Fast Streamline Search: An Exact Technique for Diffusion MRI Tractography

Etienne St-Onge¹ · Eleftherios Garyfallidis² · D. Louis Collins¹

Accepted: 10 May 2022 / Published online: 18 June 2022
© The Author(s) 2022

Abstract
In this work, a hierarchical search algorithm is proposed to efficiently compute the distance between similar tractography streamlines. This hierarchical framework offers an upper bound and a lower bound for the point-wise distance between two streamlines, which guarantees the validity of a proximity search. The proposed streamline representation enables the use of space-partitioning search trees to increase the tractography clustering speed without reducing its accuracy. The resulting approach enables a fast reconstruction a sparse distance matrix between two sets of streamlines, for all similar streamlines within a given radius. Alongside a white matter atlas, this fast streamline search can be used for accurate and reproducible tractogram clustering.

Keywords Tractography · Streamline · Polyline · White matter bundle · Binary search tree · Clustering

Introduction
In classical anatomy, the study of white matter fascicles and bundles connecting different brain regions required dissection. The non-invasive analysis of these connections has been greatly facilitated by the use of diffusion weighted MRI (Catani et al., 2002; Jones, 2008). From diffusion weighted MRI, tractography algorithms can be employed to investigate the white matter structure and connectivity (Wakana et al., 2007; Descoteaux, 2015; Jbabdi & Johansen-Berg, 2011). Representing white matter pathways, these tractography streamlines are often grouped in bundles for further analysis, such as tractometry (Bells et al., 2011; Chamberland et al., 2019a; Chamberland et al., 2019b).

Streamlines reconstructed from a tractography algorithm are composed of an ordered list of points, depicting local white matter position and trajectory. Each streamline is a polygonal chain, a set of connected line segments (also named polyline in computer graphics), with some specific characteristics that depend on the tractography algorithm. For example, most tractography algorithms reconstruct streamlines with a fixed step size (segment length) and a maximum turning angle (Tournier et al., 2012; Côté et al., 2013; Behrens et al., 2014).

Multiple tractography applications require a grouping of similar streamlines for analysis. These streamlines can be clustered based on shape similarity and proximity. Numerous algorithms and definitions of distance have been studied to improve the accuracy and efficiency of streamlines clustering (Guevara et al., 2011; Siless et al., 2013; Garyfallidis et al., 2012; Garyfallidis et al., 2016; Olivetti et al., 2017; Vázquez et al., 2020). Searching for the nearest streamline in a pre-segmented set of streamlines (called a bundle atlas) can be used to automatically dissect a tractogram into different bundles and white matter pathways (O’Donnell & Westin, 2007; Garyfallidis et al., 2018; Wang & Shi, 2019; Bertò et al., 2021). However, current approaches rely on space embedding techniques or subsampling without any distance-preserving guaranties, resulting in approximate distance.

In parallel, similar proximity search algorithms have been proposed in the data-mining field to analyze and compare time series data (Liao, 2005; Fu, 2011; Wang et al., 2013; Kotsakos et al., 2013). A multivariate time series could also be represented as a polygonal chain. Nonetheless, current
distance measures for tractography streamlines do not
directly fit in this framework. Interestingly, some bounded
dimensionality reduction techniques employed for time
series can be adapted to an existing streamline distance
measure (Yi & Faloutsos, 2000; Keogh et al., 2001; Chan
et al., 2003; Wang et al., 2013). One of these techniques, the
piecewise aggregate approximation (Keogh et al., 2001), can
be adapted to estimate Euclidean-based streamline distance,
offering a lower bound which guarantees no false dismissal.
In other words, this approximation never overestimates the
given distance; thus, it never wrongly rejects streamlines in
a radius search.

In this work, we focus on a streamline representation/
simplification that conserves important distance properties.
The resulting hierarchical representation enables the use of
standard binary search trees to increase the clustering speed.
In addition, the theoretical upper and lower bounds are used
to ensure the accuracy of the proximity search. The resulting
formulation can be applied to efficiently compute an exact
nearest neighbor (NN) or k-nearest neighbors (KNN) search
within a maximum distance.

**Methods**

This section describes the proposed hierarchical approach
to efficiently evaluate streamlines distance. For this, we first
detail the mathematical framework to compute the distance
between two streamlines. Followed by interesting mathemat-
ical properties used to optimize streamline representation
and construct the proposed hierarchical search. Afterward,
this approach is employed to search for the nearest stream-
line in a pre-segmented white matter bundle atlas, described
in the "Experiments" section.

