Which Convex Bodies are Most Chiral?

Problem stated in 2012 by Herbert Edelsbrunner and Roman Karasev

Chirality from mirror images. The quantitative study of the symmetry of convex bodies has a long tradition in geometry [3]. Here, we follow a suggestion of Buda, auf der Heyde, Mislow and quantify the asymmetry of a convex body using intersections with its mirror images [1]. Let B be a compact convex body with non-empty interior in $\mathbb{R}^n$. Given a hyperplane, ϱ, we write $B' = \varrho(B)$ for the mirror image obtained by reflecting B across ϱ. We are interested in the ratio of the n-dimensional volume of the intersection of B and B' over the volume of B. For symmetric bodies, there exist hyperplanes for which this ratio is one, and for others it is always less than one. To obtain a measure of how far the body is from being symmetric, we take the supremum over all hyperplanes and define

$$\chi(B) \quad = \quad 1 - \sup_{\varrho} \frac{\mathrm{vol(B \cap \varrho(B))}}{\mathrm{vol(B)}}.$$

This measure of chirality is a number in $[0, 1]$. It is zero for symmetric bodies, but it is not clear how close to one it can be. Note that we may alternatively consider all rigid motions of the mirror image. Taking the supremum, we define

$$\chi^*(B) \quad = \quad 1 - \sup_{\mu} \frac{\mathrm{vol(B \cap \mu(B'))}}{\mathrm{vol(B)}},$$

where B' is a mirror image of B and $\mu(B')$ is its image under a rigid motion. Every reflection can be obtained by composing a fixed reflection and a rigid motion, but the converse is not true, which implies $\chi^*(B) \leq \chi(B)$.

Problem statement. There are a number of questions one can ask, about the computational complexity of computing χ and χ^*, about extremal properties of these measures, and more. Keeping in mind that the motivation for the question comes from chemistry, the most important case is $n = 3$.

QUESTION. What is the infimum of χ over all compact convex bodies with non-empty volume in $\mathbb{R}^n$? If this infimum is attained, what is the solid body that attains it?

We can of course asks the same question for χ^*. It is not difficult to prove that $\chi(B) = \chi^*(B)$ in two dimensions; see Buda and Mislow [2]. Is this also true in three or higher dimensions?

Other measures. Beyond the specific quantification of asymmetry using the volume of the intersection with a mirror image, we may ask for other measures.

QUESTION. What can be said about functions on the family of compact convex polytopes in $\mathbb{R}^n$ that are easy to calculate, have reasonable continuity properties, are invariant under rigid motions but *not* under mirror imaging?

As a possible approach one may consider a more general object: a collection of points, p_i, and weights, w_i. Assuming that the mass center is at the origin, we may write the m-th moment as

$$M_m \quad = \quad \sum_i w_i \underbrace{p_i \otimes \cdots \otimes p_i}_{m}.$$

In other words, this is a homogeneous polynomial of degree m given by the formula $M_m(x) = \sum_i w_i \langle p_i, x \rangle^m$. Formally, for a homogeneous polynomial h, we want to quantify the condition that the $\mathrm{SO}(3)$-orbits of $h(x, y, z)$ and its mirror image, $h(-x, y, z)$, are distinct. It is clear that for degrees 1 and 2 the polynomials $h(x, y, z)$ and $h(-x, y, z)$ are always within the same $\mathrm{SO}(3)$-orbit, but for $m \geq 3$ this may be not so; see [4]. We may now interpret the above question as a request to write down $\mathrm{SO}(3)$-invariant functions of homogeneous degree m polynomials allowing to detect polynomials that cannot be transformed by $\mathrm{SO}(3)$ into their mirror images.

References

[1] A. B. BUDA, T. AUF DER HEYDE AND K. MISLOW. On quantifying chirality. *Angew. Chem.* **31** (1992), 989–1007.

[2] A. B. BUDA AND K. MISLOW. On a measure of axiality for triangular domains. *Elem. Math.* **46** (1999), 65–73.

[3] B. GRÜNBAUM. Measures of symmetry for convex sets. *Proc. Sympos. Pure Math.*, Amer. Math. Soc. **7** (1963), 233–270.

[4] M. K. HU. Visual pattern recognition by moment invariants. *IEEE Trans. Inform. Theory* **8** (1962), 179–187.