Single and Multiple Shell Sampling Design in dMRI
Using Spherical code and Mixed Integer Linear Programming
Jian Cheng, Pew-Thian Yap, Dinggang Shen

To cite this version:

HAL Id: hal-01011892
https://hal.archives-ouvertes.fr/hal-01011892
Submitted on 27 Jun 2014

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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 decades, two kinds of uniform single shell sampling scheme 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 \( \{ u_i \} \) 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 \( S^2 \) 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 generalizes 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.

Theory: Single shell case. Given the number \( K \), the SC problem is to find the \( K \) samples in single shell \( \{ u_i \} \) such that the minimal distance is maximized. See Eq (1).

\[
\max_{\{u_i\}} \min_i \min_j \arccos(u_i^T u_j) \tag{1}
\]

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 \( D \) is the continuous sphere \( S^2 \). 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 \( h_i \) is the distance constraint.

\[
\begin{align*}
\text{s.t.} & \quad \arccos(u_i^T u_j) \geq y - (2 - h_i - h_j)M, \quad \forall j > i \\
& \quad d_{ij} \leq y \leq d_{ij}(2K), \quad \sum_i h_i = K, \quad h_i = 0,1
\end{align*}
\]

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). There are \( N \) shells, and every shell has \( K \) directions from the given \( \sum_i K_i \) directions. By considering directions in different shells as a whole shell, we can maximize the angular difference of the shells. This problem can be transformed to a mixed integer linear programming as Eq (4), where \( d_{ij} \) is the distance constraint.

\[
\begin{align*}
\text{s.t.} & \quad \arccos(u_i^T u_j) \geq y - (2 - h_i - h_j)M, \quad \forall j > i, \forall s,
\end{align*}
\]

\[
\begin{align*}
\text{s.t.} & \quad \arccos(u_i^T u_j) \geq y - (2 - h_i - h_j)M, \quad \forall j > i, \forall s,
\end{align*}
\]

Experiments: Separating one subset into several subsets. We randomly generated two uniform directions, one is from sphere tessellation of 81 directions and the other one is 60 directions in CAMINO based on electrostatic energy minimization. We performed subepochs 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 2082 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 angular difference. Please note that the estimated configurations from discrete set can be improved by local search in the continuous sphere, which is our future work.