Instance-Optimal Geometric Algorithms

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Abstract

We prove the existence of an algorithm A for computing 2-d or 3-d convex hulls that is optimal for every point set in the following sense: for every set S of npoints and for every algorithm A' in a certain class A, the maximum running time of A on input $\langle s_1, \ldots, s_n \rangle$ is at most a constant factor times the maximum running time of A' on $\langle s_1, \ldots, s_n \rangle$, where the maximum is taken over all permutations $\langle s_1, \ldots, s_n \rangle$ of S. In fact, we can establish a stronger property: for every S and A', the maximum running time of A is at most a constant factor times the average running time of A' over all permutations of S. We call algorithms satisfying these properties instance-optimal in the order-oblivious and random-order setting. Such instance-optimal algorithms simultaneously subsume output-sensitive algorithms and distribution-dependent average-case algorithms, and all algorithms that do not take advantage of the order of the input or that assume the input is given in a random order.

The class A under consideration consists of all algorithms in a decision tree model where the tests involve only multilinear functions with a constant number of arguments. To establish an instance-specific lower bound, we deviate from traditional Ben–Or-style proofs and adopt an interesting adversary argument. For 2-d convex hulls, we prove that a version of the well known algorithm by Kirkpatrick and Seidel (1986) or Chan, Snoeyink, and Yap (1995) already attains this lower bound. For 3-d convex hulls, we propose a new algorithm.

To demonstrate the potential of the concept, we further obtain instance-optimal results for a few other standard problems in computational geometry, such as maxima in 2-d and 3-d, orthogonal line segment intersection in 2-d, finding bichromatic L_{∞} -close pairs in 2-d, off-line orthogonal range searching in 2-d, off-line dominance reporting in 2-d and 3-d, off-line halfspace range reporting in 2-d and 3-d, and off-line point location in 2-d.

1. Introduction

Instance optimality: our model(s). Standard worstcase analysis of algorithms has often been criticized as overly pessimistic. As a remedy, some researchers have turned towards *adaptive* analysis where the cost of algorithms is measured as a function of not just the input size but other parameters that capture in some ways the inherent simplicity or difficulty of the input instance. For example, for problems in computational geometry (the primary domain of the present paper), parameters that have been considered in the past include the output size (leading to so-called *output-sensitive* algorithms) [46], the spread of an input point set (the ratio of the maximum to the minimum pairwise distance) [38], various measures of fatness of the input objects (e.g., ratio of circumradii to inradii) [48] or clutteredness of a collection of objects [30], the number of reflex angles in an input polygon, and so on.

The ultimate in adaptive algorithms is an *instance*optimal algorithm, i.e., an algorithm A whose cost is at most a constant factor from the cost of any other algorithm A' running on the same input, for every input instance. Unfortunately, for many problems, this requirement is too stringent. For example, consider the 2-d convex hull problem, which has $\Theta(n \log n)$ worst-case complexity in the algebraic computation tree model: for every input sequence of n points, one can easily design an algorithm A' (with its code depending on the input sequence) that runs in O(n) time on that particular sequence, thus ruling out the existence of an instanceoptimal algorithm.¹

¹The length of the program for A' may depend on n in this example. If we relax the definition to permit the "constant factor" to grow as a function of the program length of A', then an instance-optimal al-

To get a more useful definition, we suggest a variant of instance optimality where we ignore the order in which the input elements are given, as formalized precisely below:

Definition 1.1 Consider a problem where the input consists of a sequence of n elements from a domain \mathcal{D} . Consider a class \mathcal{A} of algorithms. A *correct* algorithm refers to an algorithm that outputs a correct answer for every possible sequence of elements in \mathcal{D} .

For a set S of n elements in \mathcal{D} , let $T_A(S)$ denote the maximum running time of A on input σ over all n! possible permutations σ of S. Let OPT(S) denote the minimum of $T_{A'}(S)$ over all correct algorithms $A' \in \mathcal{A}$. If $A \in \mathcal{A}$ is a correct algorithm such that $T_A(S) \leq O(1) \cdot OPT(S)$ for every set S, then we say A is *instance-optimal in the order-oblivious setting*.

For many problems, the output is a function of the input as a set rather than a sequence, and the above definition is especially meaningful. In particular, for such problems, instance-optimal algorithms are automatically optimal output-sensitive algorithms; in fact, they are automatically optimal adaptive algorithms with respect to *any* parameter that is independent of the input order, all at the same time! This property is satisfied by simple parameters like the spread of an input point set S, or more complicated quantities like the expected size $f_r(S)$ of the convex hull of a random sample of size r from S [26].

For many algorithms (e.g., quickhull [52], to name one), the running time is not affected so much by the order in which the input points are given but by the input point set itself. Combinatorial and computational geometers more often associate "bad examples" with bad point sets rather than bad point sequences. All this supports the reasonableness and importance of the order-oblivious form of instance optimality.

We can consider a still stronger variant of instance optimality:

Definition 1.2 For a set S of n elements in \mathcal{D} , let $T_A^{\text{avg}}(S)$ denote the average running time of A on input σ over all n! possible permutations σ of S. Let $\text{OPT}^{\text{avg}}(S)$ denote the minimum of $T_{A'}^{\text{avg}}(S)$ over all correct algorithms $A' \in \mathcal{A}$. If $A \in \mathcal{A}$ is a correct algorithm such that $T_A(S) \leq O(1) \cdot \text{OPT}^{\text{avg}}(S)$ for every set S, then we say A is instance-optimal in the random-order setting.²

Note that an instance-optimal algorithm in the above sense is immediately also competitive against *randomized* (Las Vegas) algorithms A', by the easy direction of Yao's principle. The above definition has extra appeal in computational geometry, as it is common to see the design of randomized algorithms where the input elements are initially permuted in random order [28].

Instance-optimal algorithms in the random-order setting also imply optimal *average-case* algorithms where we analyze the expected running time under the assumption that the input elements are random and independently chosen from a common given probability distribution. (To see this, just observe that the input sequence is equally likely to be any permutation of S conditioned to the event that the set of n input elements equals any fixed set S.) An instance-optimal algorithm can deal with all probability distributions at the same time! Instance optimality also remedies a common complaint about averagecase analysis, that it does not provide information about an algorithm's performance on a specific input.

Convex hull: our main result. After making the case for instance-optimal algorithms under our definitions, the question remains: do such algorithms actually exist, or are they "too good to be true"? Specifically, we turn to one of the most fundamental and well known problems in computational geometry-computing the convex hull of a set of n points. Many $O(n \log n)$ -time algorithms in 2-d and 3-d have been proposed since the 1970s [31, 36, 52], which are worst-case optimal under the algebraic computation tree model. Optimal outputsensitive algorithms can solve the 2-d and 3-d problem in $O(n \log h)$ time, where h is the output size. The first such output-sensitive algorithm in 2-d was found by Kirkpatrick and Seidel [46] in the 1980s and was later simplified by Chan, Snoeyink, and Yap [20] and independently Wenger [55]; a different, simple, optimal output-sensitive algorithm was discovered by Chan [15]. The first optimal output-sensitive algorithm in 3-d was obtained by Clarkson and Shor [28] using randomization; another version was described by Clarkson [26]. The first deterministic optimal output-sensitive algorithm in 3-d was obtained by Chazelle and Matoušek [25] via derandomization; the approach by Chan [15] can also be extended to 3-d and yields a simpler optimal output-sensitive algorithm. There are also average-case algorithms that run in O(n) expected time for certain probability distributions [52], e.g., when the points are independent and uniformly distributed inside a circle or a constant-size polygon in 2-d, or a ball or a constant-size polyhedron in 3-d.

The convex hull problem is in some ways an ideal candidate to consider in our models. It is not difficult to think of examples of "easy" point sets and "hard" point sets (see Figure 1(a,b)). It is not difficult to think of differ-

gorithm A exists for many problems such as sorting (or more generally problems that admit linear-time verification). This follows from a trick attributed to Levin [42], of enumerating and simulating all programs in parallel under an appropriate schedule. To say that algorithms obtained this way are impractical, however, would be an understatement.

²One can also consider other variations of the definition, e.g., relaxing the condition to $T_A^{\text{avg}}(S) \leq O(1) \cdot \text{OPT}^{\text{avg}}(S)$, or replacing expected running time over random permutations with analogous highprobability statements.

ent heuristics for pruning nonextreme points, which may not necessarily improve worst-case complexity but may help for many point sets encountered "in practice" (e.g., consider quickhull [52]). However, it is unclear whether there is a single pruning strategy that works best on all point sets.

In this paper, we show that there are indeed instanceoptimal algorithms for both the 2-d and 3-d convex hull problem, in the order-oblivious or the stronger randomorder setting. Our algorithms thus subsume all the previous output-sensitive and average-case algorithms simultaneously, and are provably at least as good asymptotically as any other algorithm for every point set, so long as input order is ignored.

Techniques. We believe that our techniques—for both the upper-bound side (i.e., algorithms) and the lower-bound side (i.e., proofs of their instance optimality)—are as interesting as our results.