**Distance Between Two Streamlines**

A tractography streamline \( S = [s_1, ..., s_m] \) is defined as an
ordered series of \( m \) points, where each of those points lives
in a three-dimensional space \( s_i \in \mathbb{R}^3, i \in \{1, ..., m\} \). The
distance between two points in \( n \)-dimensions \( (x, y \in \mathbb{R}^n) \)
has generally been defined by the Minkowski distance \( (L^p\text{-norm}) \).

\[
\text{dist}_{L^p}(x, y) := \|x - y\|_p = \left( \sum_{j=1}^{n} |x_j - y_j|^p \right)^{1/p}
\]

This distance is a generalization of both the Manhattan
\( (L^1) \) and the Euclidean \( (L^2) \) distance. It satisfies the triangle
inequality for any \( p \geq 1 \), resulting in a valid metric. This can
be extended to define the maximum norm \( (L^\infty) \) as \( p \to \infty \),
dual to the \( L^1 \) norm in finite-dimensional spaces. This
research focuses on the \( L^1 \) and the \( L^2 \) norms. Nonetheless
the \( L^\infty \) provides some bounding capacity and is sometimes
used in binary search trees.

\[
\text{dist}_{L^\infty}(x, y) := \|x - y\|_\infty = \max_{j=1}^{n} (|x_j - y_j|)
\]

The proposed method utilizes the sum (or average) of
\( L^p \)-norm to compute the distance between two streamlines
\( (U = [u_1, ..., u_m], W = [w_1, ..., w_m]) \).

\[
\text{dist}_{L^p}(U, W) := \sum_{i=1}^{m} ||u_i - w_i||_p = \sum_{i=1}^{m} \left( \sum_{j=1}^{n} |u_{i,j} - w_{i,j}|^p \right)^{1/p}
\]

\[
\text{mdist}_{L^p}(U, W) := \frac{1}{m} \text{dist}_{L^p}(U, W)
\]

\[
\text{dist}_{MDF}(U, W) := \min \left( \text{dist}_{L^p}(U, W), \text{dist}_{L^p}(U, W') \right)
\]

The “\( \text{dist}_{L^p}(-, \cdot) \)” is employed to compute the average
point-wise distance. This is done to normalize the distance
by the number of points. When computed for both ascend-
ing \( (W = [w_1, ..., w_m]) \) and descending ordered points
\( (W' = [w_m, ..., w_1]) \), the average \( L^2 \) distance is equivalent to
the minimum-average direct flip (MDF) proposed by Garyfallidis
et al. (2012). The minimum-average direct flip is often used for
streamlines clustering, similarity search and registration (Olivetti
et al., 2017; Garyfallidis et al., 2018). For tractography, each
point is in a tridimensional space, but the measure could be used
in higher dimensions. The “\( \text{dist}_{L^p}(-, \cdot) \)” between two stream-
lines is depicted in Fig. 1, equivalent to the sum of the norm of
directed vectors \( (d_i = u_i - w_i) \). This sum of the norm is also
known as the \( L^{p-1} \) entry-wise matrix norm.

**Sum of Norm Properties**

In this subsection, a few interesting properties of the sum of
\( L^1 \) and \( L^2 \) are described. These characteristics are used to
modify the streamline representation while keeping impor-
tant distance properties. These mathematical remarks are
further detailed in Appendix A.

---

---
Remark 1 When using Manhattan ($L^1$) distance, comparing two lists composed of $m$ $n$-dimensional points ($u_i, w_i \in \mathbb{R}^n, i \in \{1, \ldots, m\}$) is equivalent to computing the $L^1$ distance between two $m \times n$ dimensional points ($u, w \in \mathbb{R}^{m \times n}$).

$$\text{dist}_{L^1}(U, W) = \sum_{i=1}^{m} ||u_i - w_i||_1 = ||u - w||_1$$  \hspace{1cm} (6)

Remark 2 The $L^1$ distance in $n$-dimensions can be used as an upper and a lower bound obtained from Hölder’s inequality.

$$||x||_p \leq ||x||_q \leq n^{(1/q - 1/p)}||x||_p, \text{ for } 0 < q < p$$  \hspace{1cm} (7)

From this general equation, the Euclidean ($L^2$) distance can be bounded with $L^1$ with the previous inequality ($q = 1, p = 2$). Figure 2 illustrates this inequality with bounded volume ($||x||_p \leq r$).

$$\frac{1}{\sqrt{n}} ||x||_1 \leq ||x||_2 \leq ||x||_1 \leq \sqrt{n}||x||_2$$  \hspace{1cm} (8)

The sum of distances (p-norm) follow the same rules, since all summed values are positive.

$$\frac{1}{\sqrt{n}} \sum_{i=1}^{m} ||u_i - w_i||_1 \leq \sum_{i=1}^{m} ||u_i - w_i||_2 \leq \sum_{i=1}^{m} ||u_i - w_i||_1$$  \hspace{1cm} (9)

**Streamlines Representation & Simplification**

**Resampling** Some form of resampling is required when comparing streamlines with different numbers of points with a point-wise distance. Tractography generates streamlines with a fixed step size, resulting in individual segments of equal length. Thus, to compare streamlines from start to end, each segment can be subdivided according to the least common multiple of the number of segments. This subdivision ensures an uniform distribution of points along each streamline for the point-wise distance without changing its geometry (see Fig. 3-a).

**Downsampling** Subsampling is often used to reduce streamline complexity, but in the general case, it does not offer any bounding property. Therefore, removing points before the comparison of streamlines can reduce or increase the average distance between them. This is illustrated in Fig. 3-b, where keeping the filled-in points will increase the distance, and keeping the hollow points will decrease it. Thus, some neighbors could be missed when doing a proximity search using subsampled streamlines, resulting in an approximate search.

