Programming Assignments 3 and 4 – 601.455/655 Fall 2025

Score Sheet (hand in with report) Also, PLEASE INDICATE WHETHER YOU ARE IN 601.455 or 601.655

(one in each section is OK)

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Grade Factor		
Program (40)		
Design and overall program structure	20	
Reusability and modularity	10	
Clarity of documentation and programming	10	
Results (20)		
Correctness and completeness	20	
Report (40)		
Description of formulation and algorithmic approach	15	
Overview of program	10	
Discussion of validation approach	5	
Discussion of results	10	
TOTAL	100	

CIS PA4

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1 Overview

In this assignment, we are asked to implement the matching portion of a simplified Iterative Closest Point (ICP) algorithm to match a triangle mesh of a bone to a set of points sampled from a pointing device. The problem setup includes the following objects:

1. Optical tracker base

2. A bone (the target of the ICP)

3. Rigid body A, a free moving object with optical markers and known offset to the tip A_{tip}

4. Rigid body B, an object with optical markers on its body which is firmly attached to the bone

The following data about these objects is available:

1. A triangle mesh of the bone taken from a CT scan, containing the vertices of all of the triangles and their associated indices

2. A set of readings of the optical markers on rigid bodies A and B using the optical tracker base as rigid body A is moved to be in contact to the bone at different positions.

The ultimate goal is to find the registration between the point cloud generated by sampling A_{tip} while moving rigid body A around and the triangle mesh of the bone. In PA3, we focus solely on the matching step of ICP, assuming $F_{\text{reg}} = I$. In PA4, we now estimate a nontrivial F_{reg} and use it to iteratively refine the correspondences and alignment.

For each sample frame k, the pointer tip expressed in the coordinate frame of rigid body B (which is fixed to the bone) is

$$d_k = F_{B,k}^{-1} F_{A,k} A_{\text{tip}}.$$

This is the raw point cloud produced from the tracking system.

In PA3, since $F_{\text{reg}} = I$, the matched point on the mesh is simply $c_k = \text{ClosestPoint}(d_k, \text{ mesh})$, and no additional transformation is applied.

In PA4, we estimate a rigid registration F_{reg} and therefore define a transformed source point $s_k = F_{reg}, d_k$, with correspondences recomputed as $c_k = \text{ClosestPoint}(s_k, \text{mesh})$. The pairs (s_k, c_k) are then used by the Kabsch PCR algorithm to update F_{reg} on each iteration.

Because this problem involves unknown correspondences between the point cloud and the surface mesh, the PCR algorithm cannot align d_k and c_k on the first pass. Instead, ICP alternates between recomputing correspondences and updating F_{reg} until convergence.

As a note, the Closest Point and KD-tree algorithms are reused from PA3, and the PCR algorithm is identical to the method implemented in PA1 and PA2.

2 Mathematical approach

1. **Transformation Chain:**

   We first need to find the coordinates of the optical trackers on bodies A and B in the optical tracker base frame. This is required all k samples we take. After performing PCR, we are left with F_{A_k} and F_{B_k}, which are the HTMs for both bodies for the kth sample. We are interested in finding the location of A_{tip} in the frame of body B, since that frame is static in relation to the bone. This step is needed for all k samples to generate the source point cloud, To obtain, this we can perform the following frame transformation chain for each of the k samples:

   $$F_{B_k}^{-1} F_{A_k} A_{tip}$$

   With this transformation chain, we can now construct a point cloud in the frame of rigid body B, constructed by sampling and transforming A_{tip}.

2. **Iterative Transformation Method:**

   Because we do not have known correspondences between the point cloud d_k and the mesh surface, a single application of point cloud registration (PCR) will not correctly align the two shapes. In the first iteration, we assume $F_{\text{reg}} = I$, giving

   $$s_k^{(0)} = d_k.$$

   Using these initial source points, we compute closest points $c_k^{(0)}$ on the mesh.

