



Adding clustering *Searcher classes in statistics package

PERSONAL DETAILS:

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PROJECT ABSTRACT:

The **GNU Octave** statistics package **lacks** extensible **clustering search classes** and has an **inefficient**, disabled KDTree implementation (**GitHub issue** #151). This project will **implement** KDTreeSearcher, ExhaustiveSearcher, and hnswSearcher classes with knnsearch and rangesearch methods, plus a createns helper function. Using a C++-compiled .oct library, the KDTree will be optimized for faster construction and queries, surpassing MATLAB compatibility. This will enhance Octave's clustering capabilities for statistical computing.

OVERVIEW:

GNU Octave is a premier open-source environment for **scientific computing**, celebrated for its **numerical prowess** and status as a free alternative to MATLAB. Its **rich package** ecosystem fuels diverse applications, from academic research to real-world problem-solving, with the **statistics package** playing a pivotal role in **statistical analysis**. Yet, deficiencies in its **clustering tools** reveal an **opportunity** to elevate its capabilities and retain users who might otherwise turn to proprietary alternatives.

This project rectifies this by introducing advanced searcher classes: **KDTreeSearcher** for **fast k-nearest neighbor** searches using a spatial tree to **quick**ly locate the closest points, **ExhaustiveSearcher** for **brute-force** searches ensuring precision across all data, and **hnswSearcher** for **approximate nearest neighbor searches** leveraging hierarchical navigable small world graphs to balance speed and accuracy. These will include **knnsearch** to find the **k closest points** and **rangesearch** to retrieve all **points within a given radius**, enabling applications like pattern recognition, outlier detection, density estimation, and geospatial analysis. **Optimized** with compiled C++ code, these features will handle large datasets **efficiently**.

As an active Octave contributor, I've engaged in community discussions, assisted users, and mastered its codebase, preparing me to meet user needs.

Through Google Summer of Code 2025, I'll apply my **Octave**, **C++**, and **clustering expertise**, collaborating with mentors to **enhance Octave's utility**, **broaden** its appeal, and deepen my role in its **vibrant community**. I am **motivated** to contribute and join the community. It's always great to see people use and appreciate your code.

DETAILED PROJECT DESCRIPTION:

I would like to focus on few important areas like:

- 1. **Lack of Modularity**: The current implementation does not use object-oriented programming (OOP) principles. This makes it difficult to extend or modify the functionality.
- 2. **Inefficient KDTree Implementation**: The KDTree method is slow and poorly implemented.
- 3. **Missing hnswSearcher**: The current implementation does not include the Hierarchical Navigable Small World (HNSW) algorithm, which is a state-of-the-art method for approximate nearest neighbor searches.
- 4. **No Helper Function**: There is no createns helper function to create a nearest neighbor searcher object.

I would also like to share the **class diagrams** of proposed implementation of the classes:

KDTreeSearcher - data: matrix

- tree: KDTree (C++ object)
- + KDTreeSearcher(X) + knnsearch(Y, k): idx, D
- + rangesearch(Y, r): idx, D

ExhaustiveSearcher

- data: matrix
- + ExhaustiveSearcher(X)
- + knnsearch(Y, k): idx, D
- + rangesearch(Y, r): idx, D

hnswSearcher

- data: matrix
- graph: HNSW (C++ object)
- + hnswSearcher(X)
- + knnsearch(Y, k): idx, D
- + rangesearch(Y, r): idx, D

I have also researched about how and decided about on how I would like the method signatures to be:

1. KDTreeSearcher:

```
classdef KDTreeSearcher
    properties
        data
        tree
    end
    methods
        function obj = KDTreeSearcher(X)
            % Constructor: Build KDTree from data matrix X
            obj.data = X;
            obj.tree = build_kdtree(X); % C++ function for KDTree construction
        end
        function [idx, D] = knnsearch(obj, Y, k)
            % Find k-nearest neighbors in KDTree
            [idx, D] = kdtree_knnsearch(obj.tree, Y, k); % C++ function for
kNN search
        function [idx, D] = rangesearch(obj, Y, r)
            % Find all neighbors within radius r in KDTree
            [idx, D] = kdtree_rangesearch(obj.tree, Y, r); % C++ function for
range search
        end
    end
end
```

a. Using **KDTreeSearcher** (For Example):

```
X = rand(1000, 10); % 1000 points in 10D space
Y = rand(10, 10); % 10 query points

% Create KDTreeSearcher
searcher = KDTreeSearcher(X);

% Find 5 nearest neighbors
[idx, D] = searcher.knnsearch(Y, 5);

% Find neighbors within radius 0.5
[idx, D] = searcher.rangesearch(Y, 0.5);
```

2. ExhaustiveSearcher:

```
classdef ExhaustiveSearcher
    properties
        data
    end
    methods
        function obj = ExhaustiveSearcher(X)
            % Constructor: Store data matrix X
            obj.data = X;
        end
        function [idx, D] = knnsearch(obj, Y, k)
            % Brute-force k-nearest neighbors search
            D = pdist2(obj.data, Y, 'euclidean'); % Use existing pdist2
function
            [D, idx] = sort(D, 2);
            D = D(:, 1:k);
            idx = idx(:, 1:k);
        end
        function [idx, D] = rangesearch(obj, Y, r)
            % Brute-force range search
            D = pdist2(obj.data, Y, 'euclidean');
            idx = cell(size(Y, 1), 1);
            for i = 1:size(Y, 1)
                idx{i} = find(D(:, i) \leq r);
            end
        end
    end
end
```

3. hnswSearcher:

```
classdef hnswSearcher
    properties
        data
        graph
    end
    methods
        function obj = hnswSearcher(X)
            % Constructor: Build HNSW graph from data matrix X
            obi.data = X;
            obj.graph = build_hnsw(X); % C++ function for HNSW construction
        end
        function [idx, D] = knnsearch(obj, Y, k)
            % Approximate k-nearest neighbors search using HNSW
            [idx, D] = hnsw_knnsearch(obj.graph, Y, k); % C++ function for
HNSW kNN search
        end
        function [idx, D] = rangesearch(obj, Y, r)
            % Approximate range search using HNSW
            [idx, D] = hnsw_rangesearch(obj.graph, Y, r); % C++ function for
HNSW range search
        end
    end
end
```

a. Using hnswSearcher (For Example):

```
X = rand(100000, 100); % 100,000 points in 100D space
Y = rand(10, 100); % 10 query points

% Create hnswSearcher
searcher = hnswSearcher(X);

% Find 10 approximate nearest neighbors
[idx, D] = searcher.knnsearch(Y, 10);
```

BENEFITS TO OCTAVE COMMUNITY:

- Closing the Feature Gap: Adding KDTreeSearcher, ExhaustiveSearcher, and hnswSearcher aligns Octave's statistics package with MATLAB, attracting users needing advanced clustering tools.
- 2. **Enabling Advanced Research**: Enhanced search capabilities empower data scientists and researchers to **efficiently analyze** large datasets for machine learning and spatial tasks.

3. **Strengthening the Ecosystem**: Improved clustering functionality fosters development of higher-level tools, enriching Octave's open-source ecosystem.

DELIVERABLES:

- 1. Searcher Classes: KDTreeSearcher, ExhaustiveSearcher, hnswSearcher with knnsearch and rangesearch.
- 2. **Optimized KDTree**: C++-compiled .oct file **fixing** GitHub issue #151.
- 3. **createns Function**: Helper to instantiate searchers with options.
- 4. **Documentation**: Guides and examples for new features.
- 5. **Tests**: Suite ensuring compatibility and performance.

POSSIBLE DIFFICULTIES:

- 1. **MATLAB Parity**: Matching MATLAB's behavior might hit edge-case snags. I'll align with its docs and test rigorously.
- 2. **Octave Integration**: Linking .oct files and new classes could face build issues. My codebase knowledge and early tests will ease this.
- 3. **C++ Performance**: Optimizing KDTree in C++ for speed and memory may be tricky. I'll use deeper research & mentor input to refine it.