Fig. 2 Illustration of norm inequality from remark 2 (Eq. 8). In 2D, the Euclidean distance ($L^2$), displayed in red, is bounded between $L^1/\sqrt{2}$ and $L^1$.

**Remark 3** If $\bar{u} = \frac{1}{m} \sum_{i=1}^{m} u_i$ is the mean position of a streamline, then the distance between the mean position of two streamlines is always smaller or equal to the average point-wise distance.

$$\text{dist}_{L^p}(\bar{u}, \bar{w}) = \|\bar{u} - \bar{w}\|_p \leq \frac{1}{m} \sum_{i=1}^{m} ||u_i - w_i||_p = m \text{dist}_{L^p}(U, W)$$  \hspace{1cm} (10)

Thus, averaging points together can be used to reduce the number of points to compare, without increasing the distance. This type of aggregation of points is used extensively for time series analysis, such as the piecewise aggregate approximation (Keogh et al., 2001), or Haar wavelet transform (Chan et al., 2003).

Fig. 3 a Uniformly resampling streamlines can be used to make two streamlines, with unequal number of points, directly comparable using a point-wise distance; for equal length segments, this can be computed with the least common multiple of the number of segments. b Subsampling points can reduce (gray dashed lines) or increase (red dotted lines) the average point-wise distance between two streamlines. c Averaging points (green dashed lines) never increases this distance - it can only reduce it.
Averaging As demonstrated earlier in remark 3, averaging points together never increases the average distance (“dist_{L_p}(\cdot, \cdot)”). Therefore, when searching for all similar streamlines in a given radius (r) using averaged points, it is guaranteed that the distance remains inside that radius. Consequently, computing the barycenter, or multiple mean points (“sub-barycenters”), is an effective way to reduce the number of comparisons (i.e. to reduce dimensionality) for tractography streamline proximity search. This concept of aggregating points will be used to generate a hierarchical comparison method, similar to a multiscale approach. Fig. 3-c illustrates this simplification by averaging together 3 points along each streamlines, resulting in 2 mean points to compare.

Proposed Hierarchical Streamline Representation

Based on previous remarks, we propose a new hierarchical approach for tractography streamlines proximity search (exact NN or KNN) within a maximum distance. In this subsection, the framework is detailed in three procedures: barycenter binning, simplification by averaging, and distance refinement. When this approach is employed to search for the nearest streamline in a template (pre-segmented white matter bundle atlas), these procedures are used for both: the template construction (Fig. 4), and the resulting hierarchical streamlines search (Fig. 5).

**Barycenter Binning** First, the barycenter of a streamline can be used as an initial proximity search. Because the distance between two barycenters is never greater than the “dist_{L_p}(\cdot, \cdot)” (see remark 3), it can be used to limit the proximity search (Fig. 5-c). Coordinates for all barycenters can be grouped together on a regular grid. When searching for all similar streamlines within a specified range (r), only the current grid and its neighbors (within distance r) need to be examined. The binning size can be optimized based on the amount of streamlines and the radius (r) of the proximity search; smaller bins will increase the preprocessing and construction time, but reduce the subsequent search time. Moreover, this barycenter binning provides independent bins, enabling efficient multithreading and the reduction of memory usage. Consequently, each bin can be separated and processed individually, only requiring the current and neighboring bins. When searching in a template, bins can be generated with an overlap to avoid to look at neighboring bins (see Fig. 4-D).

**Simplification by Averaging** Second, streamline points can be aggregated to create a simplified version with μ mean points (Fig. 5-b). This is done to reduce the number of dimensions when using a binary search tree, thereby “avoiding” the curse of dimensionality (Marimont and Shapiro, 1979; Verleysen and François, 2005; Pestov, 2013). When the number of mean points (μ) is a divisor of the initial number of

---

**Fig. 4** Template construction for the proposed hierarchical fast streamline search. **A** Streamlines in a given template, **B** template simplification by averaging resulting in μ mean points (mpts) per streamline, **C** barycenter (1 mean point) per streamline, **D-E** organizing streamlines using barycenter bins with an overlap greater or equal to the search radius, **F** space-partitioning tree structure for each bin using μ mean points.

© Springer
points \(m\) the remark 3 remains true; otherwise a continuous averaging needs to be done. Afterwards, each streamline’s mean points are vectorized in a \(\mu \times n\) vector, to employ both remarks 1-2. This vectorization enables the use of standard space-partitioning tree structure, which greatly increase the search speed (see Fig. 5-d). For the distance between streamlines “\(\text{mdist}_{L^2}(\cdot, \cdot)\)”, with the \(L^2\) norm per points, the searching range need to be increased by the square root of the spatial dimensionality (\(\sqrt{n}\)). Since the distance between simplified streamlines using \(\mu\) mean points is always smaller than or equal to the tractography streamline point-wise distance (remark 3), this aggregation enables the search for all similar streamlines within a certain radius, without missing any streamlines (Fig. 5-e). This results in a radius search with no false dismissals (no false negatives), where remaining false positives can be rectified with a refinement step.