On the upper-bound side, we find that in the 2-d case, a new algorithm is not necessary: a version of Kirkpatrick and Seidel's output-sensitive algorithm, or its simplification by Chan, Snoeyink, and Yap, is instance-optimal in the order-oblivious and random-order setting. We view this as a plus: these algorithms are simple and practical to implement [12], and our analysis sheds new light into their theoretical complexity. In particular, our result immediately implies that a version of Kirkpatrick and Seidel's algorithm runs in O(n) expected time for points uniformly distributed inside a circle or a fixed-size polygon-we were unaware of this fact before. (interestingly, Kirkpatrick and Seidel's paper is titled "The ultimate planar convex hull algorithm?"; our result gives a positive answer to the title question in the order-oblivious and random-order model.)

In 3-d we propose a new algorithm, as none of the previous output-sensitive algorithms seem to be instance-optimal (e.g., known 3-d generalizations of the Kirkpatrick–Seidel algorithm have suboptimal $O(n \log^2 h)$ running time [20, 37], while a straightforward implementation of Chan's algorithm [15] fails to be instance-optimal even in 2-d). Our algorithm builds on Chan's technique [15] but requires additional ideas, notably the use of *partition trees* [31, 49].

The lower-bound side requires more innovation. We are aware of three existing techniques for proving worstcase $\Omega(n \log n)$ (or output-sensitive $\Omega(n \log h)$) lower bounds in computational geometry: (i) informationtheoretical or counting arguments, (ii) topological arguments, from early work by Yao [56] to Ben-Or's theorem [10], and (iii) Ramsey-theory-based arguments, by Moran, Snir, and Manber [50]. Ben-Or's approach is perhaps the most powerful and works in the general algebraic computation tree model, whereas Moran *et al.*'s approach works for a decision tree model in which all the test functions have a bounded number of arguments. For an arbitrary input set S for the convex hull problem, the naive information-theoretical argument gives only an $\Omega(h \log h)$ lower bound on OPT(S). On the other hand, topological and Ramsey-theory approaches seem unable to give any instance-specific lower bound at all (e.g., modifying the topological approach is already nontrivial if we just want a lower bound for *some* integer input set [57], let alone for *every* input set, whereas the Ramsey-theory approach considers only input elements that come from a cleverly designed subdomain).

We end up using a different lower bound technique which is inspired by an adversary argument from a recent work by Chan [18] on an unrelated problem (time-space lower bounds for median finding). Chan [19] noted that this approach can lead to another proof of the standard $\Omega(n \log n)$ lower bounds for many geometric problems including convex hull; the proof is simple and works in an algebraic decision tree model where the test functions have at most constant degree and have at most a constant number of arguments. We build on the idea further and obtain an optimal lower bound for the convex hull problem for every input point set. The assumed model is more restrictive: the class \mathcal{A} of allowed algorithms consists of those under a decision tree model in which the test functions are multilinear and have at most a constant number of arguments. Fortunately, most standard primitive operations encountered in existing convex hull algorithms satisfy the multilinearity condition (e.g., the standard determinant test does). The final proof is quite nice, in our opinion. Interestingly it involves partition trees, which are more typically used in algorithms (as in our new 3-d algorithm) rather than in lower-bound proofs.

So, what is OPT(S), i.e., what parameter truly captures the difficulty of a point set S, asymptotically, for the convex hull problem? As it turns out, the bound has a simple expression (to be revealed in Section 3) and shares similarity with entropy bounds found in average-case (also called "expected-case") analysis of geometric data structures where query points come from a given probability distribution-these entropy-based results have been the subject of several recent papers [6, 7, 29, 35, 41]. However, lower bounds for expected-case data structures cannot be applied to our problem because our problem is off-line (lower bounds for on-line query problems usually assume that the query algorithms fit a "classification tree" framework, but an off-line algorithm may compare a query point not only with points from the data set but also with other query points). Furthermore, although in the off-line setting we can think of the query points as coming from a discrete point probability distribution, the distribution is not known in advance.³ Lastly, expected-

³Self-improving algorithms [4, 27] also cope with the issue of how to



Figure 1. (a) A "harder" point set and (b) an "easier" point set for the upper hull problem. (c) A point set with $\mathcal{H}(S)$ near $\log h$ and (d) an "easier" point set with $\mathcal{H}(S)$ near constant for the maxima problem.

case data structures achieve speedup in querying but not preprocessing.

Other results. Convex hull is just one problem for which we are able to obtain instance optimality. We show that our techniques can lead to instance-optimal results for many other standard problems in computational geometry, in the order-oblivious or random-order setting, including: (a) maxima in 2-d and 3-d, (b) reporting/counting intersection between horizontal and vertical line segments in 2-d, (c) reporting/counting pairs of L_{∞} -distance at most 1 between a red point set and a blue point set in 2-d, (e) off-line orthogonal range reporting/counting in 2-d, (e) off-line dominating reporting in 2-d and 3-d, (f) off-line halfspace range reporting in 2-d and 3-d, and (g) off-line point location in 2-d. (We are forced to put these results in Appendix A because of space limitation.)

Optimal expected-case, entropy-based data structures for the on-line version of (g) are known before [7, 41], but not for (e,f)—for example, a recent SODA'09 paper by Dujmović, Howat, and Morin [35] only obtained results for 2-d dominance counting, a special case of 2-d orthogonal range counting. Incidentally, as a consequence of our ideas, we can also get new optimal expected-case data structures for on-line 2-d general orthogonal range counting and 2-d and 3-d halfspace range reporting.

Related work. Although Fagin *et al.* [39] first coined the term "instance optimality" (when studying the problem about finding items with the k top aggregate scores in a database in a certain model), the concept has appeared before. For example, the well known "dynamic optimality conjecture" is about instance optimality concerning algorithms for manipulating binary search trees (see [32] for the latest in a series of papers). Demaine, López-

Ortiz, and Munro [34] studied the problem of computing the union or intersection of k sorted sets and gave instance-optimal results for any k for union, and for constant k for intersection, in the comparison model; see Barbay and Chen [9] for an extension to a 2-d problem on computing the convex hulls of k convex polygons. Another work about instance-optimal geometric algorithms is by Baran and Demaine [8], who addressed an approximation problem about computing the distance of a point to a curve under a certain black-box model. Other than these, there has not been much work on instance optimality in computational geometry, especially concerning the classical problems under conventional models.

The concept of instance optimality resembles competitive analysis of on-line algorithms. In fact, in the on-line algorithms literature, our order-oblivious setting of instance optimality is related to what Boyar and Favrholdt called the *relative worst order ratio* [13], and our random-order setting is related to Kenyon's *random order ratio* [43]. What makes instance optimality more intriguing is that we are not bounding the objective function of an optimization problem but the cost of an algorithm.

2. Warm-Up: 2-d Maxima

Before proving our main result on convex hull, we find it useful to study a simpler problem: maxima in 2-d. For two points p and q we say p dominates q if each coordinate of p is greater than that the corresponding coordinate of q. Given a set S of n points in \mathbb{R}^d , a point p is maximal if $p \in S$ and p is not dominated by any other point in S. For simplicity, we assume that the input is always nondegenerate throughout the paper. The maxima problem is to report all maximal points, say, from left to right.

For an alternative formulation, we can define the *or*thant at a point p to be the region of all points that are dominated by p. In 2-d, the boundary of the union of the orthants at all $p \in S$ forms a *staircase*, and the maxima

deal with unknown input probability distributions, but are not directly comparable with our results, since in their setting each point can come from a different distribution, so input order matters.

problem is equivalent to computing the staircase of S.

This problem has a similar history as the convex hull problem: many worst-case $O(n \log n)$ -time algorithms are known, Kirpatrick and Seidel's output-sensitive algorithm runs in $O(n \log h)$ time for output size h, and average-case algorithms with O(n) expected time have been analyzed for various probability distributions [11, 26, 52]. The problem is simpler in the sense that direct pairwise comparisons are sufficient. We therefore work with the class A of algorithms in the *comparison model* where we can access the input points only through comparisons of the coordinate of an input point. The number of comparisons made by an algorithm will act as a lower bound on the running time.

We define a measure $\mathcal{H}(S)$ to represent the difficulty of a point set S and prove that the optimal running time OPT(S) is precisely $\Theta(n(\mathcal{H}(S)+1))$ for the 2-d maxima problem in the order-oblivious and random-order setting.

Definition 2.1 Consider a partition Π of the input set S into disjoint subsets S_1, \ldots, S_t . We say that Π is *respectful* if each subset S_k is either a singleton or can be enclosed by an axis-aligned box B_k whose interior is completely below the staircase of S. Define $\mathcal{H}(\Pi) = \sum_{k=1}^{t} (|S_k|/n) \log(n/|S_k|)$ and let $\mathcal{H}(S)$ to be the minimum of $\mathcal{H}(\Pi)$ over all respectful partitions Π of S.

Remark 2.2 Alternatively, we could further insist in the definition that the bounding boxes B_i are nonoverlapping and cover precisely the staircase of S. However, this will not matter, as it turns out that the two definitions yield asymptotically the same quantity (this nonobvious fact is a byproduct of our lower bound proof).

 $\mathcal{H}(\Pi)$ is of course an entropy-like expression and is similar to bounds used in expected-case geometric data structures for the case of a discrete point probability distribution, although our definition itself is nonprobabilistic. A measure proposed by Sen and Gupta [53] is identical to $\mathcal{H}(\Pi_{\text{vert}})$ in which Π_{vert} is a partition of S obtained by dividing the point set S by h vertical lines at the h maximal points of S. Note that $\mathcal{H}(\Pi_{\text{vert}})$ is at most log h (see Figure 1(c)) but can be much smaller; in turn, $\mathcal{H}(S)$ can be much smaller than $\mathcal{H}(\Pi_{\text{vert}})$ (see Figure 1(d)). The complexity of the 1-d multiset sorting problem [51] also has a similar expression, but there each input multiset induces a unique partition and so the situation is even simpler.