   PCR requires pairs of corresponding points. Here, no correspondence is known beforehand, so the initial alignment is not an alignment at all. All we have to pair d_k are the closest-point projection onto the mesh. Because a good registration relies on good correspondences but better correspondences rely on better registration, we must do this iteratively. It

is like a chicken and egg problem. We obtain closest points $c_k^{(i)}$ for the ith iteration, we compute a new estimate of the bone–registration transform:

$$F_{\text{reg}}^{(i+1)} = \text{PCR}\left(\{d_k\}, \{c_k^{(i)}\}\right).$$

We then update all source points:

$$s_k^{(i+1)} = F_{\text{reg}}^{(i+1)} d_k.$$

With these updated positions, we re-query the KD-tree to obtain new closest points $c_k^{(i+1)}$, and repeat until convergence:

$$\|F_{\text{reg}}^{(i+1)} - F_{\text{reg}}^{(i)}\| < \varepsilon.$$

Our conditions for convergence are either an RMSE error of less than $1e^-5$ or a change in F_{reg} from last iteration of less than $1e^-6$.

3. **Closest Point on Triangular Mesh:**

To find the closest point on a triangle to an arbitrary point $\mathbf{a}$, we follow the method from Taylor's slides [1]. Given triangle vertices $\mathbf{p}, \mathbf{q}, \mathbf{r}$, any point on the triangle can be written

$$\mathbf{c}(\lambda, \mu) = \mathbf{p} + \lambda(\mathbf{q} - \mathbf{p}) + \mu(\mathbf{r} - \mathbf{p}).$$

We first compute the projection of $\mathbf{a}$ onto the triangle by solving the least–squares problem:

$$\min_{\lambda, \mu} \left\|\mathbf{a} - \mathbf{c}(\lambda, \mu)\right\|^2, \qquad \mathbf{A} = \begin{bmatrix} \mathbf{q} - \mathbf{p} & \mathbf{r} - \mathbf{p} \end{bmatrix}, \quad \mathbf{b} = \mathbf{a} - \mathbf{p}.$$

$$[\lambda\,, \mu] = \arg\min \left\|\mathbf{A}[\lambda\,, \mu] - \mathbf{b}\right\|^2,$$

This is solved easily enough with a numerical linear algebra library. With λ and μ, we can now divide the area around and including the triangle into two primarily areas:

(a) Point lies inside the triangle:

$$\lambda \geq 0, \qquad \mu \geq 0, \qquad \lambda + \mu \leq 1,$$

in which case $\mathbf{c}$ is the closest point.

(b) Point lies outside the triangle on one of three exterior regions:

$$\lambda < 0 : \text{Line } \mathbf{rp}, \qquad \mu < 0 : \text{Line } \mathbf{pq}, \qquad \lambda + \mu > 1 : \text{Line } \mathbf{qr}$$

In this case $\mathbf{c}$ must lie on one of the three exterior lines. An example is with this edge with vertices $\mathbf{q}$ and $\mathbf{p}$:

$$\lambda = \frac{(\mathbf{c} - \mathbf{p}) \cdot (\mathbf{q} - \mathbf{p})}{\|\mathbf{q} - \mathbf{p}\|^2}, \qquad \lambda^{(\text{seg})} = \max(0, \min(\lambda), 1), \qquad \mathbf{c} = \mathbf{p} + \lambda^{(\text{seg})}(\mathbf{q} - \mathbf{p}).$$

This is generalized for all possibilities $\mathbf{qr}, \mathbf{pq}$, and $\mathbf{rp}$.

Using this method, regardless if the point lines inside of outside the triangle, it is boxed to a point on the triangle.

Note: in our implementation, we used a kd-tree to store the triangle mesh. Since we construct the kd-tree based off of the centroid of each of the triangles but are interested in the closest point anywhere on a surface of any of the triangles, we used a method as described in [2] and [3] to construct bounding boxes around groups of triangles, and computing distance from query to bounding boxes to allow accurate search. The distance from point to bounding box is simple Euclidean distance formula, bounded below by 0 (points inside a bounding box has distance 0 to it).

3 Algorithmic approach

Algorithm 1 Iterative Closest Point for PA4

1: **Input:** Body A/B definitions, mesh vertices/triangles, sample readings
2: Build KD–tree for triangle mesh
3: **for** each dataset X **do**
4:     Parse sample readings
5:     **for** each frame k **do**
6:         Compute $F_{A,k}$ and $F_{B,k}$ via PCR
7:         Compute $d_k = F_{B,k}^{-1} F_{A,k} A_{\text{tip}}$
8:     **end for**
9:     Initialize $F_{\text{reg}} \leftarrow I$
10:     **for** iter = 1:maxIters **do**
11:         Transform points $s_k = F_{\text{reg}} d_k$
12:         For each s_k, query KD–tree for closest mesh point c_k
13:         Compute updated transform $F_{\text{reg}}^{new} = \text{PCR}(d_k, c_k)$
14:         **if** $\|F_{\text{reg}}^{new} - F_{\text{reg}}\| < \epsilon$ **or** mean error $< \tau$ **then**
15:             $F_{\text{reg}} \leftarrow F_{\text{reg}}^{new}$
16:             **break**
17:         **end if**
18:         $F_{\text{reg}} \leftarrow F_{\text{reg}}^{new}$
19:     **end for**
20:     Output final s_k, c_k, and errors
21: **end for**