**Distance Refinement** Finally, the resulting similar streamlines with their respective distances, obtained from the proximity search using simplified streamlines, can be refined by computing the complete distance (without simplification). When searching for all similar streamlines within a radius (i.e. proximity search), streamlines with a complete distance larger than the desired radius need to be filtered out (Fig. 5-f). KNN search, within a maximum radius, can be done by computing refined distances and extracting the first \(K\) streamlines.

**Experiments**

**Dataset**

**Tractography** For the evaluation, we utilized 44 subjects from the Human Connectome Project (HCP) dataset (Van Essen et al., 2013). Tractography streamlines were reconstructed using probabilistic *particle filtering tractography* (Girard et al., 2014) implemented in *Dipy* (Garyfallidis et al., 2014). Resulting streamlines were
aligned to the MNI space (ICBM 2009a, Fonov et al., 2011) using ANTs’ affine registration (Avants et al., 2008). This registration was computed from the T1-weighted image of each subject (already aligned with the distortion corrected diffusion space) to the MNI template.

**Bundle Atlas** The bundle atlas employed for the experiment is detailed in Garyfallidis et al. (2018); Yeh et al. (2018). Streamlines from this atlas were already aligned to the MNI space (ICBM 2009a, Fonov et al., 2011), which is composed of 33 bundles (9 inter-hemispheric, 12 intra-hemispheric) with a total of 210K streamlines.

**Streamlines** All streamlines were defined with 32 points \((m = 32)\), to limit the variability in our testing, and make the proposed proximity search comparable to RecoBundles (Garyfallidis et al., 2018), because RecoBundles downsamples all streamlines to a fixed number of points (12). For the proposed approach, all streamlines from the atlas were compared with both ascending and descending (flip) order, resulting in 420K streamlines. This makes the employed distance \(\text{mdist}_{L_2}(\cdot, \cdot)\) equivalent to RecoBundles’ minimum-average direct flip distance.

**Evaluation**

The proposed hierarchical streamline search was quantitatively evaluated by measuring the computation time. Each streamline search method was computed twice per subject to avoid aberrant run time, keeping the smallest time for each subject (except for longer run without binning or without mean points). This computation time is afterward averaged over all 44 subjects to compare the efficiency of the proposed method with various parameters. This computation time did not include any file loading or saving time. The proposed approach was evaluated with and without the *barycenter binning* at various *bin_size* (4mm, 8mm, 12mm). The *simplification by averaging* was compared at different numbers of mean points (2, 4, 8). Without *barycenter binning and simplification*, this is equivalent to a brute force search with quadratic time.

For each subject, multiple sets of streamlines were used to vary the total amount of streamlines (500K, 1M, 2M, 4M). The proximity search radius was evaluated from 2mm to 12mm, in 2mm steps. The proximity search was applied to 44 subjects using all 33 bundles from the atlas.

The proposed algorithm was also compared to RecoBundles (Garyfallidis et al., 2018) with various number of streamlines. RecoBundles was run with its default parameters from *Scilpy* (v1.1.0): subsampling streamlines to 12 points, a pruning distance of 8mm, and a clustering threshold of 12mm (Garyfallidis et al., 2014; Garyfallidis et al., 2016; Rheault, 2020). It should be noted that the proposed *fast streamline search* is not equivalent to RecoBundles; RecoBundles subsamples streamlines and relies on the QuickBundles clustering algorithm, resulting in an approximate search. Moreover, RecoBundles/QuickBundles prune clusters using an adapted clustering threshold for each bundle. The goal of this evaluation is to give an idea of the clustering speed of the proposed streamline search method, compared to a state-of-the-art similarity-based clustering method (RecoBundles). Computation times were measured from a single core on Intel’s 2.4GHz Skylake 6148 processor. The proposed method employs *Scipy* (v1.6.3) cKDTree for space-partitioning (Virtanen et al., 2020).

Streamline simplification errors were evaluated to compare the conventional subsampling and the proposed mean points averaging. In addition, inaccuracy was estimated using false positive and false negative rates compared to an exact brute force search from 500K streamlines. For this accuracy test, RecoBundles results were averaged from 30
runs, using different random seed, to avoid outliers with this stochastic approach. All distance values and estimated errors are reported in millimeters.

## Results

### Computation Time

Figure 6 details the computation time for streamline proximity search within 8\( \text{mm} \) (\( \text{mdist}_{L^2}(\cdot, \cdot) \leq 8 \text{mm} \)) at various numbers of streamlines (500K, 1M, 2M, 4M), searching for similar streamlines in a bundle atlas of 210K streamlines. When using both \textit{barycenter binning} and \textit{simplification}, the resulting clustering speed is comparable to RecoBundles. Figure 7 presents the computation time as a function of the search radius (from 2mm to 12mm) for 4 million streamlines. When using \textit{barycenter binning}, a \textit{simplification} with 4 mean points (nb\_mpts=4) performs slightly better for any number of streamlines (from 500K to 4M) and search radius (from 2mm to 12mm). Using less mean points (nb\_mpts=2) decrease the tree search time but increase even more the \textit{distance refinement} computation time. This is reversed with more mean points (nb\_mpts=8), since it reduces the \textit{distance refinement} time but further increases the search time. It can be observe from Figs. 6, 7, that the optimal \textit{barycenter binning} size varies in function of the number streamlines and search radius.

