Single and Multiple Shell Sampling Design in dMRI Using Spherical code and Mixed Integer Linear Programming

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Introduction. Sampling scheme is crucial in diffusion MRI data acquisition and reconstruction. A good sampling scheme can obtain good reconstruction results with less number of samples in diffusion q-space. It has been showed that for the diffusion data obtained from single shell (single b value), the uniform sampling scheme has good performance in a general case because it does not assume a preferred direction. In last decade, two kinds of uniform single shell sampling schemes are widely used in diffusion MRI field, i.e. the sphere tessellation and electrostatic energy minimization introduced in dMRI by Jones [1]. However sphere tessellation cannot handle arbitrary number of samples, and electrostatic energy minimization lacks its physical meaning related to reconstructions in dMRI. It is still unclear that why electrostatic energy matters in diffusion data reconstruction? We hope the samples in sphere have large angular difference such that the "angular resolution" in reconstruction can be as large as possible, so mathematically a more natural way is to define a uniform sampling scheme $\{\boldsymbol{u}_i\}$ such that the minimal angular difference can be as large as possible, which is essentially the Spherical Code (SC) problem[2]. Some optimal configurations for sphere $\boldsymbol{S}^2$ for different number K have been collected in [3]. Although the solutions in [3] can be directly used in dMRI, they have two main limitations. 1) They are for single sphere, not for multi-shell schemes. 2) For real applications in dMRI, sometimes we need to find one or several sets of "uniform" schemes from a given set of sampling scheme, which is the "discretized" SC problem. In this paper, we propose a general Mixed Integer Linear Programming (MILP) framework to design "uniform" sampling schemes for both single and multi-shell dMRI. Although some recent works proposed to generalized electrostatic energy minimization method to multi-shell case [4], to our knowledge, this paper is the first work to design uniform single/multi-shell sampling scheme using SC formulation.

$$\max_{\{\boldsymbol{u}_i\}_{i=1}^{K}\in\boldsymbol{D}} \min_{i\neq j} \arccos\left(|\,\boldsymbol{u}_i^T\boldsymbol{u}_j\,|\right) \qquad (1)$$

$$\begin{aligned} &\max_{y,\{h_i\}_{i=1}^{N}} y \\ s.t.\quad &\arccos(|\boldsymbol{u}_i^T\boldsymbol{u}_j|) \geq y-(2-h_i-h_j)M, \quad \forall i>j \qquad (2)\\ &d_{lb}\leq y\leq d_{ub}(2K),\quad \sum_{i=1}^{N}h_i=K,\quad h_i=0,1 \end{aligned}$$

$$\max_{\{\boldsymbol{u}_{s,i}\}\in\boldsymbol{D}} w\frac{1}{N_s}\sum_{s=1}^{N_s}\min_{i\neq j}\arccos(|\boldsymbol{u}_{s,i}^T\boldsymbol{u}_{s,j}|)+(1-w)\min_{(s,i)\neq(s',j)}\arccos(|\boldsymbol{u}_{s,i}^T\boldsymbol{u}_{s',j}|) \qquad (3)$$

$$\begin{aligned} &\max_{y,\{h_{s,i}\}} w\frac{1}{N_s}\sum_{s=1}^{N_s}y_s+(1-w)y_0 \\ s.t.\quad &\arccos(|\boldsymbol{u}_i^T\boldsymbol{u}_j|)\geq y_s-(2-h_{s,i}-h_{s,j})M,\quad \forall i>j,\forall s \qquad (4)\\ &\arccos(|\boldsymbol{u}_i^T\boldsymbol{u}_j|)\geq y_s-(2-h_{s,i}-h_{s',j})M,\quad \forall i>j,\forall s,\forall s' \\ &d_{lb,s}\leq y\leq d_{ub}(2K_s),\quad d_{lb,0}\leq y_0\leq d_{ub}(2\sum_{s=1}^{N_s}K_s) \\ &\sum_{s=1}^{N_s}h_{s,i}\leq 1,\quad \sum_{i=1}^{N}h_{s,i}=K_s,\quad h_{s,i}=0,1 \end{aligned}$$

Theory: Single shell case. Given the number K, the SC problem is to find the K samples in single shell $\{\boldsymbol{u}_i\}$ such that the minimal distance is maximized. See Eq (1). The absolute value is used because in dMRI we want to force the antipodal symmetric constraint. Note that the original SC problem assumes the search domain $\boldsymbol{D}$ is the continuous sphere $\mathbf{S}^2$. In dMRI we may need to search the solution from a given set of samples with size N. We formulate this problem as a mixed integer linear programming as Eq (2), where h_i =1 means i-th sample is chosen, d_{ub} (2K) is the theoretical upper bound for $2K$ samples given in [1], d_{lb} is an lower bound which can be chosen by some prior knowledge or any feasible solution. M is the difference between the maximal distance and the minimal distance of any two pair $\boldsymbol{u}_i$ and $\boldsymbol{u}_j$, such that the inequality constraint holds if and only if both i-th and j-th samples are chosen. This problem can be solved by GUROBI or other software. Please note that the obtained solution of this discretized SC problem can be used as an initialization of the continuous SC problem. Any local search method can be used to improve the solution in the continuous domain.