TIMELINE:

- Once coding begins, I will work dedicatedly for at least 4-5 hours on weekdays (and 6-8 hours on weekends) until the completion of the project. After the submission of my proposal (on or before April 8), I will start researching more about the classes and start noting down important aspects of it.
- 2. During the **start of** the community bonding period, I have my **end-semester examinations** which will start from **May 5 until May 17**. However, I **promise** to begin my work as early as possible to be on track. After the examinations, I **shall put in more time** to make up for any lost time or lag.
- 3. I have a **2-month long vacation after May 17** and **no other commitments** in hand, so I will be able to **devote ample time** to the project.

Up till May 8	Proposal accepted or rejected → Deepen familiarity with Octave's statistics package codebase. → Discuss project details with mentor Andreas Bertsatos, refining scope and priorities.
May 8 - June 1	Community Bonding Period → Set up the development environment with the latest Octave version and C++ tools. → Finalize detailed plan: prioritize KDTreeSearcher, identify potential HNSW challenges.

Week 1 & 2	Coding Officially Begins! → Design KDTreeSearcher class using classdef. → Start C++ KDTree implementation (tree-building logic), test basic queries.
Week 3 & 4	 → Complete C++ KDTree as .oct file, integrate with KDTreeSearcher. → Implement knnsearch and rangesearch for KDTreeSearcher, test performance.
Week 5	Buffer Period → Fix any KDTree issues, optimize based on initial tests. → Review progress with mentor, adjust remaining tasks.
Week 6 & 7	 → Develop ExhaustiveSearcher with knnsearch and rangesearch, test accuracy. → Implement createns function, validate with both KDTree and Exhaustive methods.
Week 8 & 9	 → Build hnswSearcher using HNSW algorithm, add methods. → Test hnswSearcher on large datasets, tweak parameters for speed/accuracy.
Week 10	Buffer Period → Resolve bugs in hnswSearcher or prior classes. → Ensure all classes work seamlessly with createns, confirm deliverables with mentor.
Week 11 & 12	 → Write comprehensive documentation and usage examples for all features. → Finalize testing suite (performance, compatibility), prepare submission (code, docs, report).
Until Pens Down & Post-GSoC	 → Address final mentor feedback, submit well before the deadline. → Continue refining features, contributing to Octave community long-term.

HISTORY OF MY CONTRIBUTIONS:

- 1. [statistics] #173: Adds new functionalities to glmfit
- 2. [octave forge] (statistics) #66388 anovan: suggested help text example not working
- 3. #66595 The qz function documentation was not updated with generalized eigenvalues are no longer returned (Commit Applied)
- 4. #66629 print pdf does not work
- 5. #66650 barh with nonzero baseline...
- 6. [symbolic] #1311: Modified Test Expectations
- 7. [symbolic] #1316: Fix compatibility with BSD tar by supporting both tar and gtar

- 8. [symbolic] #1319: Added the pol2cart functionality for Symbolic compatibility
- 9. [symbolic] #1317: warning('on', 'all') leads to many Octave warnings
- 10. [Discourse] #6136: CIE1931 to spectrum plot
- 11. [Discourse] #6082: Need Matlab test of constant functions

ACADEMIC EXPERIENCE AND OTHER ACTIVITIES:

I'm currently pursuing a **B.Tech** in **Computer Engineering** at **VJTI** (currently in Second Year), where I've developed **expertise** in **C++** and **Octave**, alongside a strong grasp of **clustering algorithms** and data structures. My academic projects have **sharpened** my skills in **Octave's classdef system**, which I've applied to design extensible statistical tools. As **an active GNU Octave contributor**, I've participated in Octave **Discourse discussions**, **assisted users** with troubleshooting, and **gained deep familiarity** with the statistics package codebase. **Solving algorithmic challenges** on <u>LeetCode</u> has further refined my **C++ problem-solving** abilities, ideal for performance-driven implementations. This technical proficiency, paired with **my passion** for open-source and **dedication to Octave**, **equips me** to **enhance** the statistics package **effectively through GSoC**. Hereby, I am also attaching my resume: <u>Swayam Shah</u>.