### Quantitative Comparison

Distance errors from downsampling streamlines are presented in Table 1. Overall, the proposed mean points results in a smaller mean absolute/squared error. Table 2 depicts the number of false positives and false negatives for each method at various resampling. Since the mean points approach did not increase the distance between two streamlines (from a positive minimum difference in Table 1), it resulted in zero false negatives when using a brute force approach. Without refinement, the \textit{fast streamline search} is equivalent in accuracy to an exhaustive search with simplified streamlines. It can be noted that the proposed \textit{fast streamline search} with refinement and mean points simplification results in an exact search, based on the “\text{mdist}_{L^2}(\cdot, \cdot)” measure. Thus, only computation time varies when changing the bin size or the number of mean points, resulting distances and clustered streamlines do not change.

### Qualitative Comparison

Figure 8 shows streamlines extracted using both the proposed method (radius of 4mm, 6mm or 8mm) and RecoBundles. Both clusters were obtained from the Corticospinal tract (CST) in the bundle atlas. Results for other bundles are displayed in Appendix B (Figure 9, 10 and 11).

### Table 1 Distance errors when using subsampling or mean points at various number of points (4, 8, 16). Comparing the estimated distance to the exact distance (with 32 points), from 500K streamlines to the left Corticospinal tract (CST) bundle in the atlas. The average error for each approach is presented with both mean absolute error (MAE) and mean squared error (MSE). The minimum and maximum differences are obtained from the exact distance minus the distance with resampled streamlines. All distance values and estimated errors are in millimeters.

| Resampling | Nb. Points | MAE | MSE | Min Diff. | Max Diff. |
|------------|------------|-----|-----|-----------|-----------|
| Subsample  | 16         | 0.7529 | 0.6730 | -3.0529   | 1.4244    |
| Subsample  | 8          | 2.4034 | 6.7801 | -9.3363   | 3.4591    |
| Subsample  | 4          | 6.4656 | 48.6004 | -26.4175 | 12.9009   |
| Mean Points| 16         | 0.0360 | 0.0015 | 0.0006    | 0.5940    |
| Mean Points| 8          | 0.1773 | 0.0362 | 0.0019    | 2.7803    |
| Mean Points| 4          | 0.7210 | 0.6087 | 0.0043    | 8.1184    |
Table 2  Number of false positive (left) : false negative (right) using a brute force search, Recobundles and the proposed fast streamline search (FSS) without or with refinement. The 8mm radius search was done using 500K streamlines and the left Corticospinal tract (CST)

| resampling    | nb. pts | brute force | Recobundles | FSS no refine | FSS refined |
|---------------|---------|-------------|-------------|---------------|-------------|
| none          | 32 0 : 0 0 | 0 : 1465    | 0 : 0       | 0 : 0         | 0 : 0       |
| subsample     | 16 0 : 22 0 | 0 : 1465    | 0 : 22      | 0 : 22        | 0 : 22      |
| subsample     | 8 0 : 75 4 | 0 : 1264    | 0 : 75      | 0 : 75        | 0 : 75      |
| subsample     | 4 1 : 152 6 | 0 : 1346    | 1 : 152     | 0 : 152       | 0 : 152     |
| mean points   | 16 2 : 0 0 | 0 : 1461    | 2 : 0       | 0 : 0         | 0 : 0       |
| mean points   | 8 12 : 0 14 | 0 : 1181    | 12 : 0      | 0 : 0         | 0 : 0       |
| mean points   | 4 40 : 0 18 | 0 : 1284    | 40 : 0      | 0 : 0         | 0 : 0       |

**Discussion**

Overall, the proposed approach using 4 mean points results in the fastest computation time on average. Streamlines simplification with 4 mean points is a good trade-off between distance refinement computation time and tree search speed. In addition, the optimal barycenter binning size varies in function of the search radius, the number of streamlines and also from one subject to another. Nonetheless, not using this barycenter binning generally results in slower performance (green lines in Figs. 6 and 7) and is highly dependent of the bin size. Directly using all streamlines points (32), without simplification.

**Fig. 8** Results of the proximity search for the left Corticospinal tract (CST) from single HCP subject: a) the bundle atlas from Garyfallidis et al. (2018); Yeh et al. (2018), b) RecoBundles result, c) RecoBundles result (in green) showing in purple streamlines missing in RecoBundles (false negatives) but present in the proposed technique with an exact search of 6mm radius. The proposed proximity search, \( \text{mdist}\left(\cdot, \cdot\right) \leq r \), using a radius of: d) 4mm, e) 6mm, and f) 8mm. Streamlines are colored based on the local orientation (x,y,z to RGB) with the exception of c)

| a) Left CST Atlas | b) RecoBundles | c) Comparison |
|-------------------|----------------|--------------|
| d) 4mm search     | e) 6mm search  | f) 8mm search |

\( \text{Springer} \)
(orange line in Fig. 6), results in a poor computation time and heavy memory usage for the binary search tree. Bins of 8mm and 12mm without simplification are not displayed since they were significantly slower than binning at 4mm.