Algorithm 2 FindClosestPoint($\mathbf{a}$, $\mathbf{p}$, $\mathbf{q}$, $\mathbf{r}$)

1: $\mathbf{qp} \leftarrow \mathbf{q} - \mathbf{p}$
2: $\mathbf{rp} \leftarrow \mathbf{r} - \mathbf{p}$
3: Solve the least-squares problem:

$$\mathbf{a} - \mathbf{p} \approx \lambda \, \mathbf{qp} + \mu \, \mathbf{rp}.$$

4: Extract (λ, μ).

5: **if** $\lambda \geq 0$ **and** $\mu \geq 0$ **and** $\lambda + \mu \leq 1$ **then**
6:     **return** $\mathbf{c}^* = \mathbf{p} + \lambda \, \mathbf{qp} + \mu \, \mathbf{rp}$
7: **end if**

8: $\mathbf{c} \leftarrow \mathbf{p} + \lambda \, \mathbf{qp} + \mu \, \mathbf{rp}$

9: **if** $\lambda < 0$ **then**
10:     **return** ProjectOnSegment($\mathbf{c}$, $\mathbf{p}$, $\mathbf{r}$)
11: **else if** $\mu < 0$ **then**
12:     **return** ProjectOnSegment($\mathbf{c}$, $\mathbf{p}$, $\mathbf{q}$)
13: **else**
14:     **return** ProjectOnSegment($\mathbf{c}$, $\mathbf{q}$, $\mathbf{r}$)
15: **end if**

Algorithm 3 ProjectOnSegment($\mathbf{c}, \mathbf{u}, \mathbf{v}$)

   $\mathbf{d} \leftarrow \mathbf{v} - \mathbf{u}$
2: $t \leftarrow \dfrac{(\mathbf{c} - \mathbf{u}) \cdot \mathbf{d}}{\|\mathbf{d}\|^2}$
   $t \leftarrow \min(1, \max(0, t))$
4: **return** $\mathbf{u} + t \, \mathbf{d}$

Description of kd-tree

We decided to store the triangle mesh in a kd-tree (defined in ./utils/kdtree.py) to allow faster nearest-neighbor matching for points (as compared to brute-force linear search). The kd-tree is designed to work in 3D, two children per node, one triangle per node, split along the median of each axis in round robin fashion. We also found the implementation of bounding boxes as described in [2] and [3] to be necessary to match the performance of brute force search. Based off of our examination of the datasets which showed roughly uniform distribution of points along each axis and our implementation of our kd-tree, our nearest-neighbor search should be $O(log \text{ n})$ on average.

The kd-tree is an object with two functions, whose algorithms are described below. Their purposes are to construct a kd-tree from a traingle mesh, and search for a closest point on the triangle mesh given a 3D point.

Description of kd-tree node

Each node is defined as follows with private fields:

```
class KDTreeNode
tri_idx :  triangle index stored in current node
point :  centroid for splitting
left, right :  subtree nodes
axis :  splitting axis (0,1, or 2)
bbox_min, bbox_max :  bounding-box limits
```

Algorithm 4 BuildKDTree(tri_indices, depth)

1: **if** |tri_indices| = 0 **then**
2:     **return** None
3: **end if**
4: axis ← depth mod 3
5: sorted_idx ← argsort(centroids[tri_indices, axis])
6: tri_indices ← tri_indices[sorted_idx]
7: median_idx ← $\lfloor$|tri_indices|/2$\rfloor$
8: median_tri ← tri_indices[median_idx]
9: centroid ← centroids[median_tri]
10: bbox_min ← min(tri_bbox_min[tri_indices])
11: bbox_max ← max(tri_bbox_max[tri_indices])
12: **if** |tri_indices| = 1 **then**
13:     **return** KDTreeNode([median_tri], centroid, None, None, axis, bbox_min, bbox_max)
14: **end if**
15: left ← BuildKDTree(tri_indices[:median_idx], depth + 1)
16: right ← BuildKDTree(tri_indices[median_idx+1:], depth + 1)
17: **return** KDTreeNode([median_tri], centroid, left, right, axis, bbox_min, bbox_max)