2.1. Upper bound

We use a slight variant of Kirkpatrick and Seidel's output-sensitive maxima algorithm [45] (in their original algorithm, only points from Q_{ℓ} are pruned in line 4):

maxima(Q):

- 1. if |Q| = 1 then return Q
- 2. divide Q into the left and right halves Q_{ℓ} and Q_r by the median x-coordinate
- 3. *discover* the point q with the maximum y-coordinate in Q_r (computable in linear time)
- 4. *prune* all points in Q_{ℓ} and Q_r that are dominated by q
- 5. return the concatenation of $maxima(Q_\ell)$ and $maxima(Q_r)$

We call maxima(S) to start. It is straightforward to show that the algorithm runs in time $O(n \log h)$, or $O(n(\mathcal{H}(\Pi_{vert}) + 1))$ time, as was done by Sen and Gupta [53]. Upper-bounding the running time by $O(n(\mathcal{H}(\Pi) + 1))$ for an *arbitrary* respectful partition Π of S requires a bit more finesse:

Theorem 2.3 *The above 2-d maxima algorithm runs in* $O(n(\mathcal{H}(S) + 1))$ *time.*

Proof: Consider the recursion tree of the algorithm and let X_j denote the sublist of all maximal points of S discovered during the first j recursion levels, in left-to-right order. Let $S^{(j)}$ be the subset of S that *survives* recursion level j, i.e., the set of points that have not been pruned during the first j recursion levels and $n_j := |S^{(j)}|$. Observe that (i) there can be at most $\lceil n/2^j \rceil$ points of $S^{(j)}$ with x-coordinates between any two consecutive points in X_j , and (ii) all points of S that are strictly below the staircase of X_j have been pruned during levels $0, \ldots, j$ of the recursion. The running time is asymptotically bounded by $\sum_{j=0}^{\log n} n_j$.

Let Π be any respectful partition of S. Look at a subset S_k in Π . Let B_k be a box enclosing S_k whose interior lies below the staircase of S. Fix a level j. Suppose the upper-right corner of B_k has x-coordinate between two consecutive points q_i, q_{i+1} in X_j . By (ii), the only points in B_k that can survive level j must have x-coordinates between q_i and q_{i+1} . Thus, by (i), the number of points in S_k that survive level j is at most min $\{|S_k|, \lceil n/2^j \rceil\}$. Since the S_k 's cover the entire point set, with a double summation we have

$$\sum_{j=0}^{\log n} n_j \leq \sum_k \sum_{j=0}^{\log n} \min\left\{ |S_k|, \lceil n/2^j \rceil \right\} \leq \sum_k O\left(|S_k| \log(n/|S_k|) + |S_k| + |S_k|/2 + |S_k|/4 + \cdots \right)$$
$$= O\left(\sum_k |S_k| (\log(n/|S_k|) + 1) \right) = O(n(\mathcal{H}(\Pi) + 1)).$$

2.2. Lower bound

For the lower-bound side, we first provide an intuitive justification for the bound $n\mathcal{H}(S)$ and point out the subtlety in obtaining a rigorous proof. Intuitively, to certify that we have a correct answer, the algorithm must gather evidence for each point p eliminated why it is not a maximal point, by indicating at least one witness point in S which dominates p. We can define a partition Π by placing points with a common witness in the same subset. It is easy to see that this partition Π is respectful. The entropy bound $n\mathcal{H}(\Pi)$ roughly presents the number of bits required to encode the partition Π , so in a vague sense, $n\mathcal{H}(S)$ represents the length of the shortest "certificate" for S. Unfortunately, there could be many valid certificates for a given input set S (due to possibly multiple choices of witnesses for each nonmaximal point). If hypothetically all branches of an algorithm lead to a common partition Π , then a straightforward informationtheoretic or counting argument would indeed prove the lower bound. The problem is that each leaf of the decision tree may give rise to a different partition Π . In the full version of this paper, we will show that despite the aforementioned difficulty, it is possible to obtain a proof of instance optimality via this approach, but the proof requires a more sophisticated counting argument, and also works with a different definition of $\mathcal{H}(S)$. Moreover, it is limited specifically to the 2-d maxima problem and does not extend to 3-d maxima, let alone to nonorthgonal problems like convex hull.

In this subsection, we describe a different proof, which generalizes to the other problems that we consider. The proof is based on an interesting and simple *adversary* argument. Here, we concentrate on the order-oblivious setting. The proofs for the corresponding results in the random-order setting will appear in the full version of the paper.

Theorem 2.4 OPT $(S) = \Omega(n(\mathcal{H}(S) + 1))$ for the 2-d maxima problem in the comparison model.

Proof: We prove that a specific respectful partition described below not only asymptotically achieves the minimum entropy among all the respectful partitions, but also provides a lower bound for the running time of any comparison based algorithm that solves the 2-d maxima problem. The construction of the partition uses k-d trees [31] to define a tree \mathcal{T} of axis-aligned boxes, generated top-down as follows: The root stores the entire plane. For each node storing box B, if B is strictly below the staircase of S, or if B contains just one point of S, then B is a leaf. Otherwise, if the node is at an odd (resp. even) depth, divide B into two subboxes by the median x-coordinate (resp. y-coordinate) among the points of S inside B. The two subboxes are the children of B. Note

that each box at depth j of \mathcal{T} contains at least $\lfloor n/2^j \rfloor$ points of S.

Our claimed partition, denoted by $\Pi_{\text{kd-tree}}$, is one formed by the leaf boxes in this tree \mathcal{T} (i.e., points in the same leaf box are placed in the same subset). Clearly, $\Pi_{\text{kd-tree}}$ is respectful. We will prove that for any correct algorithm in \mathcal{A} , there exists a permutation of S on which the algorithm requires at least $\Omega(n\mathcal{H}(\Pi_{\text{kd-tree}}))$ comparisons.

The adversary constructs a bad permutation for the input by simulating the algorithm; each comparison made by algorithm is resolved such that the algorithm is forced many comparisons. During the simulation, we maintain a box B_p in \mathcal{T} for each point p. If B_p is a leaf, the algorithm knows the exact location of p inside B_p . But if B_p is an internal node, the only information the algorithm knows about p is that p lies inside B_p . In other words, p can be assigned any point in B_p without affecting the outcome of the previous comparisons made.

For each box B in \mathcal{T} , let n(B) be the number of points p with B_p contained in B. We maintain the invariant that $n(B) \leq |S \cap B|$. If $n(B) = |S \cap B|$, we say that B is *full*. If B_p is a leaf we assign p to an arbitrary point in $S \cap B_p$ that has previously not been assigned; we then call p a *fixed* point. The invariant ensures that all the points inside a leaf can be fixed.

Assume the algorithm asks for a comparison, say, of the x-coordinates, between two points p and q. The main case is when neither B_p nor B_q is a leaf. In this case, the comparison is simulated in the following way:

- 1. If B_p (resp. B_q) is at even depth, we arbitrarily reset B_p (resp. B_q) to one of its children that is not full. Thus assume that B_p and B_q are both at odd depths.
 - W.l.o.g., suppose that the median x-coordinate of B_p is less than the median x-coordinate of B_q . We reset B_p to the left child B'_p of B_p and B_q to the right child B'_q of B_q ; if either B'_p or B'_q is full we go to step 2. Now, the knowledge that p and q lie in B'_p and B'_q allows us to deduce that p has a smaller x-coordinate than q. Thus, the adversary declares to the algorithm that x-coordinate of p is smaller than that of q and continues with the rest of the simulation.
- An exceptional case occurs if B'_p is full (or similarly B'_q is full). Here, we reset B_p instead to the sibling B''_p of B'_p but the comparison is not necessarily resolved yet, so we go back to step 1.

Note that in both steps the invariant is maintained. This is because both B_p and B'_p cannot be full: we have $|S \cap B_p| = |S \cap B'_p| + |S \cap B''_p|$ and since B_p is assigned to p we have $|S \cap B_p| \ge n(B_p) \ge n(B'_p) + n(B''_p) + 1$ implies that either $n(B'_p) < |S \cap B'_p|$ or $n(B''_p) < |S \cap B'_p|$. It remains to handle the case when B_p or B_q is a leaf. Note that if both B_p and B_q are leaves, then all the points inside them are fixed and p and q are assigned to specific points within B_p and B_q , meaning the comparison is already resolved. Otherwise, w.l.o.g., assume B_p is a leaf. We follow step 1 except that now since p has been fixed, we compare the actual x-coordinate of p to the median x-coordinate of B_q , and reset only B_q .

We now prove a lower bound on the number of comparisons, T, that the algorithm makes. Let D be the sum of the depth of B_p over all points $p \in S$. We will lower bound T in terms of D. Each time we reset a box to one of its children in step 1 or 2, D increments; we say that an ordinary (resp. exceptional) increment occurs at the parent box if this is done in step 1 (resp. step 2). Each comparison generates only O(1) ordinary increments. To take exceptional increments into account, we use a little amortization argument: At each box B in \mathcal{T} , the number of ordinary increments has to reach at least $||S \cap B|/2|$ first, before exceptional increments can occur, and the number of exceptional increments is at most $[|S \cap B|/2]$. Thus, the total number of exceptional increments is asymptotically at most the total number of ordinary increments, which is O(T). It follows that D = O(T), i.e., $T = \Omega(D)$.