Theory: Multi-shell case. The above discretized SC method for single shell can be generalized to multi-shell case, by defining the cost function as Eq. (3), where there are N_s shells, and every shell has K_s different directions from the given $\sum_s K_s$ directions. By considering all directions in different single shells as a whole shell, we can maximize the angular resolution between shells, thus w is the compromise weight between the single shell term and the multi-shell term. Similarly with Eq (1), Eq (3) also can be transformed to a mixed integer linear programming problem in Eq (4), where $h_{s,i}$=1 means direction $\boldsymbol{u}_i$ is chosen by s-th shell. Compared to Eq (2), Eq(4) incorporates some constrains to avoid ambiguity between shells. Note that although the solution of Eq (4) is from a given discrete set of directions, it can be used as an initialization to obtain better solution in continuous multi-shells. The formulation (4) can be also used for single shell scheme to separate a given single shell sampling scheme into several parts, as the tool subsetpoints in CAMINO [5], which is very slow because the simulated-annealing is used. If w=1, these separated parts have no angular exclusion.

	Shell 1 (28)	Shell 2 (28)	Shell 3 (28)	Global (84)
[4] (search from $\boldsymbol{S}^2$)	22.2°	22.2^2	22.0°	13.2°
[4] (incremental)	19.2°	19.7°	19.3°	4.7°
MILP (search from 321 directions)	**23.8°**	**23.8°**	**24.3°**	**13.3°**
Incremental learning (from 20482 directions)	19.3°	21.3°	21.1°	10.5°

Theory: Solve mixed integer linear programming (MILP). Note that although in general the MILP problem is NP hard, it can be solved using branch and cut method to iteratively solve the relaxed LP program. We use GUROBI [6] to solve Eq (3) and (4). In our experiments, we found that GUROBI can solve the proposed MILP problem efficiently to obtain a feasible solution in less than 10 minutes, and in some cases it stops with the global solution in 10 minutes, but in some other cases it may take a long time to obtain the global solution. In practice, we iteratively increase the lower bound d_{lb} to find a feasible solution obtained in 10 minutes. The experiments showed that the feasible solution in 10 minutes is good enough.

Theory: **Incremental configuration estimation**. Similarly with [4], both Eq (1) and Eq (3) can be solved greedily using incremental strategy. We can first pick one direction, and then in each step incrementally choose the next one direction from the remaining candidates to maximize the cost functions, which is extremely fast.

Experiments: **Separation one subset into several subsets.** We randomly mixed two uniformly directions, where one is from sphere tessellation of 81 directions and the other one is 60 directions in CAMINO based on electrostatic energy minimization. We performed subsetpoints in CAMINO and Eq (4) with w=1 to separate the 141 directions into two sets with 60 and 81 directions. Eq (4) obtained the global solution which is the same as the ground truth within 5 seconds. However after one hour, the solution by CAMINO still detects 25 wrong directions within the 60 directions.

Experiments: Schemes for multi-shell case. We test the algorithm Eq (4) and its incremental estimation to generate multi-shell sampling with 3 shells, 28 directions per shell. MILP Eq (4) selects 28x3 directions from 321 uniform directions of sphere tessellation, and the incremental learning selects them from 20482 directions. The minimal angles between directions in the results can be seen in Table 1. Table 1 also shows the results from [4], where the result of multi-shell scheme using electrostatic energy minimization is directly copied from the table in [4], and the result of incremental learning is from the website of the author of [4]. It can be seen that our MILP method and its incremental estimation obtained larger separation angle for all three single shells and the global shell including all directions,

Conclusion: We propose a general mixed integer linear programming framework to design single/multi-shell sampling schemes for dMRI. It outperforms the state-of-the-art methods in CAMINO and [4]. To our knowledge, it is the first work in dMRI to design sampling schemes by maximizing the minimal angle. Please note that the estimated configurations from discrete set can be improved by local search in the continuous sphere, which is our future work.

Reference: [1] Jones DK, Optimal strategies for measuring diffusion in anisotropic systems by magnetic resonance imaging, MRM 1999.[2]http://mathworld.wolfram.com/SphericalCode.html [3] http://www2.research.att.com/~njas/packings/ [4] Caruyer E, Design of multishell sampling schemes with uniform coverage in diffusion MRI, MRM 2013. [5] Cook PA, Camino: Open-Source Diffusion-MRI Reconstruction and Processing, ISMRM 2006 [6] http://www.gurobi.com/