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Computations of Entropy Bounds: Multidimensional Geometric Methods

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Abstract
The entropy bounds for constructive upper bound on the needed number-of-bits for solving a dichotomy is represented by the quotient of two multidimensional solid volumes. For minimization of this upper bound exact calculation of the volume of this quotient is needed. Three methods for exact computing of the volume of a given $nD$ volume are presented: 1) general method for calculation any $nD$ volume by slicing it into volumes of decreasing dimension is presented 2) a method applying appropriate curvilinear coordinate system is described for volume bounded by symmetrical curvilinear hypersurfaces (spheres, cones, hyperboloids, ellipsoids, cylinders, etc.) 3) an algorithm for dividing any $nD$ complex into simplices and computing of the volume of the simplices is presented, supplemented by a general formula for calculation of volume of an $nD$ simplex. These mathematical methods enable exact calculation of volume of any complicated multidimensional solids. The methods allow for the calculation of the minimal volume and lead to tighter bounds on the needed number-of-bits.

1 WHY COMPUTATION OF MULTIDIMENSIONAL VOLUMES IS NEEDED?
There is a long studied problem of finding the smallest size neural network which can realize an arbitrary function given by a set of $m$ vectors (i.e. examples or points) in $n$ dimensions.

Many results have been obtained for neural networks having a threshold activation function, [1] for lower as well as upper entropy bound [2, 3]. A different approach

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for classification problems has been presented in [4, 5, 6], and is based on computing
the entropy (i.e., number-of-bits) of the given data-set. Establishing bounds on the
needed number-of-bits for solving a dichotomy is important for engineering appli-
cations. Knowledge of the bounds can improve certain constructive neural learning
algorithms [7] and eventually result in reducing the area of future VLSI implementa-
tions of neural networks [1, 8]. The entropy bounds for constructive upper bound
on the needed number-of-bits for solving a dichotomy is represented by the quo-
tient of two multidimensional solid volumes. For minimization of this upper bound
methods for exact calculation of the volume of this quotient are needed. In the
geometrical language this is a problem of volume calculation for a multidimensional
solid. Such problem can always be exactly solved, sometimes analytically, more
frequently numerically. The methods for performing such volume calculations are
presented in this paper. First, the general method of slicing the volume into the
lower-dimensional ones is presented. It can be applied to any multidimensional solid
regardless its shape. An example of volume calculations by this method is shown.
Next, the way of simplification of calculations is discussed for solids bounded by
highly symmetrical curved hypersurfaces. This method applies to multidimensional
simplices and complexes only, it allows for easy automation of the whole procedure:
the algorithm will be given below. An example of volume calculation for a complex
in shown. Finally, the methods are summarized in the conclusion.

2 GENERAL METHOD FOR CALCULATION OF ANY
MULTIDIMENSIONAL VOLUME: SLICING

For any n-dimensional solid there is an effective general method for the calculation
of the volume based on recursive slicing the nD solid into (n - 1)D solids. After k
steps we obtain (n - k)D solids of known volumes. In the worst possible case we
have to apply n steps down to a length of a sector of 1D line. In order to obtain
the volume of the nD solid one needs to integrate backwards k-times. There is no
guarantee that these integrations can always be done analytically (it depends on
the boundaries). Even if the analytical integration is not possible, numerical results
can always be obtained. On the other hand, this method is relatively complicated,
time consuming, and could not lead to analytical formula, even in some cases in
which such formula exists. The other methods presented in this paper do not have
such wide applicability, but usually significantly simplify calculations.

Example: volume of a part of an (n + 1)D sphere

Let us consider as a simple example, calculation of a volume of a part of (n + 1)D
sphere of radius r.

To find the volume we have to integrate over the angle \( \phi \) in the range \((0, \phi_0)\) in the
(n + 1)-th dimension. This is an integral of the function which describes the volume
of n-dimensional spheres constituting the (n + 1)D one.