Algorithm 5 ClosestPoint(p)

 1: best ← None
 2: stack ← [root]   ▷ DFS stack
 3: **while** stack is not empty **do**
 4:     node ← stack.pop()
 5:     **if** node = None **then**
 6:         **continue**
 7:     **end if**
 8:     **if** best ≠ None **then**
 9:         box_dist ← point_bbox_distance(p, node.bbox_min, node.bbox_max)
10:         **if** box_dist ≥ best[0] **then**
11:             **continue**   ▷ This subtree gets pruned
12:         **end if**
13:     **end if**
14:     **for all** tri_idx ∈ node.tri_indices **do**
15:         ($v0, v1, v2$) ← vertices[triangles[tri_idx]]
16:         q ← find_closest_point($p, v0, v1, v2$)
17:         dist ← $\|p - q\|$
18:         **if** best = None **or** dist < best[0] **then**
19:             best ← (dist, q, [tri_idx])
20:         **end if**
21:     **end for**
22:     diff ← p[node.axis] − node.point[node.axis]
23:     **if** diff < 0 **then**
24:         near, far ← node.left, node.right
25:     **else**
26:         near, far ← node.right, node.left
27:     **end if**
28:     stack.append(far)
29:     stack.append(near)
30: **end while**
31: (dist, closest_point, tri_idx) ← best
32: **return** closest_point, dist, tri_idx[0]

---

4 Overview of structure

We structured our code in PA4 to rely on helper functions (namely algorithms like PCR) and the kd tree data structure. The entirety of PA4 is run in a series of 2 loops in main.py, where we loop through all data sets and iteratively solve for a transformation to align our mesh and point cloud. Please run main.py in its entirety to generate the output files for this PA.

1. **Main script**
   main.py
   In PA4, `main.py` performs the following steps:

   (a) Load rigid body marker files and mesh files.

   (b) Build a kd-tree to store the triangle mesh.

   (c) Load a dataset.

   (d) Perform PCR between the two rigid bodies for each sample frame.

   (e) Calculate A_{tip} points in the frame of rigid body B (compute d_k).

   (f) Apply a registration transformation F_{reg} (initialized as identity).

   (g) Perform an iterative ICP procedure:

       i. Compute $s_k = F_{\text{reg}} d_k$.

       ii. Find closest points on the triangle mesh for each s_k using the kd-tree.

       iii. Update F_{reg} via PCR between d_k and the closest points.

       iv. Check convergence and repeat if necessary.

   (h) Output results in the required format.

   (i) Repeat steps c through h for all datasets.

2. **Utility Scripts**

   ./utils/calculate_errors.py

   ```
   function rms = calculate_rms_error(pc1, pc2)
   function [F_diff, angle_err, trans_err] =
   calculate_error_transformation(Fa, Fb)
   function stats = calculate_error_stats(pc1, pc2)
   function print_error_stats(stats)
   ```

   This file provides basic error–evaluation utilities for PA3/PA4. It computes RMS point–cloud error, rotational and translational differences between two rigid transforms, and summary statistics for point-wise residuals.

./utils/icp.py

```
function c = project_on_segment(c, p, q)
function c = find_closest_point(a, p, q, r)
function [q_closest, d, idx] = linear_search_closest_poin
ts_on_mesh(p, V, T)
function test_closest_point_on_triangle()
```

This file implements closest point computations on triangles and triangle
meshes by constructing a linear search. It includes small unit test validates
correctness on all triangle regions.

./utils/kdtree.py

```
function d = point_aabb_distance(p, aabb_min, aabb_max)
class KDTreeNode
class KDTreeTriangles
method build_kdtree(tri_indices)
method closest_point(p)
method _closest_point_recursive(p, node)
```

This file constructs a per-triangle kd-tree to speed up closest-point queries
on a mesh. Each node stores triangle indices, centroid split axis, and a
bounding box for improved pruning. Queries descend the KD-tree, skip-
ping subtrees whose bounding boxes cannot contain a closer point, and
use find_closest_point to compute the exact closest point on each can-
didate triangle. The kd-tree object defined here encompasses both the
structure, building of, and execution of a closest point search in a kd-tree
containing a triangle mesh.