Depicted in Tables 1-2, the proposed framework (bar-ycenter binning, simplification by averaging and distance refinement) accurately find all similar streamlines without any false positives or false negatives. Results are visually comparable (Fig. 8) to existing approaches that use an approximate similarity search (RecoBundles), where further comparison are displayed in Appendix B.

Despite this comparison, some part of this fast streamlines search algorithm could be directly integrated inside QuickBundles and RecoBundles to further improve their clustering speed when matching bundle centroids. Additionally, mean points could be employed in other tractography approaches, instead of subsampling, to reduce simplification errors when computing the distance between streamlines.

The proposed lower and upper bound definitions could be further improved using specific properties of tractography streamlines, such as the step size and maximum curving angle. However, these values would change from one tractography algorithm to another. As mentioned previously, tractography streamlines normally have a fixed segment length, however some researchers compress streamlines with the Ramer–Douglas–Peucker algorithm (Hershberger & Snoeyink, 1992) or a similar variant for tractography (Presseau et al., 2015) to save disk space. It should be noted, that compression algorithms modify streamlines thus they will change the original distance.

Other approaches could be used to further reduce the number of points (or dimensions) required when employing a search tree (O’Donnell & Westin, 2007; Olivetti et al., 2012; Wang & Shi, 2019; Legarreta et al., 2021). Nevertheless, those dimensionality reduction techniques on tractography streamlines do not preserve distances nor guarantee any lower/upper limits on distance, resulting in an approximate neighbor search.
Applications This proposed approach would be useful in a clinical setting when the search accuracy is critical, especially when missing streamlines (from false negatives) could significantly alter the analysis. This type of hierarchical search will become necessary when working with large tractograms, because computing an exhaustive search would be unfeasible. Still, before comparing streamlines, validating the tractography reconstruction and brain registration is crucial for clinical applications.

Limitation & Future Work This proposed method and streamlines simplification were specifically designed for the sum (or average) of Minkowski p-norm. This hierarchical approach might be adaptable to other streamlines similarity measures described by Olivetti et al. (2017), however it would requires a redefined simplification algorithm along with new upper and lower bounds.

Conclusion The proposed framework efficiently and accurately search for all similar tractography streamlines inside a given radius. This method can be used to cluster streamlines into bundles, based on an given white matter atlas. The use of simplification by averaging (mean points) combined with a space-partitioning search tree significantly reduces the query time, with no false dismissals. Furthermore, barycenter binning provides independent bins, enabling efficient multithreading and the reduction of memory usage. Finally, this proposed method guarantees accurate results and is comparable in speed to existing approaches using approximate similarity search.

Information Statement Sharing
The datasets employed in this experiment is available at HumanConnectome.org, from the Human Connectome Project (HCP) (Van Essen et al., 2013). The bundle atlas is available at zenodo.org/record/3613688 (Garyfallidis et al., 2018; Yeh et al., 2018).

Resulting streamlines generated during the current study are available from the corresponding author on reasonable request. Where both the tractography algorithm and RecoBundles segmentation were computed with Dipy at dipy.org (Garyfallidis et al., 2014). An open source implementation of the proposed Fast Streamline Search is available in Dipy.

Appendix

A. Sum of Norm Properties with Detailed Equations

Proof (Remark 1) The dist$_{L^1}(U, W)$ is equivalent to computing the $L^1$ distance between two $m \times n$ dimensional points ($u, w \in \mathbb{R}^{m \times n}$).

$$\text{dist}_{L^1}(U, W) = \sum_{i=1}^{m} ||u_i - w_i||_1$$

$$= \sum_{i=1}^{m} \sum_{j=1}^{n} |u_{ij} - w_{ij}|$$

$$= ||u - w||_1$$

$\square$
Proof (Remark 2) The $L^1$ distance in $n$-dimensions can be used as an upper and a lower bound the $L^2$ distance, from Hölder’s inequality ($x \in \mathbb{R}^n$).

$$\|x\|_p \leq \|x\|_r \leq n^{(1/r - 1/p)} \|x\|_p$$

where $0 < r < p$

$$\|x\|_2 \leq \|x\|_1 \leq \sqrt{n} \|x\|_2$$

$r = 1, \, p = 2$

$$\frac{1}{\sqrt{n}} \|x\|_2 \leq \frac{1}{\sqrt{n}} \|x\|_1 \leq \|x\|_2$$

division by $\frac{1}{\sqrt{n}}$

□

Proof (Remark 3) The distance between the mean position ($\bar{u} = \frac{1}{m} \sum_{i=1}^{m} \mathbf{u}_i$) of two streamlines is always smaller or equal to the average point-wise distance. This can be obtained from $L^p$-norm properties ($1 \leq p < \infty$, $x, y \in \mathbb{R}^n$, $\lambda \in \mathbb{R}$).

