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Effective contact measures☆

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HIGHLIGHTS

- Introduces a new concept of effective contact measure as an approximation of surface contact area.
- Proposes 3 new concepts of effective contact measures.
- Discusses application to alignment problems.

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ABSTRACT

Contact area is an important geometric measurement in many physical systems. It is also difficult to compute due to its extreme sensitivity to infinitesimal perturbations. In this paper, we propose a new concept called an *effective contact measure*, which acts as a smooth version of contact area. Effective contact measures incorporate a notion of scale into the definition of contact area, allowing one to consider the degree of contact at different sizes. We show how effective contact measures can yield useful statistics for a number of applications, including analysis of multiphase materials and docking/alignment problems.

1. Introduction

Let us say that a pair of solids, $S, T \subseteq \mathbb{R}^n$ are in *contact* if their closures intersect but not their interiors[1]:

$$(\kappa S \cap \kappa T) \neq \emptyset$$
$$(\iota S \cap \iota T) = \emptyset.$$

If S and T are in contact, then define their *contact area* to be the $(n-1)$-Hausdorff measure of their intersection:

$$\mu^{n-1}(S \cap T).$$

The goal of this paper is to study some approximations of contact area and their computations. In these approximations, we will consider both perturbation of the shapes and the situation where the shapes are nearly in contact (i.e. they may be slightly separated or interpenetrating, violating the strict contact condition).

1.1. Motivation

There are a number of reasons that one might be interested in contact area. As a motivating example, consider the problem of analyzing a sample of some multiphase material. In general, some of the phases may be insulated from one another, while others may be directly touching. The extent to which any two phases are in contact has a direct physical significance in heat transfer [1], electrical resistance [2], material strength [3], mechanical wear [4] and microscopic friction [5]. Another application of contact area is the solution of docking problems. Suppose we are given two solids – for example, pieces of a jigsaw puzzle – and say that we want to figure out how to align them such that they fit together while touching as much as possible. Finding such alignments could be used as a subproblem for higher level assembly and planning operations, like box packing [6] or recovering assembly constraints [7], for example.

1.2. Challenges

The main issue with the direct definition of contact area is that it is unstable with respect to small perturbations of the shapes involved. This seems to have been first noticed by Bowden [8], and is similar to the behavior of the surface area or curvature [9,10] of a solid. From a practical standpoint, this instability causes problems when using numerical optimization to find docking configurations.

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[1] We use the symbols κ, ι, δ to denote closure, interior and boundary operators respectively. We call a bounded set a *solid* if it is compact and regular; $S = \kappa\iota S$.

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It also means the calculation of the contact area becomes highly dependent on the scale at which the objects involved are measured and represented, where results at finer scales may diverge greatly from those which are sampled more coarsely.

1.3. Contributions

Our proposed solution to these problems is to introduce a new concept which we call an "effective contact measure". Effective contact measures allow us to consider contact area at different scales and in situations where objects are nearly touching or even slightly penetrating. This avoids the use of highly sensitive calculations like surface area. The bulk of this paper is devoted to studying various formulations of effective contact measure. We also show that many of these quantities can be computed efficiently using the Fourier transform which makes them attractive for problems like alignment or nesting. In the final portion of the paper, we discuss some of these applications in more detail and experimentally compare the behavior of our various constructions on several examples in 2D and 3D.

2. Related work

In physics and mechanical engineering there has been a great deal of work in relating various physical quantities to contact area, as discussed in Section 1.1. But outside the applied sciences, the concept of contact area does not appear to have received much attention in its own right. Perhaps the most closely related set of ideas to our approach is the concept of a curvature measure [11,9], as defined in the field of geometric measure theory and integral geometry. However, a key difference is that curvature measures consider only the change of a single body within a fixed localizing region, while in a contact area measure we consider simultaneous perturbations of both sets.

To the best of our knowledge, the direct application of contact area to alignment or docking problems does not appear to have been investigated in either a theoretical or computational context. In spirit, the most closely related research to this work is cross correlation based alignment for protein docking [12,13]. These techniques model the alignment problem as one of maximizing the overlap of pseudo electric charge potentials defined over the surface of some molecule, with complex weights added to the interiors to penalize interference and reward docking. Variations of this idea are currently used in state of the art systems of finding probably docking configurations in drug discovery [14,15]. This same sort of operation is at the heart of our approach to contact area, though we do not use the same approach to defining the "electric fields" and give the operation a very different interpretation. Finally, it bears mentioning that Kazhdan used spherical harmonics to align pairs of 3D models up to a rotation [16] by cross correlating their surface normals. This technique can be interpreted as a special case of the Laplacian contact area we propose in the later section.

