Experimental lower bounds for three simplex chirality measures in low dimensions*

David Bremner † David Gay †

Abstract

Three proposed simplex chirality measures—intersection, union, and inflation—are explored experimentally in $\mathbb{R}^2$ and $\mathbb{R}^3$. The intersection measure in $\mathbb{R}^2$ (solved analytically by Buda and Mislow in 1991) serves as a control case. We attempt to discover an approximate lower-bound on the degree of chirality (i.e. the "most chiral" simplex) and present our findings. While an analytic solution in $\mathbb{R}^d$ for these measures remains open, we provide evidence suggesting the probable geometries for $d = 2, 3$.

1 Introduction

A geometric object G embedded in $\mathbb{R}^d$ is called *chiral* if the object's mirror image G' cannot be perfectly superimposed with G through rigid motion in $\mathbb{R}^d$. An object which can be superimposed with its mirror is called *achiral* (see Fig. 1). For a fixed number of dimensions d and a geometric object G, a *chirality measure* χ (in $\mathbb{R}^d$) is a function $\chi : G \to \mathbb{R}$ such that $\chi(G) = 0$ when G is achiral, and $\chi(G) = -\chi(G')$ [2]. The *degree of chirality* of object G is defined as $|\chi(G)|$.

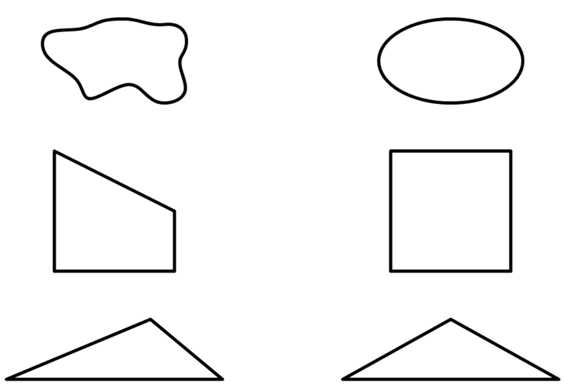

Figure 1: Examples of chiral objects (left) and achiral objects (right) in $\mathbb{R}^2$.

Our motivation for investigating chirality measures comes from cheminformatics, where the "handedness" of various chiral molecules (i.e. stereoisomers) is important to their identification and functional description [4], [7]. These molecules may be modeled as simplicial complexes in $\mathbb{R}^3$, with an overall chirality measure formed by considering the chirality measures of the constituent 3-simplices (tetrahedra). Discussions at the 2001 Bellairs Winter Workshop on Computational Geometry led to the proposal of three candidate chirality measures for tetrahedra—the intersection, (convex hull of) union, and inflation measures—though the question of which is superior was not resolved. A definition of each of these measures follows (see also Fig. 2).

For a polytope P, let $V(P)$ denote the content ("hypervolume") of P and let $\mathrm{conv}(P)$ denote the convex hull of P. For a d-simplex S, and a given chirality measure χ, let T^* be a rigid motion that maximizes $|\chi(S)|$. The *intersection measure for* $\mathbb{R}^d$ is defined as

$$\chi^d_\cap(S) \stackrel{\text{def}}{=} 1 - \frac{V\big(S \cap T^*(S')\big)}{V(S)}.$$

The *union measure for* $\mathbb{R}^d$ is defined as

$$\chi^d_\cup(S) \stackrel{\text{def}}{=} 1 - \frac{V(S)}{V\big(\mathrm{conv}(S \cup T^*(S'))\big)}.$$

The *inflation measure for* $\mathbb{R}^d$ is defined as

$$\chi^d_I(S) \stackrel{\text{def}}{=} h,$$

where h is the smallest non-negative real such that

$$\big((1+h)\cdot S\big) \cup T^*(S') = \big((1+h)\cdot S\big).$$

In 1991, Buda and Mislow analyzed the intersection measure in $\mathbb{R}^2$, $\chi^2_\cap$, and discovered that the degree of chirality of the most-chiral triangle (which can only be obtained in the limit, as the triangle's height approaches zero) is $(\sqrt{2}-1)/(\sqrt{2}+1)$, and conjectured that a similar limiting result would hold in higher dimensions [2].