./utils/parse.py

```
function [markers, tip, N] = parse_rigid_bodies(path)
function [V, T] = parse_mesh(path)
function [A_tr, B_tr, Ns] = parse_readings(path, NA, NB)
function [d_k, c_k] = parse_output(path)
```

This file provides all input–output parsing utilities for PA4. It loads rigid-
body definitions, surface-mesh vertex and triangle lists, tracker sample
readings for bodies A and B, and previously generated output files. All
routines convert the assignment's text formats into clean NumPy arrays
for downstream computation.

`./utils/pcr.py`

```
function F = point_cloud_registration(a, b)
function random_pcr_test()
```

This file implements the rigid point–cloud registration method used in all previous PAs. It relies on correspondence, which is not guaranteed for this scenario. A built-in randomized unit test verifies correctness by comparing the recovered transform against a known ground-truth transformation.

`./utils/write_out.py`

```
function write_p3_output(d_points, c_points, errors,
path)
```

This file formats and writes the PA4 output file in the exact specification required by the assignment.

3. **Testing Scripts**

`./tests/compare_outputs.py`

```
function compare_output(letter)
```

This test script compares the PA4 output files against the provided debug "ground truth" outputs. This is our primary method of validating our ICP algorithm.

`./tests/kdtree_test.py`

```
function test_triangle_kdtree()
```

This script provides unit tests for the triangle kd-tree implementation. It constructs simple meshes, queries closest points, and verifies correctness against analytically known solutions for interior, exterior, and multi-triangle cases. These tests validate pruning logic and exact closest-point evaluation on triangles.

`./tests/closest_point_test.py`

```
function assert_close(x, y, msg)
function run_tests()
```

This script provides a correctness test for the triangle closest–point routine. It evaluates all barycentric regions (interior, vertices, and all three edges), including near-edge projections, and compares results against analytically computed ground truth using `project_on_segment`.

5 Validation Approach

In general, we used the following equations implemented in `calculate_errors.py` to evaluate our algorithms:

$$e_{\mathrm{rms}} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left\| \mathbf{pc}_1^{(i)} - \mathbf{pc}_2^{(i)} \right\|^2}.$$

$$\mathrm{mean} = \frac{1}{N} \sum_{i=1}^{N} \left\| \mathbf{pc}_1^{(i)} - \mathbf{pc}_2^{(i)} \right\|.$$

$$\mathrm{std} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left(\left\| \mathbf{pc}_1^{(i)} - \mathbf{pc}_2^{(i)} \right\| - \mathrm{mean} \right)^2}.$$

1. **Comparing Outputs**

   Datasets A-F contain sample output files. We can treat these files are "ground truths" to validate out generated output files. For each dataset, we compute a RMS error between the encoded s_k and c_k point clouds.

2. **Validating Closest Point Algorithm**

   The primary ethos when testing our Closest Point Algorithm is to generate known triangle, place points on the inside face and outside face (three regions of the outside face), and determine if the algorithm correctly solves for the correct point.

3. **Validating kd-Tree** Our approach to validating our kd-tree implementation focused on building the tree, and performing a nearest point search. Since these two functions are so closely aligned and dependent on each other, we test them in conjunction.
   We first test with a mesh of just one triangle. This test case helped us verify that we are instantiating the kd-tree at all, and the ability to generate a root node. Then, we tried two test queries, one for a point inside

the triangle, and one outside. These two options cover all possibilities, where the distance from the query point to the triangle is either positive or zero (a query for a point on the boundary of triangle will also result in distance of zero). We verified the correctness of our code by comparing the code's output with out manually computed expected outputs.

We then move on to testing the kd-tree on a mesh with multiple triangles. In this case, there is three triangles. Again, we tested querying a point inside one of the triangles, and another point outside of all of the triangles, again verifying by hand. We believe this covers all cases, as this case shows the ability to give a node two children and still correctly calculate nearest point on mesh.

Finally, the ultimate test for our kd-tree was comparing its performance to the brute force linear search for nearest point on a triangle mesh on the real dataset. We discuss this in more detail in the results section, but briefly speaking, the kd-tree implementation achieved the same accuracy and faster runtime when compared to the brute force linear search, which is verification enough that our implementation is correct for the given problem.