3. Effective contact area

3.1. Basic requirements

We choose to cast our theory of effective contact measures in the language of bimeasures. The motivation for bimeasures comes from a desire to extend measures from one to many sets. At minimum, a bimeasure satisfies the following definition:

Definition 1. A *bimeasure* is a real valued binary function K on solids such that for all compact regular sets $S, T \subseteq \mathbb{R}^n$, K satisfies the following axioms:

(i) *(Null–Emptyset)* $K(\emptyset, S) = K(S, \emptyset) = 0$.

(ii) *(Additive)* Given $S_1, S_2, T_1, T_2 \subseteq \mathbb{R}^n$ where $S_1 \cap S_2 = \emptyset$ and $T_1 \cap T_2 = \emptyset$,

$$K(S_1 \cup S_2, T_1 \cup T_2) = K(S_1, T_1) + K(S_1, T_2) + K(S_2, T_1) + K(S_2, T_2).$$

We want to define bimeasures which capture some notion of contact size between a pair of solids. But a bimeasure is a very general type of structure, and so for our goals it is reasonable to impose some additional constraints upon the bimeasures and the class of solids that we will be investigating. Inspired by the ideas of Edalat and Lieutier [17], we would like to ensure that our functions are computable by convergent sequences of solids, for example in the Hausdorff topology. Hence the following two definitions.

Definition 2. A sequence $S_0, S_1, \ldots \subseteq \mathbb{R}^n$ converges to $S \subseteq \mathbb{R}^n$ (in the Hausdorff topology) [18] if for any $\epsilon > 0$, there exists some $k \in \mathbb{N}^+$ such that for all $i > k$,

$$S \subseteq S_i \oplus \epsilon B^n \quad \text{and} \quad S_i \subseteq S \oplus \epsilon B^n$$

where $\oplus$ denotes the Minkowski sum and $B^n = \{x \in \mathbb{R}^n : |x| \leq 1\}$ is the unit ball.

Definition 3. A bimeasure is *continuous* (in the Hausdorff topology) if for any pair of convergent sequences, $\{S_i\}$, $\{T_j\}$ approaching S, T respectively, we have:

$$\lim_{i,j\to\infty} K(S_i, T_j) = K(S, T).$$

Continuity is a necessary requirement for a bimeasure to be robustly computable [17]. Without this property, small perturbations in the input shapes can have arbitrarily large effects on the result. The desire for continuity is also the reason why we must look beyond the most naive measures of contact area. In fact one can see that the Hausdorff area of the intersection fails to be continuous from the following simple example. Given two plates which are separated by some finite distance t, they determine a sequence of solids which converge to a pair of plates that are exactly in contact. For any $t > 0$, the two plates are not in contact and so $\mu^{n-1}(S \cap T)$ is 0; however in the limit where they touch it $\mu^{n-1}(S \cap T)$ jumps to the area of the intersection, and so the measure is obviously not continuous.

3.2. Effective contact area

The fact that the Hausdorff measure of the intersection of two solids is discontinuous is the main technical necessity for pursuing this research. Our proposed solution to this problem is to first replace the measure of the intersection with an integral of indicator functions, and then to apply smoothing that the resulting function is continuous. This smoothing introduces a concept of scale, where coarser scales correspond to more smoothing, while fine values give a sharper measure which in the limit converges to the exact contact area. A side effect of this smoothing is that we recover finite effective contact area in the case where the solids involved *are not in strictly contact*, that is they might not intersect or their interiors may be slightly overlapping. Formalizing this concept is the basis for our new definition of an effective contact measure,

Definition 4. An *effective contact measure* is a family of bimeasures $\{K_h : h > 0\}$ such that for $h > 0$ each K_h is continuous, and that for any pair of solids of finite reach which are *in contact*,[2] there exists a real number $C > 0$ such that,

$$\lim_{h\to 0} K_h(S, T) = C\mu^{n-1}(S \cap T).$$

[2] See introduction.