For fixed number of dimensions d and chirality measure χ, let Δ^d_χ be an achiral d-simplex and Γ^d_χ be a most-chiral d-simplex. Thus, $\chi^2_\cap(\Delta) = 0$ and $\chi^2_\cap(\Gamma) \approx 0.172$.

Our objective is to discover an experimental approximation of the most-chiral d-simplex Γ for each of the three proposed measures in both $\mathbb{R}^2$ and $\mathbb{R}^3$, with the above known case serving as a control. The general approach we have taken, for each case, is to generate a large series of random simplices and their mirrors, performing an optimization process on each pair in order to discover an approximate worst-case (and corresponding approximation of the most-chiral simplex).

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†Faculty of Computer Science, University of New Brunswick, Fredericton, New Brunswick, Canada, E3B 4A1, email: {bremner, dave.gay}@unb.ca

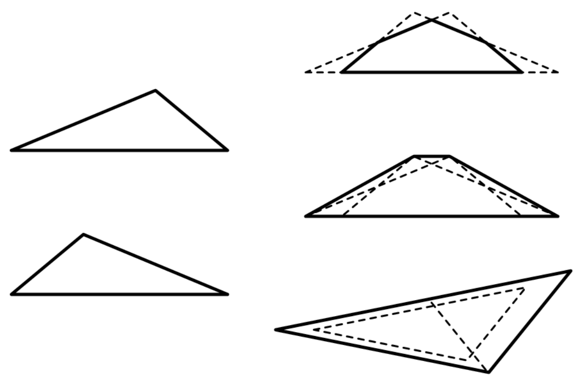

Figure 2: Pictorial representation of the three measures in $\mathbb{R}^2$. Left: a scalene triangle and its mirror. Right: intersection, union, inflation.

2 Method and Implementation

The optimization method chosen was an iterative-stochastic method, involving three nested loops. The outer "trial" loop generated random, non-degenerate simplices S and tracked worst-case information. The middle "epoch" loop generated random seed values for the transformation T and checked for early-exit conditions. The inner "optimize" loop was based on a standard gradient-descent with momentum optimization [6], with the following variations: several additional randomized vectors at each gradient calculation were added to prevent the optimizer getting stuck at saddle points, a gradient scaling factor was exponentially decayed to allow the optimizer to "settle" on the arrived-at minimum.

In order to avoid numerical degeneracy, the randomly generated simplices were translated to position the centroid[1] at the origin and scaled such that the span of the largest dimension was equal to the interval [-1, 1]. Moreover, simplices with hypervolumes less than a fixed threshold—0.1 and 0.01 were chosen for $\mathbb{R}^2$ and $\mathbb{R}^3$, respectively—were considered degenerate.

The Qhull library [1] (version 3.1) was used to find hypervolumes, convex hulls and intersections (via intermediate half-space representation) of the various polytopes used in the project. All programming was done in portable C++, with Borland C++ Builder 3. The JavaView viewer applet [5] was also used extensively during the course of the project.

Note that the use of Qhull for all central operations allows experimental trials to be performed in arbitrarily dimensions, though only $\mathbb{R}^2$ and $\mathbb{R}^3$ were considered in this implementation, enabling some local optimizations. As the number of degrees of freedom increases, however, the optimization process becomes much more expensive and less stable, suggesting that an analytic solution should be pursued for higher dimensions.

In the case of the intersection metric, it was possible that the transformation T would yield a null intersection, in which case the discovery of a gradient vector was impossible. This situation was remedied by zeroing the momentum term and repeatedly halving the translation component of T until the intersection was non-null. Finally, several further optimizations inspired by the branch-and-bound approach were implemented, reducing the time required to run a large series of trials from weeks to hours (on a consumer-grade workstation).

[1] Subsequent results suggested the incenter would be more appropriate in the case of the inflation measure.