Thus, it remains to prove our lower bound for D. We do this by showing that the algorithm cannot terminate if there exists a box B_q which is not a leaf: Since B_p is not a leaf it contains at least two points and is not completely underneath the staircase of S. We can either move a non-maximal point upward or a maximal point downward inside B_p and obtain a different input that is consistent with the comparisons made but has a different set of maximal points. The algorithm would be incorrect on this input: a contradiction.

Thus, at the end of the simulation, each B_p has depth $\Theta(\log(n/|S \cap B_p|))$. It follows that

$$T = \Omega(D) = \Omega\left(\sum_{\text{leaf } B} |S \cap B| \log(n/|S \cap B|)\right)$$
$$= \Omega(n\mathcal{H}(\Pi_{\text{kd-tree}})) = \Omega(n\mathcal{H}(S)).$$

Remark 2.5 The above proof is inspired by an adversary argument by Chan [18] for a 1-d problem (the original proof maintains a dyadic interval for each input point, while the new proof maintains a box from a hierarchical subdivision). The proof still holds for weaker versions of the problem, e.g., where we can report the maxima in any order, or we just want the number of maximal points (or the parity of the number). The lower-bound proof easily extends to any fixed dimension and can be easily modified to allow comparisons of different coordinates of any two points $p = (x_1, \ldots, x_d)$ and $q = (x'_1, \ldots, x'_d)$.

e.g., testing whether $x_i < x'_j$, or even $x_i < x'_j + a$ for any constant a. (For a still wider class of test functions, see the next section.)

3 Convex Hull

We now turn to our main result on 2-d and 3-d convex hull. It suffices to consider the problem of computing the upper hull of an input point set S in \mathbb{R}^d $(d \in \{2, 3\})$, since the lower hull can be computed by running the upper hull algorithm on a reflection of S.

We work with the class \mathcal{A} of algorithms in a *multilinear decision tree* model where we can access the input points only through tests of the form $f(p_1, \ldots, p_c) > 0$ for a multilinear function f, over a constant number of input points p_1, \ldots, p_c . We recall the following standard definition:

Definition 3.1 A function $f : (\mathbb{R}^d)^c \to \mathbb{R}$ is *multilinear* if the restriction of f is a linear function from \mathbb{R}^d to \mathbb{R} when any c-1 of the c arguments are fixed. Equivalently, f is multilinear if $f((x_{11}, \ldots, x_{1d}), \ldots, (x_{c1}, \ldots, x_{cd}))$ is a multivariate polynomial function in which each monomial has the form $x_{i_1j_1} \cdots x_{i_kj_k}$ where i_1, \ldots, i_k are all distinct (i.e., we cannot multiply coordinates from the same point).

Most of the 2-d and 3-d convex hull algorithms we know of fit this framework. For example, it supports the standard determinant test (for deciding whether p_1 is above the line through p_2, p_3 , or the plane through p_2, p_3, p_4), since the determinant is a multilinear function. For another example, in 2-d we can compare the slope of the line through p_1, p_2 and the slope of the line through p_3, p_4 by testing the sign of the function $(y_2 - y_1)(x_4 - x_3) - (x_2 - x_1)(y_4 - y_3)$, which is clearly multilinear. (See Appendix .1, however, for situations where non-multilinear test functions arise.)

We adopt the following modified definition of $\mathcal{H}(S)$ (as before, it will not matter whether we insist that the simplices Δ_k below are nonoverlapping):

Definition 3.2 A partition Π of S is *respectful* if each subset S_k in Π is either a singleton or can be enclosed by a simplex Δ_k whose interior is completely below the upper hull of S. Define $\mathcal{H}(S)$ to be the minimum of $\mathcal{H}(\Pi) := \sum_k (|S_k|/n) \log(n/|S_k|)$ over all respectful partitions Π of S.

3.1. Lower bound

The lower-bound proof for convex hull builds on the proof for maxima from Section 2.2 but is more involved, because a k-d tree construction no longer suffices when

addressing nonorthogonal problems. However, known tools in computational geometry provide an appropriate analog:

Lemma 3.3 For every set Q of n points in \mathbb{R}^d and $1 \leq r \leq n$, we can partition Q into r subsets Q_1, \ldots, Q_r each of size $\Theta(n/r)$ and find r convex polyhedral cells $\gamma_1, \ldots, \gamma_r$, each of size $O(\log r)$, such that Q_i is contained in γ_i , and each hyperplane intersects at most $O(r^{1-\varepsilon})$ cells. Here, $\varepsilon > 0$ is a constant that depends only on d.

Proof: (Option 1) We can use Matoušek's partition theorem [49], which provides the best constant, namely, $\varepsilon = 1/d$. Each cell γ_i is a simplex but the cells may overlap. (Note that our application requires that the subset sizes are lower-bounded by $\Omega(n/r)$, which is guaranteed by Matoušek's construction.)

(Option 2) For d = 2 or 3, a more elementary solution follows from the 4-sectioning or 8-sectioning theorem [36, 58]: for every *n*-point set Q in \mathbb{R}^2 , there exist 2 lines that divide the plane into 4 regions each with n/4 points; for every *n*-point set Q in \mathbb{R}^3 , there exist 3 planes that divide space into 8 regions each with n/8 points. Since in \mathbb{R}^2 a line can intersect at most 3 of the 4 regions and in \mathbb{R}^3 a plane can intersect at most 7 of the 8 regions, a simple recursive application of the theorem yields $\varepsilon \approx 1 - \log_4 3$ for d = 2 and $\varepsilon \approx 1 - \log_8 7$ for d = 3. Each resulting cell γ_i may have $O(\log r)$ facets, but the cells do not overlap.

We need another fact, this time, a straightforward geometric property about multilinear functions:

Lemma 3.4 If $f : (\mathbb{R}^d)^c \to \mathbb{R}$ is multilinear and has a zero in $\gamma_1 \times \cdots \times \gamma_c$ where each γ_i is a convex polytope in \mathbb{R}^d , then f has a zero $(p_1, \ldots, p_c) \in \gamma_1 \times \cdots \times \gamma_c$ such that all but at most one point p_i is a polytope's vertex.

Proof: Let $(p_1, \ldots, p_c) \in \gamma_1 \times \cdots \times \gamma_c$ be a zero of f. Suppose some p_i does not lie on an edge of γ_i . If we fix the other c-1 points, the equation f=0 becomes a hyperplane, which intersects γ_i and thus must intersect an edge of γ_i . We can move p_i to such an intersection point. Repeating this process, we may assume that every p_i lies on an edge $\overline{u_i v_i}$ of γ_i . Represent the line segment parametrically as $\{(1-t_i)u_i + t_iv_i \mid 0 \le t_i \le 1\}$.

Next, suppose that some two points p_i and p_j are not vertices. If we fix the other c-2 points and restrict p_i and p_j to lie on $\overline{u_i v_i}$ and $\overline{u_j v_j}$ respectively, the equation f = 0 becomes a multilinear function in two parameters $t_i, t_j \in [0, 1]$. The equation has the form $at_i t_j + a' t_i + a'' t_j + a''' = 0$ and is a hyperbola, which intersects $[0, 1]^2$ and must thus intersect the boundary of $[0, 1]^2$. We can move p_i and p_j to correspond to such a boundary intersection point. Then one of p_i and p_j is now a vertex. This process can be repeated.

We are now ready for the main proof. Again, we focus on the order-oblivious setting and leave the random-order setting to Appendix **??**.

Theorem 3.5 OPT $(S) = \Omega(n(\mathcal{H}(S)+1))$ for the upper hull problem in the multilinear decision tree model.

Proof: We define a *partition tree* \mathcal{T} as follows: Each node v stores a pair $(Q(v), \gamma(v))$, where Q(v) is a subset of S enclosed inside a convex polyhedral cell $\gamma(v)$. For each node v, let $\Gamma(v)$ denote the intersection of $\gamma(u)$ over all ancestors u of v. The root stores (S, \mathbb{R}^d) . If $\Gamma(v)$ is strictly below the upper hull of S, or if |Q(v)| drops below a constant, then v is a leaf. Otherwise, fix a parameter r = b and partition Q(v) by Lemma 3.3 to get b subsets Q_1, \ldots, Q_b and cells $\gamma_1, \ldots, \gamma_b$. The pairs (Q_i, γ_i) are the children of v. For a node v at depth j of the tree \mathcal{T} we have $|Q(v)| \ge n/\Theta(b)^j$ and since $\Gamma(v)$ is the intersection of at most j convex polyhedra of size polylogarithmic in b, it has $O(j \log b) = O(bj)$ facets.