6 Results

Dataset	RMSE s_k	RMSE c_k
A	0.006436	0.005881
B	0.006210	0.005636
C	0.006500	0.006249
D	0.008253	0.007237
E	0.023163	0.019756
F	0.019547	0.016627

Table 1: RMSE comparison between "Ground Truth" debug output and generated output for datasets A–F.

When comparing the outputs for debug data sets A-F in Table 1, we see very low error. This indicates our ICP algorithm works very well. Maximally, the highest mean error at convergence came from Dataset E being 0.0679 mm away from the mesh. We feel this is a fairly pleasant result and potentially accurate enough for medical applications.

Pictured in Figure 1 is the convergence over iterations for each of our datasets. Each label is in the form (mean error at convergence, number of iterations of reach convergence). AS we can see, all datasets converge nicely.

Alan and Justin both contributed equally to this PA. Both partners research the class lecture slides on the ICP method and implemented the algorithm collaboratively.
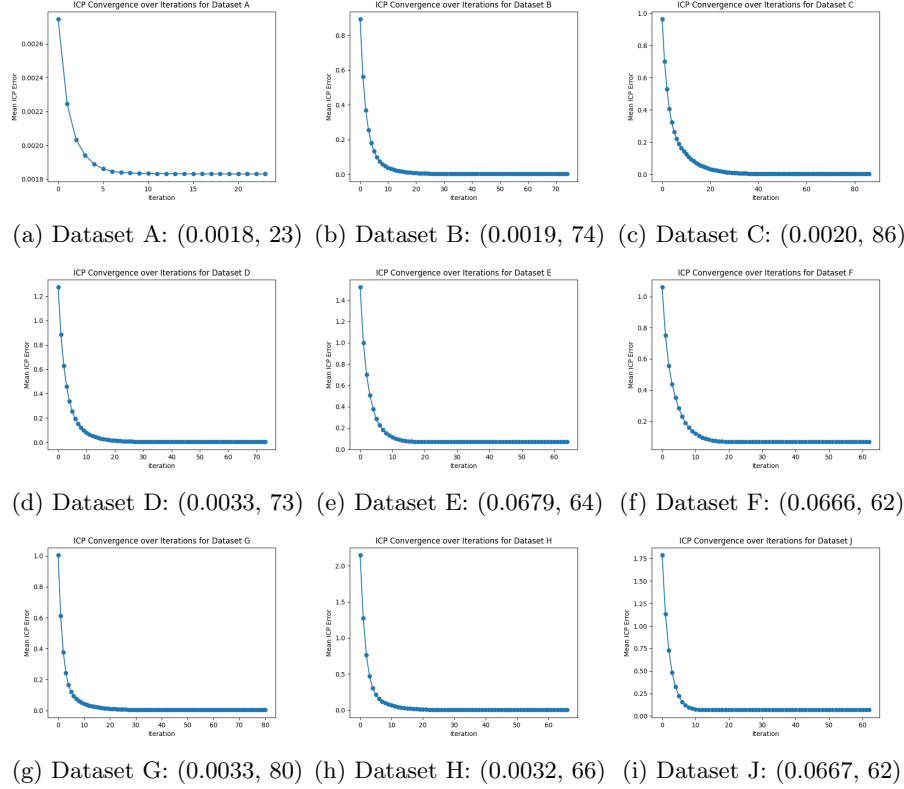
(a) Dataset A: (0.0018, 23) (b) Dataset B: (0.0019, 74) (c) Dataset C: (0.0020, 86)

(d) Dataset D: (0.0033, 73) (e) Dataset E: (0.0679, 64) (f) Dataset F: (0.0666, 62)

(g) Dataset G: (0.0033, 80) (h) Dataset H: (0.0032, 66) (i) Dataset J: (0.0667, 62)

Figure 1: Convergence and final mean error/iterations for Datasets A-J

7   References

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[3] "KD-Trees," Accessed: Nov. 13, 2025. [Online]. Available: https://cgvr.cs.uni-bremen.de/teaching/geom_notes_from_lorenzo/KD-Trees.pdf

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Ayushi Sinha 2," Oct. 2025. Accessed: Nov. 13, 2025. [Online]. Available: `https://ciis.lcsr.jhu.edu/lib/exe/fetch.php?media=courses:455-655:lectures:registration_part_1.pdf`

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[6] GeeksforGeeks, "Search and Insertion in K Dimensional tree," GeeksforGeeks, Oct. 31, 2014. `https://www.geeksforgeeks.org/dsa/search-and-insertion-in-k-dimensional-tree/`