3 Experimental Results

Early experiments revealed that the global minimum would not necessarily always be discovered (a problem with all stochastic optimization problems whose performance surfaces have local minima). In an effort to mitigate this possibility, the number of trials per simplex was chosen to be relatively high (25 trials per triangle, 100 trials per tetrahedron). To obtain a reasonably diverse sampling, 1000 non-degenerate simplices were generated for each of the six cases. Finally, an upper-bound based on early testing was chosen for each case, to provide an early-exit speed-up.

As the inherent instabilities of a randomized high-dimensional performance-surface-descent optimizer leads occasionally to the detection of a "false positive", several clearly incorrect results were discarded. Moreover, spot-checking of candidate results in the $\mathbb{R}^3$ cases revealed that the global minimum was usually not actually discovered, suggesting that the values obtained have a lower reliability. An abridged, graphical representation of the experimental results for each case is presented in Figs. 4–9 (the x-axis is the sample number, ordered by the discovered worst-case value, the horizontal line depicts the estimated lower-bound, after false-positives were discarded). After false positives were removed, the discovered worst-cases for each measure were (σ representing the appropriate simplex): $\chi^2_\cap(\sigma) = 0.1702$, $\chi^2_\cup(\sigma) = 0.2920$, $\chi^2_I(\sigma) = 0.2841$, $\chi^3_\cap(\sigma) = 0.4110$, $\chi^3_\cup(\sigma) = 0.5934$, $\chi^3_I(\sigma) = 0.5726$.

4 Analysis

The first item of note is that the experimentally obtained result for the degree of chirality of the intersection measure (0.1702) is very close to the theoretical limiting value (~ 0.1716). Second, the degrees of chirality of the union and inflation measures were both similar enough to one another to warrant the investigation of a possible interrelationship. Third, the discovered most-chiral simplices in all cases strongly resembled one another (in particular, triangles tended toward the limiting case described by Buda and Mislow in [2]). Further inquiry suggested the conjecture that the tetrahedra were also tending toward a limiting case Λ, with geometry described in Fig. 3.

To discover if this conjecture merited further investigation, the analytically-discovered triangle K and proposed tetrahe-

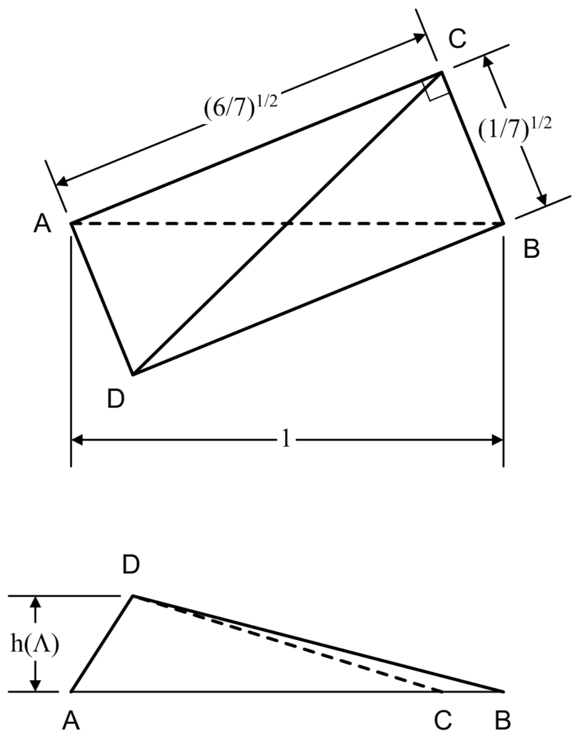

Figure 3: Presumed geometry of the most-chiral tetrahedron Λ. As $h(\Lambda)$ (the distance between D and the plane ABC) approaches zero, triangle ABD approaches congruence with triangle BAC.

dron Λ were supplied to the optimizer for a series of verification trials. Initially, the area of K was set to 0.1 and the volume of Λ set to 0.01. Decreasing the area of K to 0.01 and the volume of Λ to 0.001 caused the inflation measure to become unstable, yielding valid results only for the intersection and union measures (see Table 1). The near equality of the union and inflation evaluations suggests that they may indeed share a lower-bound, though this is difficult to verify due to the erratic behaviour of the optimizer with that measure as the simplices approach degeneracy.