$$\|x + y\|_p \leq \|x\|_p + \|y\|_p$$

Triangle inequality (11)

$$\|\lambda x\|_p = |\lambda| \|y\|_p$$

Positive homogeneity (12)

Using $\mathbf{u}_i, \mathbf{w}_i \in \mathbb{R}^n, i \in \{1, ..., m\}$, such that $\mathbf{d}_i = \mathbf{u}_i - \mathbf{w}_i$.

$$\|\bar{u} - \bar{w}\|_p = \left\| \frac{1}{m} \sum_{i=1}^{m} \mathbf{u}_i - \frac{1}{m} \sum_{i=1}^{m} \mathbf{w}_i \right\|_p$$

$$= \frac{1}{m} \left\| \sum_{i=1}^{m} (\mathbf{u}_i - \mathbf{w}_i) \right\|_p$$

from (12)

$$\leq \frac{1}{m} \sum_{i=1}^{m} \|\mathbf{u}_i - \mathbf{w}_i\|_p$$

from (11)

□

B. Streamline Search Comparison

Acknowledgements Acknowledgements to Gabrielle Grenier, Maxime Toussaint, Daniel Andrew, Alex Provost for their help and insights. Thanks to the Fonds de recherche du Québec - Nature et technologies (FRQNT), the Canadian Institutes of Health Research (MOP-111169) and the Natural Sciences and Engineering Research Council of Canada (NSERC) for research funding.

Declarations

Conflict of Interest We have no conflict of interest to declare.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article’s Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article’s Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit http://creativecommons.org/licenses/by/4.0/.

References

Avants, B. B., Epstein, C. L., Grossman, M., & Gee, J. C. (2008). Symmetric diffeomorphic image registration with cross-correlation: evaluating automated labeling of elderly and neurodegenerative brain. Medical Image Analysis, 12, 26–41.

Behrens, T. E., Sotiropoulos, S. N., & Jbabdi, S. (2014). Mr diffusion tractography. In Diffusion MRI (pp. 429–451). Elsevier.

Bells, S., Cercignani, M., Deoni, S., Assaf, Y., Pasternak, O., Evans, C. J., Leemans, A., & Jones, D. K. (2011). Tractometry–comprehensive multi-modal quantitative assessment of white matter along specific tracts. In 19th International Society of Magnetic Resonance in Medicine (ISMRM) (p. 1). volume 678.

Berti, G., Bullock, D., Astolfi, P., Hayashi, S., Zigiottlo, L., Annichiarico, L., et al. (2021). Classifyber, a robust streamline-based linear classifier for white matter bundle segmentation. NeuroImage, 224, 117402.

Catani, M., Howard, R. J., Pajevic, S., & Jones, D. K. (2002). Virtual in vivo interactive dissection of white matter fasciculi in the human brain. Neuroimage, 17, 77–94.

Chamberland, M., Raven, E. P., Genc, S., Duffy, K., Descoteaux, M., Parker, G. D., et al. (2019a). Dimensionality reduction of diffusion mri measures for improved tractometry of the human brain. NeuroImage, 200, 89–100.

Chamberland, M., St-Jean, S., Tax, C. M., & Jones, D. K. (2019b). Obtaining representative core streamlines for white matter tractometry of the human brain. In International Conference on Medical Image Computing and Computer-Assisted Intervention (pp. 359–366). Springer.

Chan, F.-P., Fu, A.-C., & Yu, C. (2003). Haar wavelets for efficient similarity search of time-series: with and without time warping. IEEE Transactions on knowledge and data engineering, 15, 686–705.

Côté, M.-A., Girard, G., Boré, A., Garyfallidis, E., Houde, J.-C., & Descoteaux, M. (2013). Tractometer: towards validation of tractography pipelines. Medical image analysis, 17, 844–857.

Descoteaux, M. (2015). High angular resolution diffusion imaging (hardi). Wiley Encyclopedia of Electrical and Electronics Engineering, (pp. 1–25).

Fonov, V., Evans, A. C., Botteron, K., Almli, C. R., McKinstry, R. C., Collins, D. L, & Brain Development Cooperative Group. (2011). Unbiased average age-appropriate atlases for pediatric studies. Neuroimage, 54(1), 313–327.

Fu, T.-C. (2011). A review on time series data mining. Engineering Applications of Artificial Intelligence, 24, 164–181.

Garyfallidis, E., Brett, M., Amiribekian, B., Rokem, A., Van Der Walt, S., Descoteaux, M., Nimmo-Smith, I., & Contributors, D. (2014). Dipy, a library for the analysis of diffusion mri data. Frontiers in neuroinformatics, 8.

Garyfallidis, E., Brett, M., Correa, M. M., Williams, G. B., & Nimmo-Smith, I. (2012). Quickbundles, a method for tractography simplification. Frontiers in neuroscience, 6, 175.

Garyfallidis, E., Côté, M.-A., Rheault, F., & Descoteaux, M. (2016). Quickbundlesx: sequential clustering of millions of streamlines in multiple levels of detail at record execution time. 24th International Society of Magnetic Resonance in Medicine (ISMRM).