Let $\Pi_{\text{part-tree}}$ be the partition formed by the subsets Q(v) at the leaves v in \mathcal{T} . Let $\Pi_{\text{part-tree}}$ be a refinement of this partition obtained as follows: for each leaf v at depth j, we triangulate $\Gamma(v)$ into $(bj)^{O(1)}$ simplices and subpartition Q(v) by placing points of Q(v) from the same simplex in the same subset; if |Q(v)| drops below a constant, we subpartition Q(v) causes the entropy to decrease by at most $O((|Q(v)|/n)\log(bj)^{O(1)}) = O((|Q(v)|/n)\log\log(n/|Q(v)|))$ for a constant b. The total decrease in entropy is thus $o(\mathcal{H}(\Pi_{\text{part-tree}}))$. So $\mathcal{H}(\Pi_{\text{part-tree}}) = \Theta(\mathcal{H}(\Pi_{\text{part-tree}}))$. Clearly, $\Pi_{\text{part-tree}}$ is respectful.

The adversary constructs a bad permutation for the input points as follows. During the simulation, we maintain a node v_p in \mathcal{T} for each point p. If v_p is a leaf, the algorithm knows the exact location of p inside $\Gamma(v_p)$. But if v_p is an internal node, the only information the algorithm knows about p is that p lies inside $\Gamma(v_p)$.

For each node v in \mathcal{T} , let n(v) be the number of points p with v_p in the subtree rooted at v. We maintain that $n(v) \leq |Q(v)|$. If n(v) = |Q(v)|, we say that v is *full*. If v_p is a leaf, we fix p to an arbitrary unassigned point in $Q(v_p)$. The invariant ensures that such an assignment can always be made.

Suppose the simulation encounters a test " $f(p_1, \ldots, p_c) > 0$?".

1. Consider a *c*-tuple $(v'_{p_1}, \ldots, v'_{p_c})$ where v'_{p_i} is a child of v_{p_i} . We say that the tuple is *bad* if *f* has a zero in $\gamma(v'_{p_1}) \times \cdots \times \gamma(v'_{p_c})$, and *good* otherwise.

We prove the existence of a good tuple by bounding the the number of bad tuples from above: If we fix all but one point p_i , the restriction of f can have a zero in at most $O(b^{1-\varepsilon})$ cells of the form $\gamma(v'_{p_i})$, by Lemma 3.3 and the multi-linearity of f. There are $O(b^{c-1} \text{ polylog } b)$ choices of c-1 vertices of the cells of the form $\gamma(v'_{p_1}), \ldots, \gamma(v'_{p_c})$. By Lemma 3.4, it follows that the number of bad tuples is at most $O(b^{c-1} \text{ polylog } b \cdot b^{1-\varepsilon}) = O(b^{c-\varepsilon} \text{ polylog } b)$. As the number of tuples is $\Theta(b^c)$, if b is a sufficiently large constant, then we can guarantee that some tuple $(v'_{p_1}, \ldots, v'_{p_c})$ is good. We reset v_{p_i} to v'_{p_i} for each $i = 1, \ldots, c$. Since the tuple is good, the sign of f is determined and the comparison is resolved.

2. In the exceptional case when some v'_{p_i} is full, we reset v_{p_i} instead to an arbitrary non-full child that is not full, and go back to step 1.

The above description can be easily modified in the case when some of the nodes v_{p_i} are leaves, i.e., when some of the points p_i are already fixed (we just have to lower cby the number of fixed points).

Let T be the number of tests made. Let D be the sum of the depth of v_p over all points $p \in S$. The rest of the argument is almost identical to one described for 2-d maxima: The same amortization argument as before (after adjustments of constant factors), proves $T = \Omega(D)$. We observe that the algorithm cannot terminate if there exists a box B_q which is not a leaf; thus, at the end of the simulation, each node v_p has depth $\Theta(\log(n/|Q(v_p)|))$. It follows that $T = \Omega(D) = \Omega(\sum_{\text{leaf } v} |Q(v)| \log(n/|Q(v)|)) = \Omega(n\mathcal{H}(\Pi_{\text{part-tree}})) = \Omega(n\mathcal{H}(\widetilde{\Pi}_{\text{part-tree}})) = \Omega(n\mathcal{H}(S))$.

3.2. Upper bound

In 2-d, an $O(n(\mathcal{H}(S)+1))$ upper bound can be established by using a version of Kirkpatrick and Seidel's (or Chan, Snoeyink, and Yap's) convex hull algorithm. The analysis is similar enough to that for 2-d maxima from Section 2.2 and will be presented in the full version of this paper. For the rest of this section we focus on the 3-d case.

Unlike in 2-d, it is unclear if any of the known algorithms can be modified for this purpose. For example, it is already nontrivial how to get an $O(n\mathcal{H}(\Pi_{vert}))$ upper bound for the specific partition Π_{vert} where points underneath the same upper-hull facet are placed in the same subset. Fortunately, informed by our lower-bound proof, we discover a solution based on partition trees.

We need the following subroutine by Chan [15, 16], which is obtained by applying a simple grouping trick in

conjunction with standard data structures (see also [14]).

Lemma 3.6 We can answer a sequence of r linear programming queries over a given set of n halfspaces in \mathbb{R}^3 in total time $O(n \log r + r \log n)$.

Our new upper hull algorithm is as follows:

- 1. $Q \leftarrow S$
- 2. for $j = 0, 1, \ldots, \lceil \log(\delta \log n) \rceil$ do
- 3. partition Q by Lemma 3.3 to get $r_j := 2^{2^j}$ subsets Q_1, \ldots, Q_{r_j} and cells $\gamma_1, \ldots, \gamma_{r_j}$
- 4. for each i do
- 5. if γ_i is strictly below the upper hull of Q then *prune* all points in Q_i from Q
- 6. return the upper hull of the remaining set Q

Line 3 takes $O(|Q| \log r_j)$ time by known algorithms for Lemma 3.3 (either option) [49]. The test in line 5 reduces to deciding whether each vertex of γ_i is strictly below the upper hull of Q. This can be done (without knowing the upper hull beforehand) by answering a 3-d linear programming query in the dual. Using Lemma 3.6, we can perform lines 4–6 collectively in time $O(|Q| \log r_j + r_j \operatorname{polylog} r_j \log n)$; note that $\sum_j r_j = O(n^{\delta})$, and so the second term is negligible by choosing a constant $\delta < 1$. Line 6 is done by running any $O(|Q| \log |Q|)$ time algorithm; note that $\log |Q| = O(\log r_j)$ in the last iteration.

Theorem 3.7 *The above 3-d upper hull algorithm runs in* $O(n(\mathcal{H}(S) + 1))$ *time.*

Proof: Let n_j be the size of Q just after iteration j. The total running time is asymptotically bounded by $\sum_j n_{j-1} \log r_j$.

Let Π be any respectful partition of S. Look at a subset S_k in Π . Let Δ_k be a simplex enclosing S_k whose interior lies below the upper hull of S. Fix an iteration j. Consider the subsets Q_1, \ldots, Q_{r_j} and cells $\gamma_1, \ldots, \gamma_{r_j}$ at this iteration. If a cell γ_i is competely inside Δ_k , then all points inside γ_i are pruned. Since $O(r_j^{1-\varepsilon})$ cells γ_i intersect the boundary of Δ_k , the the number of points in S_k that remain in Q after iteration j is at most min $\{|S_k|, O(r_j^{1-\varepsilon} \cdot n/r_j)\} = \min\{|S_k|, O(n/r_j^{\varepsilon})\}$. The S_k 's cover the entire point set, so with a double summation we have

$$\sum_{j} n_{j} \log r_{j+1} \leq \sum_{k} \sum_{j} \min \left\{ O(2^{j}) |S_{k}|, \frac{n}{2^{\Omega(\varepsilon^{2^{j}})}} \right\}$$
$$= O(n(\mathcal{H}(\Pi) + 1)).$$

Remark 3.8 Variants of the algorithm are possible. For example, instead of recomputing the partition in line 3 at each iteration from scratch, a better option is to build the partitions hierarchically as a tree. Nodes are pruned as the tree is generated level by level.

One minor technicality is that the above description of the algorithm does not discuss the low-level test functions involved. In Appendix .1, we explain how a modification of the algorithm can indeed be implemented in the multilinear model.

The same approach works for 3-d maxima as well. In the comparison model, the partitions can be constructed by a k-d tree construction, and linear programming queries are replaced by queries to test whether a point lies underneath the staircase, which can be done via an analog of Lemma 3.6.

4 Discussion

Although we have argued for the order-oblivious form of instance optimality, we are not denigrating adaptive algorithms that exploit the order of the input. Indeed, for some geometric applications, the input order may exhibit some sort of locality of reference which can speed up algorithms. There are various parameters that one can define to address this issue, but it is unclear how a unified theory of instance optimality can be developed for orderdependent algorithms for, say, the convex hull problem.

We do not claim that the algorithms described here are the best in practice, because of possibly larger constant factors (especially those that use Matoušek's partition trees), although some variations of the ideas might actually be useful. In some sense, our results can be interpreted as a theoretical explanation for why heuristics based on bounding boxes and BSP trees perform so well (e.g., see [5] on experimental results for the red/blue segment intersection problem).

Note that specializations of our techniques to 1-d also can easily lead to instance-optimal results for the multiset-sorting problem and the problem of computing the intersection of two (unsorted) sets. Adaptive algorithms for similar 1-d problems (e.g., [51]) were studied in settings different from ours.

Not all standard geometric problems admit nontrivial instance-optimal results in the order-oblivious setting. For example, computing the Voronoi diagram of n points or the trapezoidal decomposition of n disjoint line segments, both having $\Theta(n)$ sizes, requires $\Omega(n \log n)$ time for every point set by the naive information-theoretical argument. Computing the $(L_{\infty}$ -)closest pair for a *monochromatic* point set requires $\Omega(n \log n)$ time for every point set by our adversary lower-bound argument.