The first step is to find the volumes of the slices. We follow Maurin [11] for this
calculation. The nD sphere can be sliced by the planes \( x_n = \text{const} \). The slices are
(n - 1)D spheres which are reduced \( \sqrt{1 - \frac{x_n^2}{r^2}} \) times with respect to the (n - 1)D
one of the same radius r. Therefore, we have the following expression for volume of
the nD sphere:

\[
|K^n| = \int_{-r}^{r} \sqrt{1 - \frac{x_n^2}{r^2}} dK^{n-1}(x_n)
\]

where \( |K^{n-1}| \) is the volume of (n - 1)D sphere in our slicing, and r is the radius of
the nD sphere. We substitute $x_n = r \sin t$, then $\sqrt{1 - \frac{x_n^2}{r^2}} = \cos t$, and:

$$|K^n| = 2 \int_0^\frac{\pi}{2} r |K^{n-1}| \cos^n t \, dt = 2 |K^{n-1}| r \int_0^\frac{\pi}{2} \cos^n t \, dt = 2^n r^n \prod_{i=1}^{\frac{n}{2}} \int_0^\frac{\pi}{2} \cos^i t \, dt \quad (2)$$

There are only two possible cases.

For $n = 2k$ the product of the integrals gives:

$$|K^{2k}| = \frac{\pi^k}{k!} r^{2k}, \quad (3)$$

while for $n = 2k + 1$ it gives:

$$|K^{2k+1}| = 2^{k+1} \frac{\pi^k}{(2k+1)!!} r^{2k+1}. \quad (4)$$

The final integral in the $(n+1)$-dimension gives the volume we are looking for:

$$V_{n+1} = \int_0^{\phi_n} r |K^n| \sin^{n+1} \phi \, d\phi = r |K^n| \int_0^{\phi_n} \sin^{n+1} \phi \, d\phi$$

$$= r |K^n| \left\{ (-1)^{\frac{n+1}{2}} \sum_{k=0}^{\frac{n-1}{2}} (-1)^k \left( \begin{array}{c} n+1 \k \end{array} \right) \frac{\cos((n+1-2k)\phi_n)}{n+1-2k} \right\} \quad \text{for } n+1 \text{ odd}$$

$$= r |K^n| \left\{ (-1)^{\frac{n+1}{2}} \sum_{k=0}^{\frac{n-1}{2}} (-1)^k \left( \begin{array}{c} n+1 \k \end{array} \right) \frac{\sin((n+1-2k)\phi_n)}{n+1-2k} + \frac{1}{2\pi r^n} \left( \frac{n+1}{2\pi} \right) \phi_n \right\} \quad \text{for } n+1 \text{ even}$$

Fig. 1. Volume of a part of 3-dimensional sphere.

3 SOLIDS BOUNDED BY $n - 1$ D CURVED HYPERSURFACES

The preliminary step for simplification of computing the volume of a solid bounded by curved hypersurfaces is to look for symmetries of these surfaces. The solids under
consideration in the calculation of the entropy bounds from [9, 6] are fortunately highly symmetric.

In case when the surfaces are parts of spheres, paraboloids, hyperboloids, cylinders, cones, the problem can be significantly simplified by a proper choice of a curvilinear orthogonal coordinate system, such that the bounding curved hypersurface becomes a surface of a fixed coordinate. The choice is not always obvious — even in low dimensions — but finding such a coordinate system is highly rewarding: it tremendously simplifies calculations. Here is a simple example of a curvilinear coordinate system in 3D built of mutually orthogonal families of ellipsoids, and one- and two-sheet hyperboloids:

![Coordinate system built of orthogonal families of ellipsoids and one- and two-sheet hyperboloids]

Fig 2. Coordinate system built of orthogonal families of ellipsoids and one- and two-sheet hyperboloids

4 SOLIDS BOUNDED BY \( n - 1 \)D HYPERPLANES

4.1 Volumes of Simplices

Any \( n \)D body bounded by \((n-1)\)D hyperplanes is a complex. An \( n \)D complex with minimal possible number of vertices, i.e. \( (n+1) \), is called a simplex. The general formula for the calculation of the volume of a simplex is:

\[
V_n = \frac{1}{n} h_n V_{n-1} = \ldots = \frac{1}{n!} \prod_{i=1}^{n} h_i
\]

where \( h_i \) is the height of an \( i \)-dimensional simplex with its spot on \( i-1 \) dimensional simplex with volume \( V_{i-1} \) (its basis).

4.2 Complex: a sum of simplices

Any complex can be divided into a sum of simplices [12].
The partition is not unique. This non-uniqueness gives us the freedom to choose that specific partitioning which is convenient for a particular case. There are two possible approaches to this problem: The first is a general algorithm which works in all cases, but is a rather long, tedious method – symbolic computer calculations are recommended. Another possibility is to take advantage of the symmetries of the particular complex, if there are any.