Garyfallidis, E., Côté, M.-A., Rheault, F., Sidhu, J., Hau, J., Petit, L., et al. (2018). Recognition of white matter bundles using local and global streamline-based registration and clustering. NeuroImage, 170, 283–295.
Towards quantitative connectivity analysis: reducing tractography biases. Neuroimage, 98, 266–278.

Guevara, P., Poupon, C., Rivière, D., Cointepas, Y., Descoteaux, M., Thirion, B., & Mangin, J.-F. (2011). Robust clustering of massive tractography datasets. Neuroimage, 54, 1975–1993.

Hershberger, J. E., & Snoeyink, J. (1992). Speeding up the Douglas-Peucker line-simplification algorithm. Department of Computer Science Vancouver, BC: University of British Columbia.

Jbabdi, S., & Johansen-Berg, H. (2011). Tractography: where do we go from here? Brain connectivity, 1, 169–183.

Jones, D. K. (2008). Studying connections in the living human brain with diffusion mri. cortex, 44, 936–952.

Keogh, E., Chakrabarti, K., Pazzani, M., & Mehrotra, S. (2001). Dimensionality reduction for fast similarity search in large time series databases. Knowledge and information Systems, 3, 263–286.

Kotsakos, D., Trajcevski, G., Gunopulos, D., & Aggarwal, C. C. (2013). Time-series data clustering.

Legarreta, J. H., Petit, L., Rheault, F., Theaud, G., Lemaire, C., Descoteaux, M., & Jodoin, P.-M. (2021). Filtering in tractography using autoencoders (finta). Medical Image Analysis, 72, 102126.

Liao, T. W. (2005). Clustering of time series data-a survey. Pattern recognition, 38, 1857–1874.

Marimont, R., & Shapiro, M. (1979). Nearest neighbour searches and the curse of dimensionality. IMA Journal of Applied Mathematics, 24, 59–70.

O’Donnell, L. J., & Westin, C.-F. (2007). Automatic tractography segmentation using a high-dimensional white matter atlas. IEEE transactions on medical imaging, 26, 1562–1575.

Olivetti, E., Berto, G., Gori, P., Sharmin, N., & Avesani, P. (2017). Comparison of distances for supervised segmentation of white matter tractography. In 2017 International Workshop on Pattern Recognition in Neuroimaging (PRNI) (pp. 1–4). IEEE.

Olivetti, E., Nguyen, T. B., & Garyfallidis, E. (2012). The approximation of the dissimilarity projection. In 2012 Second International Workshop on Pattern Recognition in NeuroImage (pp. 85–88). IEEE.

Pestov, V. (2013). Is the k-nn classifier in high dimensions affected by the curse of dimensionality? Computers & Mathematics with Applications, 65, 1427–1437.

Presseau, C., Jodoin, P.-M., Houde, J.-C., & Descoteaux, M. (2015). A new compression format for fiber tracking datasets. NeuroImage, 109, 73–83.

Rheault, F. (2020). Analyse et reconstruction de faisceaux de la matière blanche. Computer Science. Université de Sherbrooke.

Siless, V., Medina, S., Varoquaux, G., & Thirion, B. (2013). A comparison of metrics and algorithms for fiber clustering. In 2013 International Workshop on Pattern Recognition in Neuroimaging (pp. 190–193). IEEE.

Tournier, J.-D., Calamante, F., & Connelly, A. (2012). Mrtrix: diffusion tractography in crossing fiber regions. International journal of imaging systems and technology, 22, 53–66.

Van Essen, D. C., Smith, S. M., Barch, D. M., Behrens, T. E., Yacoub, E., Ugurbil, K., Consortium, W.-M. H. et al. (2013). The wu-minn human connectome project: an overview. Neuroimage, 80, 62–79.

Vázquez, A., López-López, N., Sánchez, A., Houenou, J., Poupon, C., Mangin, J.-F., et al. (2020). Fclust: Fast fiber clustering for large tractography datasets for a detailed study of brain connectivity. NeuroImage, 220, 117070.

Verleysen, M., & François, D. (2005). The curse of dimensionality in data mining and time series prediction. In International workshop on artificial neural networks (pp. 758–770). Springer.

Wang, J., & Shi, Y. (2019). A fast fiber k-nearest-neighbor algorithm with application to group-wise white matter topography analysis. In International Conference on Information Processing in Medical Imaging (pp. 332–344). Springer.

Wang, X., Mueen, A., Ding, H., Trajcevski, G., Scheuermann, P., & Keogh, E. (2013). Experimental comparison of representation methods and distance measures for time series data. Data Mining and Knowledge Discovery, 26, 275–309.

Yeh, F.-C., Panesar, S., Fernandes, D., Meola, A., Yoshino, M., Fernandez-Miranda, J. C., et al. (2018). Population-averaged atlas of the macro-scale human structural connectome and its network topology. NeuroImage, 178, 57–68.

Yi, B.-K., & Faloutsos, C. (2000). Fast time sequence indexing for arbitrary lp norms. In VLDB 2000, Proceedings of 26th International Conference on Very Large Data Bases, September 10-14, 2000, Cairo, Egypt (pp. 385–394).

Publisher’s Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.