An open problem is to strengthen our lower bound proofs to allow for a more general class of test functions

beyond multilinear functions, e.g., arbitrary fixed-degree algebraic functions.

It remains to see how widely applicable the concept of instance optimality is. To inspire further work, we mention the following geometric problems for which we currently are unable to obtain instance-optimal results: (a) reporting all intersections between a set of disjoint red (nonorthogona) line segments and a set of disjoint blue line segments in 2-d; (b) computing the L_2 - or L_{∞} closest pair between a set of red points and a set of blue points in 2-d; (c) computing the diameter or the width of a 2-d point set; (d) computing the lower envelope of a set of (perhaps disjoint) line segments in 2-d.

Finally, we should mention that all our current results concern at most logarithmic-factor improvements. Obtaining some form of instance-optimal results for problems with $\omega(n \log n)$ worst-case complexity (e.g., offline triangular range searching, 3SUM-hard problems, ...) would be even more fascinating.

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On the multilinear model .1

Many commonly encountered test functions in geometric algorithms are multilinear. For example, in 3-d, the predicate ABOVE (p_1, \ldots, p_4) which returns true iff p_1 is above the plane through p_2, p_3, p_4 , reduces to testing signs of multilinear functions.

generally, More that function say а \mathbb{R}^{d} is quasi-multilinear if $(\mathbb{R}^d)^c$ f : \rightarrow $f(p_1, \ldots, p_c) = (f_1(p_1, \ldots, p_c), \ldots, f_d(p_1, \ldots, p_c))$ where $f_i = h_i(p_1, \ldots, p_c)/g(p_1, \ldots, p_c)$ in which $f_1, \ldots, f_d, g : (\mathbb{R}^d)^c \to \mathbb{R}$ are multi-linear functions. For example, in 3-d, the function $PLANE(p_1, \ldots, p_4)$ which returns the dual of the plane through p_1, \ldots, p_4 , or the function INTERSECT (p_1, \ldots, p_4) which returns the intersection of the dual planes of p_1, \ldots, p_4 , are quasi-multilinear. We can get more quasi-multilinear and multilinear functions by composition: e.g., if f_1,\ldots,f_4 : $(\mathbb{R}^3)^4$ ightarrow \mathbb{R}^3 are quasi-multilinear, then INTERSECT $(f_1(p_1, \ldots, p_4), \ldots, f_4(p_{13}, \ldots, p_{16}))$ is quasi-multilinear in p_1, \ldots, p_{16} , by expanding all the determinants. More elaborately, a predicate such as

also reduces to multilinear tests. However, we may run into problems if a point occurs more than once, e.g.,

ABOVE
$$(p_{17}, p_{18}, p_1, \text{INTERSECT}(\text{PLANE}(p_1, \dots, p_4), \text{PLANE})$$

since expansion of the determinants may yield monomials of the wrong type. In most 2-d algorithms, this kind of tests does not arise. Unfortunately, they can occasionally happen in our 3-d upper hull algorithm in Section 3.2. We describe some modifications to the algorithm that can avoid these problematic tests.

First, for the partition construction, it would be easier to choose the second option in the proof of Lemma 3.3. By perturbing the dividing planes, one can show the existence of 3 planes each passing through 3 input points, where the 9 points are distinct, so that each of the resulting 8 regions contains $n/8 \pm O(1)$ points. A bruteforce algorithm can find the 3 planes in polynomial time. We can reduce the construction time by using the standard technique of ε -approximations [47] (at the expense of a small change in the constant). It can be checked that known constructions for ε -approximations fits in the multilinear model (it suffices to check the implementation of the "subsystem oracle"). As a result, we can ensure that the cells are all defined by planes that pass through 3 input points, where no two planes share a common defining point. A vertex v of a cell is an intersection of 3 such planes and is defined by a set of 9 distinct input points, denoted DEF(v).

A problem occurs in testing whether a vertex v of a cell γ_i lies below the upper hull, specifically, when we

try to compare v against a feature that share a common defining point. For this reason, we weaken the test in line 5: we prune only when each vertex v of γ_i lies strictly below the upper hull of Q - DEF(v). It can be checked that some version of Lemma 3.6 can support O(r) such queries in the multilinear model, in $O(n \log r + rn^{1-\alpha})$ time for some $\alpha > 0$.

Since the pruning condition is weaker, the analysis needs more effort. We assume that the partition in line 3 is generated hierarchically in the following way: first we find a partition of Q by Lemma 3.3 with $\sqrt{r_i}$ subsets Q'_{ℓ} and cells γ'_{ℓ} ; then for each subset Q'_{ℓ} , we find a partition of Q'_{ℓ} again by Lemma 3.3 with $\sqrt{r_j}$ subsubsets Q_i and cells γ_i .

In the second paragraph of the proof of Theorem 3.7, we proceed differently. Suppose a point p lies in the subset Q'_{ℓ} and the subsubset Q_i . Observe that if the corresponding cells γ'_{ℓ} and γ_i are both completely inside Δ_k , then all points inside γ_i are pruned. This is because for each vertex v of the cell γ_i , the defining points DEF(v) are contained in $Q'_{\ell} \subset \gamma'_{\ell}$ and so cannot appear on the upper hull of Q; the vertex v lies strictly below the upper hull $\begin{array}{c} \text{Opt} Q, \text{ which coincides with the upper hull of } Q - \text{DEF}(v). \\ \text{ABOVE}(p_{17}, p_{18}, p_{19}, \text{INTERSECT}(\text{PLANE}(p_1, \dots, p_4), \text{PLANE}(p_5, \dots, p_8), \mathcal{O}(\underbrace{\mathcal{PLANE}(p_{13}, \mathcal{PLANE}(p_1, \dots, p_{16}))}_{\text{At most}}) \\ \text{At most} \mathcal{O}(\underbrace{\sqrt{r_j}}_{j} \underbrace{\mathcal{PLANE}(p_{13}, \mathcal{PLANE}(p_1, \dots, p_{16}))}_{j}) \\ \end{array} \right) \\ \end{array}$ of Δ_k . At most $O(\sqrt{r_j} \cdot \sqrt{r_j}^{1-\varepsilon})$ cells γ_i intersect the boundary of Δ_k . Hence, the number of $\min_{\substack{E \in [p_{3k}], P_{4k} \in [p_{1k}] \\ \min \left\{ |S_k|, O(\sqrt{r_j} + n/\sqrt{r_j} + \frac{p_{1k}}{\sqrt{r_j}}), \sqrt{r_j} - \varepsilon \cdot n/r_j \right\} = }$ $\min\left\{|S_k|, O(n/r_j^{\varepsilon/2})\right\}$. The rest of the proof is then the same, after readjusting ε .

Appendix 2: Other Applications Α

We can apply our techniques to obtain instanceoptimal algorithms for a number of geometric problems in the order-oblivious and random-order setting:

- 1. Off-line halfspace range reporting in 2-d and 3-d: given a set S of n points and halfspaces, report the subset of points inside each halfspace. Algorithms with $\Theta(n \log n + K)$ running time [24, 17, 1] are known for total output size K (the 3-d algorithm is randomized).
- 2. Off-line dominance reporting in 2-d and 3-d: given a set S of red/blue points, report the subset of red points dominated by each blue point. The problem has similar complexity as in item 1.
- 3. Orthogonal segment intersection in 2-d: given a set S of n horizontal/vertical line segments, report all intersections between the horizontal and vertical segments, or count the number of such intersections.

The problem is known to have worst-case complexity $\Theta(n \log n + K)$ in the reporting version, for output size K, and complexity $\Theta(n \log n)$ in the counting version [31, 52].

- 4. Bichromatic L_∞-close pairs in 2-d: given a set S of n red/blue points in 2-d, report all pairs (p, q) where p is red, q is blue, and p and q have L_∞-distance at most 1, or count the number of such pairs. Standard techniques in computational geometry [31, 52] yield algorithms with the same complexity as in item 3.
- 5. Off-line orthogonal range searching in 2-d: given a set *S* of *n* points and axis-aligned rectangles, report the subset of points inside each rectangle, or count the number of such points inside each rectangle. The worst-case complexity is the same as in item 3.
- 6. Off-line point location in 2-d: given a set S of n points and a planar connected polygonal subdivision of size O(n), report the face in the subdivision containing each point. Standard data structures [31, 52, 54] imply a worst-case running time of Θ(n log n).

For each of the above problems, it is not difficult to see that certain input sets are indeed "easier" than others, e.g., if the horizontal segments and the vertical segments respectively lie inside two bounding boxes that are disjoint, then the orthogonal segment intersection problem can be solved in O(n) time.

Note that although some of the above problems may be reducible to others in terms of worst-case complexity, the reductions may not make sense in the instanceoptimality setting. For example, an instance-optimal algorithm for a problem does not imply an instance-optimal algorithm for a restriction of the problem in a subdomain, because in the latter case, we are competing against algorithms that have to be correct only for input from this subdomain.

