^n \cdot a(n)$ (see *Proposition 3* and 4 as well as [9]), and the volume of the largest polyhedron is upper bounded by the volume of the two cones (given by *Proposition 8*):

$$\#bits_{example} = \left\lceil \log\left\{\frac{V(D,n)}{V_{2_cones}(p,n)}\right\}\right\rceil = \left\lceil \log\left\{\frac{2 \cdot \alpha (n-1) \cdot D^n \cdot a(n)}{\alpha (n-1) / n / p^n / (p+1)^{n-1}}\right\}\right\rceil$$
$$= \left\lceil 1 + n \log D + \log \{a(n)\} + \log n + n \log p + (n-1) \log(p+1)\right\rceil.$$

The bounds for log $\{a(n)\}$ follow from the fact that $a(n) = \int_{\pi/2}^{\pi/6} (\cos\theta)^n d\theta$ (??); because $\theta \in [\pi/6, \pi/2], (\sqrt{3}/2 + \pi/12) - \theta/2 \le \cos\theta \le \sqrt{3}/2 = \cos(\pi/6)$. Here again we have to compute an upper bound as log $\{a(n)\}$ is negative for any *n*:

$$\log \{a(n)\} < \log \left\{ \int_{\pi/6}^{\pi/2} (\sqrt{3}/2)^n \, d\theta \right\} = \log \left\{ \left(\frac{\sqrt{3}}{2} \right)^n \frac{\pi}{3} \right\} = 0.0665 - 0.2075 \, n$$

and by taking d = 1/(2p), which is the minimum value, the result follows:

$$\begin{aligned} \#bits_{example} &> \lceil 1 + n \log D + 0.0665 - 0.2075 \ n + \log n + n \log p + (n - 1) \log(p + 1) \rceil \\ &= \left\lceil n \log D - 0.2075 \ n + \log n + n \log \left(\frac{1}{2d}\right) + (n - 1) \log \left(1 + \frac{1}{2d}\right) + 1.0665 \right\rceil \end{aligned}$$

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$$= \left[n \log (D/d) - 0.2075 n + \log n - n + (n-1) \log \left(\frac{2d+1}{2d} \right) + 1.0665 \right]$$

> $\left[n \log (D/d) - 1.2075 n + \log n + (n-1) + 1.0665 \right]$
= $\left[n \log (D/d) - 0.2075 n + \log n + 0.0665 \right].$

By multiplying with max $(m_+, m_-) \ge m/2$, and the proof is concluded.

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4. Conclusions

Based on the entropy of the data-set, this paper has presented a new nonconstructive proof on the *number-of-bits* required for solving a dichotomy problem. The resulting lower bounds are tighter than the ones previously known. It seems very promising that the bound proved in *Proposition 10* is in fact lowering the $n\log(D/d)$ term!

Because the proofs for the *number-of-bits* are constructive, they can be used in conjunction with results like the ones presented in [19] for designing a constructive algorithm. There is still one problem: the shape of the bounding spaces does not lend itself easily to practical applications. Bounding the space with a ball, or the intersection of two balls which, as we have seen, is theoretically possible — is computationally too difficult. For all practical cases, the simplest bounding space is a hypercube (or an intersection of hypercubes). Unfortunately, by using the intersection of two hypercubes we have to pay by a logarithmic factor of logn (for the *number-of-bits*). We are working on this particular aspect by trying to use other co-ordinates (e.g., polar co-ordinates instead of the rectangular ones).

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1. Sec. 1. 1. 1. 4.

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