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Novel Single and Multiple Shell Gradient Sampling Schemes for Diffusion MRI Using Spherical Codes

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Introduction. Data sampling schemes are for diffusion MR acquisition and reconstruction. Diffusion weighted (DW) data is normally acquired on single or multiple shells in q-space. The samples in different shells are typically distributed uniformly, because they should be invariant to the orientation of structures in tissue, or the laboratory coordinate frame. The Electrostatic Energy Minimization (EEM) method was originally proposed for single shell sampling scheme in dMRI [1], and was recently generalized to the multi-shell case, called generalized EEM (gEEM) [2], which has been successfully used in the Human Connectome Project (HCP). Three algorithms based on the Spherical Code (SC) concept were proposed in [3] to maximize the minimal angle between different samples in single or multiple shells, which demonstrated better angular separation and rotational invariance than the gEEM method. In this abstract, we propose two novel algorithms based on the SC concept, i.e., Iterative Maximum Overlap Construction (IMOC) to generate a sampling scheme from discretized sphere, and a constrained non-linear optimization (CNLO) method to update a given initial scheme on a continuous sphere. Compared with Incremental Spherical Code (ISC) and Mixed Integer Linear Programming (MILP) methods in [3] which were developed for a discretized sphere, IMOC obtains a larger angular separation than ISC and is more efficient than MILP that is known to be NP hard. Compared with the RGD method that relies on taking the gradient of a discontinuous function, the optimization in CNLO is more robust because the cost function and constraints are all continuous. Experiments demonstrated that the proposed two methods both provide larger separation angles and better rotational invariance than the methods in [2].

Method: Constrained Non-Linear Optimization (CNLO). The SC problem on a single shell is to find K samples \( \{u_i\} \) such that the minimal angular distance between these samples is maximized [3]. Eq (1) guarantees the antipodal symmetric constraint in sampling due to the absolute value operator in inner product between samples. The problem in the multi-shell case is considered in Eq (2), where the cost function is a combination of the minimal separation angle in every shell and the minimal separation angle in the combined shell containing all spherical samples. We propose solving these two problems using constrained non-linear optimization (CNLO) respectively in Eq (3) and Eq (4) with the constraints that the separation angles between samples are larger than the corresponding minimal angle. With given initial samples, CNLO can be solved using sequential quadratic programming (SQP) implementation in the NLopt library [4].

Method: Iterative Maximum Overlap Construction (IMOC). The Incremental Spherical Code (ISC) [3] is proposed to obtain reasonable uniform coverage if the MRI acquisition is terminated at any time and one is left with only a subset of the desired DWI data. Similarly with the incremental method in [2], in each iteration step ISC chooses the best sample that is furthest from the chosen samples in previous iterations. However ISC does not yield a good result with large separation angles when the full scheme is used. Consider a simple example in a circle \( S^1 \) in 2D space with the number \( K=3 \), the optimal sample set has the minimal separation angle of 60°, but ISC produces the sample set with the minimal separation angle of 45°. See Fig. 1(a). Here we propose IMOC to iteratively search the minimal separation angle and generate samples with maximal spherical overlap on the sphere. See the IMOC algorithm in the following table for the single shell case. A similar algorithm for the multi-shell case is omitted due to space limitations here. It is obvious that IMOC yields the optimal solution in the 2D case in Fig. 1(b). For the single- or multi-shell sampling scheme estimation problem in 3D space, the implementation of IMOC requires a discretization of the sphere and a KD-tree search for nearest neighbors. Our implementation of IMOC requires a few seconds on an ordinary laptop.

<table>
<thead>
<tr>
<th>Method</th>
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<tr>
<td>CNLO</td>
<td>Constrained Non-Linear Optimization</td>
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<tr>
<td>IMOC</td>
<td>Iterative Maximum Overlap Construction</td>
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Fig. 1 (a) and (b) are results from ISC and IMOC. The red number is the sample order in each step.