A.1 Reporting problems

Many of the problems listed above belong to the following common framework. Let $\mathcal{R} \subset \mathbb{R}^d \times \mathbb{R}^{d'}$ be a relation for some constant dimensions d and d'. We say that a red point $p \in \mathbb{R}^d$ and a blue point $q \in \mathbb{R}^{d'}$ interact if $(p,q) \in \mathcal{R}$. We consider the reporting problem: given a set S containing red points in \mathbb{R}^d and blue points in $\mathbb{R}^{d'}$ of total size n, report all K interacting red/blue pairs of points in S. Note that by scanning the output pairs, we can collect the subset of all blue points that interact with each red point, in O(K) additional time.

We say that a red (resp. blue) cell γ is *uninteresting* to S if every red (resp. blue) point in γ interacts with exactly the same subset of blue (resp. red) points in S. We redefine $\mathcal{H}(S)$ as follows:

Definition A.1 A partition Π of S is *respectful* if each subset S_k in Π either is a singleton or is a monochromatic subset of points that can be enclosed by a simplex Δ_k that is uninteresting to S. Define $\mathcal{H}(S)$ to be the minimum of $\mathcal{H}(\Pi) := \sum_k (|S_k|/n) \log(n/|S_k|)$ over all respectful partitions Π of S.

It is straightforward to modify the proofs from Section 3.1 and Section ?? to show an OPT(S), OPT^{avg}(S) = $\Omega(n(\mathcal{H}(S) + 1) + K)$ lower bound for this problem: We now keep two partition trees, one for each color. If $\Gamma(v)$ is uninteresting to S, we make v a leaf. At the end, if some red (resp. blue) node v_p is not a leaf, we can move p to some point inside $\Gamma(v_p)$ and change the answer. (The $\Omega(K)$ term in the lower bound is obvious, by the way.)

For the upper-bound side, we need three requirements about \mathcal{R} for some constant $\alpha > 0$:

- (A) There is a worst-case algorithm for the reporting problem that runs in $O(n \log n + K)$ time.
- (B) There is a data structure for the blue (resp. red) points in S, with $O(n \log n)$ preprocessing time, such that we can report all κ blue (resp. red) points interacting with a query red (resp. blue) point in $O(n^{1-\alpha} + \kappa)$ time.
- (C) There is a data structure for the blue (resp. red) points in S, with $O(n \log n)$ preprocessing time, such that we can test whether a query red (resp. blue) simplex γ is uninteresting to S in $O(n^{1-\alpha})$ time.

Under these assumptions, it is straightforward to modify the algorithm from Section ?? to an $O(n(\mathcal{H}(S)+1)+$ K)-time algorithm: In line 3, we partition the red points of Q first. In line 5, if some red cell γ_i is uninteresting to Q, then we find the subset Z of blue points interacting with an arbitrary red point in γ_i , output all pairs between the red points of Q_i and the blue points of Z, and prune the red points of Q_i from Q. The test requires querying the data structure in (C) (after triangulating γ_i); the subset Z can be found by querying the data structure in (B). The grouping technique by Chan [16] yields an analog of Lemma 3.6 with running time $O(n \log r + rn^{1-\alpha})$ for r queries of type (C), and $O(n\log r + rn^{1-\alpha} + \kappa)$ for r queries of type (B) with total output size κ (since the problems in (B) and (C) are "decomposable"). Before moving to the next iteration, we redo lines 3–5, this time partitioning the blue points of Q and pruning red points. At the end, in line 6, we switch to the algorithm in (A). The same analysis then goes through, by choosing a constant $\delta < \alpha$.

Note that for orthogonal problems in the comparison model, we can make all the cells (all the γ 's and Δ 's) axis-aligned boxes, by reverting to a k-d tree construction.

We now check that the requirements are satisfied for some specific reporting problems.

- Off-line halfspace range reporting in 2-d and 3-d: It suffices to consider lower halfspaces in the input. Color the given points red, and map the given lower halfspaces to blue points by duality. The data structure problem in (B) is just halfspace range reporting. The data structure problem in (C) is equivalent to testing whether a query simplex intersects a given set of hyperplanes (lines in 2-d or planes in 3-d); this reduces to ray shooting (or segment emptiness) queries in a hyperplane arrangement, for which there are known results [3, 49]. Requirement (A) is satisfied in 2-d and 3-d (the 3-d algorithm is randomized).
- Off-line dominance reporting in 2-d and 3-d: The data structure problem in (B) is just dominance reporting. The data structure problem in (C) is equivalent to testing whether all the corners of a query box are dominated by the same number of points from a given point set. This reduces to orthogonal range counting [2, 31, 52].
- Orthogonal segment intersection in 2-d: Map each each horizontal line segment $\overline{(x', y)(x'', y)}$ to a red point $(x', x'', y) \in \mathbb{R}^3$ and each vertical line segment (x,y')(x,y'') to a blue point $(x,y',y'') \in$ \mathbb{R}^3 . These mappings to \mathbb{R}^3 are bijective. The data structure problem in (B) corresponds to reporting the vertical segments from a given set that intersect a query horizontal segment. The data structure problem in (C) is more complicated: for a query box $\gamma = [\xi_1, \xi_2] \times [\xi_3, \xi_4] \times [\xi_5, \xi_6]$, we want to decide whether there exists a horizontal segment $\overline{(x',y)(x'',y)}$ with $(x',x'',y) \in \gamma$ that intersects a given set of vertical segments. This is equivalent to testing whether a query rectangle $[\min\{\xi_1,\xi_3\}, \max\{\xi_2,\xi_4\}] \times [\xi_5,\xi_6]$ intersects a given set of vertical segments. Both data structure problems reduce to orthogonal intersection searching (which in turn reduces to orthogonal range searching by lifting to a higher dimension, and thus admits data structures with $O(n \log n)$ preprocessing time and $O(n^{\varepsilon})$ query time). Clearly, the resulting algorithm works in the comparison model.
- Bichromatic L_∞-close pairs in 2-d: The problem in
 (B) corresponds to reporting all points of a given point set that are inside a query square of side

length 2. The problem in (C) corresponds to deciding, for a query box $\gamma = [\xi_1, \xi_2] \times [\xi_3, \xi_4]$, whether $[\xi_1-1, \xi_2+1] \times [\xi_3-1, \xi_4+1]$ contains a point from a given set. Both data structure problems reduce to orthogonal range searching.

Note that here the resulting algorithm requires slightly more general tests of the form mentioned in Remark 2.5, which are allowed in the lower-bound proof.

Off-line orthogonal range reporting in 2-d: Color the given points red, and map each rectangle with corners (x₁, y₁), (x₁, y₂), (x₂, y₁), (x₂, y₂) to a blue point (x₁, x₂, y₁, y₂) ∈ ℝ⁴. The mapping to ℝ⁴ is bijective. The blue data structure problem in (B) corresponds to reporting all points from a given set that are inside a query rectangle. The red data structure problem in (B) corresponds to reporting all rectangles from a given set that contain a query point.

The red data structure problem in (C) corresponds to deciding, for a query box $\gamma = [\xi_1, \xi_2] \times [\xi_3, \xi_4] \times$ $[\xi_5,\xi_6] \times [\xi_7,\xi_8]$, whether all rectangles with corners $(x_1, y_1), (x_1, y_2), (x_2, y_1), (x_2, y_2), (x_1, x_2, y_1, y_2) \in$ γ , contain the same number of points from a given set. This is equivalent to testing whether rectangle $[\min\{\xi_1,\xi_3\},\max\{\xi_2,\xi_4\}]$ the Х $[\min\{\xi_5,\xi_7\},\max\{\xi_6,\xi_8\}]$ contains the same number of points from a given set as the rectangle $[\max\{\xi_1,\xi_3\},\min\{\xi_2,\xi_4\}]$ Х $[\max\{\xi_5,\xi_7\},\min\{\xi_6,\xi_8\}].$

The blue data structure problem in (C) corresponds to deciding, for a query point $\gamma = [\xi_1, \xi_2] \times [\xi_3, \xi_4]$, whether γ intersects any rectangle from a given set.

All these data structure problems reduce to orthogonal range/intersection searching.

A.2 Counting problems

We can also consider counting problems where we want the total number of interacting red/blue pairs. We just need to change requirement (A) to the existence of a counting algorithm that runs in $O(n \log n)$ time, and requirement (B) to the existence of a similar counting data structure without the $O(\kappa)$ -term penalty. These requirements are satisfied by orthogonal segment intersection counting, bichromatic L_{∞} -close pairs, and off-line orthogonal range counting. The same lower- and upperbound proofs yields $\Theta(n(\mathcal{H}(S) + 1))$.

If we want individual counts, i.e., the number of red points that interact with each blue point, we need a further assumption—that the data structure in (B) can operate in the semigroup model [2]. (This assumption is true for

the specific problems mentioned in the preceding paragraph.) This way, we can report all interacting red/blue pairs as a disjoint union of bicliques $P_i \times Q_i$ with total sizes $\sum_i (|P_i| + |Q_i|)$ bounded by $O(n(\mathcal{H}(S) + 1))$, without the O(K)-term penalty. We can keep a counter for each blue point, scan through each biclique, and add the number of red points in the biclique to the counter of each blue point in the biclique, in total additional time $O(\sum_i (|P_i| + |Q_i|))$, which is absorbed in the overall cost. We assume that the algorithm in requirement (A) can produce individual counts but does not need to be the semigroup model. At the end (line 6), we can add the individual counts produced by this algorithm to the corresponding counters of each blue point.