4.3 Calculation of Volume of nD Complex: General Algorithm

A general algorithm for finding the volume of any nD complex possessing \( k \) vertices \( (k > n + 1) \) is based on partitioning the complex into a sum of simplices, and works as follows:

- Choose one vertex, \( v_1 \).
- Consider the set of \( k - 1 \) elements consisting of all remaining vertices.
- Take all the possible subsets of this set, containing \( n - 1 \) elements each.
- The vertex \( v_1 \) and any such subset define uniquely an \( n - 1 \)-D hyperplane. Take all the hyperplanes obtained in this way. They define the faces of the simplices onto which the complex is partitioned.
- Calculate and add the volumes of the simplices.

The algorithm allows for the automation of the whole procedure, including the calculation of the volumes of the simplices. The partitioning into simplices obtained by using a direct computer program might not always be the optimal one in terms of ease of calculations, nevertheless it always leads to an exact solution.

4.4 Example: Highly Symmetrical Complex

Symmetries of the complex under consideration may significantly simplify calculations. Fortunately, the n-dimensional complexes of practical application for entropy calculations usually possess high symmetry, for example, a complex used by Beiu & Draghici [9], for bounding the number-of-bits. The n-dimensional complex considered by them consists of two hyperprisms, which have as common basis an \( n - 1 \)-dimensional complex.

The sum of the heights of these hyperprisms is the same in every dimension and equal to \( h \):

\[
h = h_1 + h_2 = d
\]

were \( d \) is the smallest Euclidean distance between points from opposite classes.

This means that every simplex with height \( h_1 \), has its counterpart, a simplex with the same basis \( b \) and height \( h - h_1 \). The sum of their volumes is equal to a volume of a simplex with height \( h \). The sum of the volumes of these bases for all such pairs is also known: this is the \( (n - 1) \)-D complex described above. To find the volume of this complex one has to repeat the same procedure in \( (n - 1) \)-dimension, \( (n - 2) \), down to 1-dimension. In this particular case it leads us to the following simple formula:

\[
V(h, n) = \frac{h^n}{n!}.
\]  

Taking into account that \( h = d \), \( V(d, n) = \frac{d^n}{n!} \), we are lead to the following lower entropy bound [9, 13]:

\[
\# \text{ bits}_{\text{example}} = \left\lfloor \log \{V(D, n)/V(d, n)\} \right\rfloor
\]

\[
= \left[ 1 + \log \alpha(n - 1) + n \log D + \log a(n) + n \log p + \log n! \right]
\]
where $V(D, n)$ is volume of the intersection of two spheres in n-dimensions, having the same radius $D$ and placed in such a way that the center of each one of them is on the boundary of the other one. $D$ is the largest Euclidean distance between examples from opposite classes.

This result has been already applied for calculation of the lowest currently known upper entropy bound [13].

![Diagram](image)

Fig. 3 The highly symmetric complex from [5] in 3D with 2D basis. The heights $h$ in all three dimensions are dashed.

5 CONCLUSIONS

There is a number of methods for calculations of multidimensional volume. In this paper three most appropriate for the problem of entropy bounds calculations were discussed. The "slicing" is the most general, it can be used for any multidimensional volume calculation. In general case it leads to numerical results only, due to the fact that many integrals can not be analytically calculated. In many cases this is not the simplest method possible. Particularly for solids bounded by highly symmetrical curvilinear hypersurfaces (ellipsoids, paraboloids, spheres, cylinders), a choice of a proper curvilinear coordinate system dramatically simplifies calculations. For calculation of volumes of multidimensional simplices a simple generalization of the formula for calculation of volume of a tetrahedron is applicable. For volumes of multidimensional complexes the only difficulty is to divide the complex into sum of simplices of the same dimension. This partition is always possible and it is not unique, an algorithm for such a division was presented. The formulas for complexes and simplices allow for obtaining exact analytical results in volume calculation, and are definitely simpler than the slicing method.

Using the methods presented in this paper, the exact calculation of a quotient of two volumes of multidimensional solids becomes feasible. It leads to a tighter lower bound on the number-of-bits (entropy) for solving a dichotomy problem. It has applications to constructive neural learning and VLSI efficient implementations of neural networks.
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