Additional observations: the degree of chirality of the intersection measure tends towards $(\sqrt{6}-1)/(\sqrt{6}+1) \approx 0.4202$ in $\mathbb{R}^3$, and the degree of chirality of both the union/inflation measures tend towards $1-1/\sqrt{2} \approx 0.2929$ in $\mathbb{R}^2$ and $1-1/\sqrt{6} \approx 0.5918$ in $\mathbb{R}^3$. This leads to a final conjecture about the general form of these equations[2], namely that the lower bound for the degree of chirality measures are as follows: for $\mathbb{R}^d$, the worst-case (i.e. most-chiral) degree of chirality of the intersection measure is

$$\frac{\sqrt{d!}-1}{\sqrt{d!}+1},$$

[2] The "law of small numbers" suggests that it is unwise in the extreme to suggest this form based on a short sequence: it should be understood merely as a possible source of intuition when approaching the analytic solution.

Measure	$V(K)=0.1$	$V(K)=0.01$
$\chi^2_\cap$	0.1531	0.1719
$\chi^2_\cup$	0.2653	0.2929
χ^2_I	0.2653	—

Measure	$V(\Lambda)=0.01$	$V(\Lambda)=0.001$
$\chi^3_\cap$	0.4067	0.4279
$\chi^3_\cup$	0.5773	0.5951
χ^3_I	0.5774	—

Table 1: Experimental results for the various measures and areas/volumes.

and the worst-case degree of chirality of the union/inflation measure is

$$1-\frac{1}{\sqrt{d!}} \quad = \quad \frac{\sqrt{d!}-1}{\sqrt{d!}}.$$

Interestingly, these forms satisfy the $d=1$ case, where all 1-simplices (line segments) are achiral.

5 Acknowledgements

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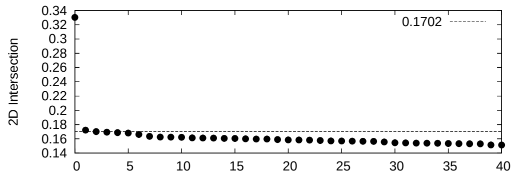

Figure 4: Experimental results for $\chi^2_\cap$.

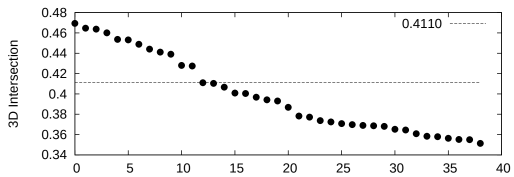

Figure 5: Experimental results for $\chi^3_\cap$.

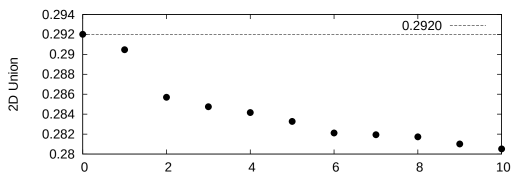

Figure 6: Experimental results for $\chi^2_\cup$.

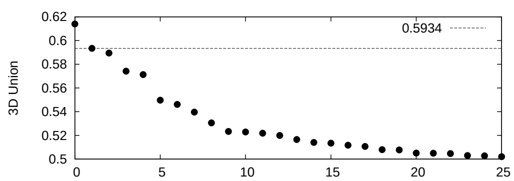

Figure 7: Experimental results for $\chi^3_\cup$.

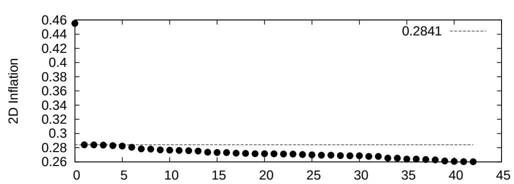

Figure 8: Experimental results for χ^2_I.

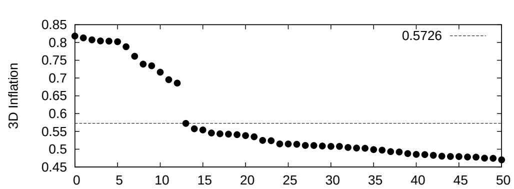

Figure 9: Experimental results for χ^3_I.