A.3 Detection problems?

We can also consider detection problems where we simply want to decide whether there exists an interacting red/blue pair. Here, we redefine $\mathcal{H}(S)$ by redefining "uninteresting": a red (resp. blue) cell γ is now considered *uninteresting to* S if no red (resp. blue) point in γ interacts with any blue (resp. red) points in S. We change requirements (A) and (B) to the existence of counting algorithms and data structures without the O(K) and $O(\kappa)$ terms.

The proof of the upper bound $O(n(\mathcal{H}(S) + 1))$ is the same, but the proof of the lower bound $\Omega(n(\mathcal{H}(S) + 1))$ only goes through for instances with a NO answer: at the end, if some red (resp. blue) node v_p is not a leaf, we can move p to some point inside $\Gamma(v_p)$ and change the answer from NO to YES.

YES instances are problematic, but this is not a weakness of our technique but of the model: on every input set S with a YES answer, OPT(S) is in fact O(n). To see this, consider an input set S for which there exists an interacting pair (p, q). An algorithm that is "hardwired" with the ranks of p and q in S with respect to, say, the x-sorted order of S can first find p and q from their ranks by linear-time selection, verify that p and q interact in constant time, and return YES if true or run a bruteforce algorithm otherwise. Then on every permutation of this particular set S, the algorithm always takes linear time. Many problems admit $\Omega(n \log n)$ worst-case lower bounds even when restricted to YES instances, and for such problems, instance optimality in the order-oblivious setting is therefore not possible on all instances.

A.4 More off-line/on-line querying problems

We now study problems from another framework. Let \mathcal{M} be a mapping from points in \mathbb{R}^d to "answers" in some space; the answer $\mathcal{M}(q)$ of a point $q \in \mathbb{R}^d$ may or may

not have constant size depending on the context. We consider the following *off-line querying* problem: given a set S of n points in \mathbb{R}^d , compute $\mathcal{M}(q)$ for every $q \in S$. In addition, we consider the following *on-line querying* problem: given a set S of n points in \mathbb{R}^d , build a data structure for S so that we can compute $\mathcal{M}(q)$ for any query point $q \in \mathbb{R}^d$, while trying to minimize the average query cost over all $q \in S$.

We redefine $\mathcal{H}(S)$ by redefining "uninteresting": a cell γ is now considered *uninteresting to* \mathcal{M} if every point q in γ has the same answer $\mathcal{M}(q)$.

For the off-line problem, our lower-bound proof gives $\Omega(n(\mathcal{H}(S)+1))$ even if \mathcal{M} has been preprocessed in advance. For the on-line problem, the same proof shows that running a sequence of n queries over some permutation of S requires $\Omega(n(\mathcal{H}(S)+1))$ time, even if the set S (not the permutation) has been preprocessed in advance. So, the average query time is $\Omega(\mathcal{H}(S)+1)$. (In contrast, lower bounds for the on-line problem do not necessarily translate to lower bounds for the off-line problem.)

For the upper-bound side, we need two requirements about \mathcal{M} for some constant $\alpha > 0$ and some parameter m describing the size of \mathcal{M} . We assume that \mathcal{M} has been preprocessed in some data structure.

- (A) Given $q \in \mathbb{R}^d$, we can compute $\mathcal{M}(q)$ in $O(\log m + \kappa)$ worst-case time for output size κ .
- (C) Given a simplex γ , we can test whether γ is uninteresting to \mathcal{M} in $O(m^{1-\alpha})$ time.

The algorithm this time is actually simpler, because there is only one color. Instead of using a 2^{2^j} progression, we use a straightforward *b*-way recursion, for some fixed parameter *b* (the resulting recursion tree mimics the tree \mathcal{T} from the lower-bound proof in Theorem 3.5, on purpose):

off-line-queries (Q, Γ) , where $Q \subset \Gamma$:

- 1. if |Q| drops below n/m^{δ} then return answers directly
- 2. partition Q by Lemma 3.3 to get b subsets Q_1, \ldots, Q_b and cells $\gamma_1, \ldots, \gamma_b$
- 3. for each i do
- 4. if $\gamma_i \cap \Gamma$ is uninteresting to \mathcal{M} then
- 5. compute $\mathcal{M}(q)$ for an arbitrary point $q \in \gamma_i \cap \Gamma$
- 6. output $\mathcal{M}(q)$ for the points in Q_i

7. else off-line-queries $(Q_i, \gamma_i \cap \Gamma)$

We call off-line-queries (S, \mathbb{R}^d) to start. Line 1 takes $O(|Q| \log m + \kappa)$ time for output size κ by switching to the data structure for (A); note that each point in Q in this case has participated in $\Omega(\log m)$ levels of the recursion, and we can account for the first term by charging each

point unit cost for every level it participates in. Line 2 takes O(|Q|) time for a constant b by known constructions [49]. Line 4 takes $O(m^{1-\alpha} \operatorname{polylog} m)$ time $(\gamma_i \cap \Gamma$ has $O(\operatorname{polylog} m)$ vertices), by (C); this cost is negligible by choosing a sufficiently small constant $\delta < \alpha$, since the recursion tree has $O(m^{\delta})$ nodes. Line 5 takes $O(\log m + \kappa)$ time for output size κ , by (A); the $O(\log m)$ term is again negligible.

For the on-line problem, we just build a data structure corresponding to the recursion tree generated above, in addition to the data structure for (A); the extra space is $O(m^{\delta})$.

Theorem A.2 The above off-line querying algorithm runs in $O(n(\mathcal{H}(S) + 1) + K)$ time for total output size K. For the on-line querying problem, it produces a data structure that has average query cost $O(\mathcal{H}(S) + 1 + \kappa)$ for output size κ .

Proof: Let n_j be number of points in S that *survive* level j, i.e., participate in subsets Q at level j of the recursion. The total running time for the off-line problem is asymptotically bounded by $\sum_j n_j$. Similarly, for the on-line problem, the total query cost over all $q \in S$ is asymptotically bounded by $\sum_j n_j$.

Let Π be any respectful partition of S. Look at a subset S_k in Π . Let Δ_k be a simplex enclosing S_k that is contained inside one face of M. Fix a level j. Let Q_i 's and γ_i 's be the subsets Q and cells γ at level j. Each Q_i has size at most $n/\Theta(b)^j$. The number of γ_i 's that intersect each side of Δ_k is at most $O(b^{1-\varepsilon})^j$. Thus, the number of points in S_k that survive level j is at most $\min\{|S_k|, O(b^{1-\varepsilon})^j \cdot n/\Theta(b)^j\}$. Since the S_k 's cover the entire point set, with a double summation we have, for a sufficiently large constant b,

$$\sum_{j} n_{j} \leq \sum_{k} \sum_{j} \min \left\{ |S_{k}|, \lceil n/\Theta(b)^{\varepsilon_{j}} \rceil \right\}$$
$$= O(n(\mathcal{H}(\Pi) + 1)). \square$$

For the on-line problem, the above approach works, after straightforward modifications, for weighted point sets S where we want to minimize the weighted average query cost. In principle, the approach works not only for discrete point sets S but also for continuous probability distributions, since the query bound does not depend on the size n of S explicitly and can be imagined to approach infinity. "Average query cost" over a finite set of query point distribution. (The preprocessing time can also be made independent of n, under some computational assumptions about the distribution.)

Below, we briefly mention applications to some specific off-line/on-line querying problems. • Off-line/on-line point location queries in 2-d: For the off-line planar point location problem, the data structure for requirement (A) only needs O(m) preprocessing time and space [44, 22, 54]. The data structure problem in (C) reduces to testing whether a triangle is contained in a face of the subdivision; this reduces to ray shooting (or segment emptiness) queries in a polygonal subdivision, for which there are known results [23]. The total running time is $O(n(\mathcal{H}(S) + 1))$, including preprocessing, if the subdivision has size m = O(n). (For this problem, output sizes can be ignored.)

For the on-line version, we immediately get optimal $O(\mathcal{H}(S) + 1)$ average query cost, with an O(m)-space data structure for a subdivision of size m. This on-line point location result is already known [6, 7, 29, 41] (some of these previous work even optimize the constant factor in the query cost).

- On-line halfspace range reporting queries in 2-d and 3-d: Here, we map query lower halfspaces to points by duality. The known data structure for (A) needs O(m) space [24, 1]. The data structure for (C) is the same as in Section A.1. We get optimal O(H(S) + 1 + κ) average query cost for output size κ, with an O(m)-space data structure for a given point set of size m in 2-d or 3-d. This result is new.
- On-line dominance reporting queries in 2-d and 3-d: The story is similar to halfspace range reporting.
- On-line orthogonal range reporting/counting queries in 2-d: Here, we map query rectangles to points in 4-d as in Section A.1. The known data structure for (A) needs $O(m \log m)$ preprocessing time and O(m) space [21]. The data structure for (C) is the same as in Section A.1. We get optimal $O(\mathcal{H}(S) + 1 + \kappa)$ average query cost for output size κ , with an O(m)-space data structure for a given point set of size m in 2-d. (For counting, $\kappa = O(1)$.) The resulting algorithm works in the comparison model. This result is apparently new, as it extends Dujmović, Howat, and Morin's recent result on 2-d dominance counting [35] and unintentionally answers one of their main open problems (and at the same time improves their space bound from $O(m \log m)$ to O(m)).