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].

$$\max_{\{\boldsymbol{u}_i\}} \min_{i\neq j} \cos^{-1}(|\boldsymbol{u}_i^T \boldsymbol{u}_j|) \qquad (1)$$

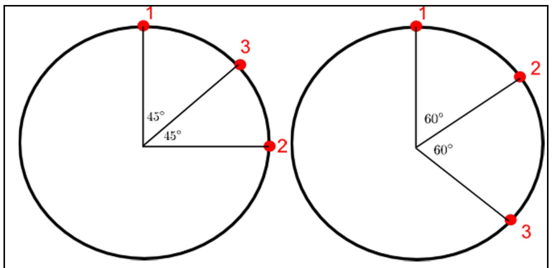
$$\max_{\{\boldsymbol{u}_{s,i}\}} w \frac{1}{N_s}\sum_{s=1}^{N_s} \min_{i\neq j} \cos^{-1}\left(|\boldsymbol{u}_{s,i}^T \boldsymbol{u}_{s,j}|\right) + (1-w)\min_{(s,i)\neq(s',j)} \cos^{-1}\left(|\boldsymbol{u}_{s,i}^T \boldsymbol{u}_{s',j}|\right) \qquad (2)$$

$$\max_{\{\boldsymbol{u}_i\},\theta}\ \theta \qquad (3)$$
$$\text{s.t.}\quad \cos^{-1}(|\boldsymbol{u}_i^T \boldsymbol{u}_j|) \geq \theta, \forall\, i<j;\quad \boldsymbol{u}_i^T\boldsymbol{u}_i = 1,\ \forall\, i$$

$$\max_{\{\boldsymbol{u}_{s,i}\},\{\theta_s\},\theta_0} w\frac{1}{N_s}\sum_{s=1}^{N_s}\theta_s + (1-w)\theta_0 \qquad (4)$$
$$\text{s.t.}\quad \cos^{-1}(|\boldsymbol{u}_{s,i}^T \boldsymbol{u}_{s,j}|) \geq \theta_s, \forall\, s,\ \forall\, i<j;\quad \cos^{-1}(|\boldsymbol{u}_{s,i}^T \boldsymbol{u}_{s',j}|) \geq \theta_0,\ \forall\, s,s',\ \forall\, i<j;\quad \boldsymbol{u}_{s,i}^T\boldsymbol{u}_{s,i} = 1, \forall\, s,i$$

Method: Constrained Non-Linear Optimization (CNLO). The SC problem on a single shell is to find K samples $\{\boldsymbol{u}_i\}$ 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) implemented 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 $\mathbb{S}^1$ in 2D space with the number K=3, the optimal sample set has the minimal separation angle of 60^o, but ISC produces the sample set with the minimal separation angle of 45^o. 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.



(a) **(b)**

Fig.1 (a) and (b) are results from ISC and IMOC. The red number is the sample order in each step.

Iterative Maximum Overlap Construction (IMOC):
Input: number K
Output: K samples in single shell
// binary search θ from $(0,\theta_{\text{up}})$. θ_{up} is the upper bound [3].
$\theta^0 = 0,\ \theta^1 = \theta_{\text{up}}$;
Do {
  $\theta = (\theta^0 + \theta^1)/2$;
  [IsSatisfied, $\{\boldsymbol{u}_i\}$] = **MOC**(θ, K);
  If IsSatisfied **: then** $\theta^0 = \theta$; **Else :** $\theta^1 = \theta$;
} **while** (θ does not change)

Maximum Overlap Construction (MOC) :
Input: θ, K
Output: IsSatisfied, $\{\boldsymbol{u}_i\}$
// Define the coverage of $\boldsymbol{x}$ as $C(\boldsymbol{x},\theta) := \{\boldsymbol{y} \mid \cos^{-1}(|\boldsymbol{y}^T\boldsymbol{x}|) < \theta\}$
Initialize coverage set CS as an empty set;
For i = 1 : K :
{ **If** CS==$\mathbb{S}^2$ **: then** IsSatisfied=**False**; **return**;
  If i ==1**: then** choose any $\boldsymbol{u}_1$**;**
  Else : Choose $\boldsymbol{u}_i$ in ($\mathbb{S}^2$-CS) such that the overlap set $C(\boldsymbol{u}_i,\theta) \cap$ CS has the largest area;
  CS = CS $\cup\ C(\boldsymbol{u}_i,\theta)$;}
IsSatisfied=**True**; **return**;

Experiments: Schemes for multi-shell case. We test the proposed CNLO and IMOC methods to generate multi-shell sampling with 3 shells, 28 directions per shell. The minimal angles between directions in the results are in the table to the right. MILP+RGD means RGD uses the initialization from MILP, and IMOC+CNLO means CNLO uses the initialization from IMOC. The results shown by methods in [3] are directly copied from [3]. It can be seen that the IMOC yields a larger separation angle than ISC and MILP, and IMOC+CNLO produces the largest separation angle. Note that the separation angle in each shell by IMOC+CNLO is also larger than the EEM method implemented in CAMINO, considering the minimal separation angle in the single shell sampling scheme with 28 samples in CAMINO is 25.7° [3,5].

	Shell 1 (28)	Shell 2 (28)	Shell 3 (28)	Combined Shell (84)
ISC [3]	21.3°	19.3°	21.1°	10.5°
MILP [3]	23.8°	23.8°	24.2°	13.3°
MILP+RGD [3]	25.7°	25.7°	25.4°	13.6°
IMOC	**24.3°**	**24.3°**	**24.3°**	**14.0°**
IMOC+CNLO	26.3°	25.9°	26.6°	14.6°

Conclusion: We propose two methods, IMOC and CNLP, based on SC concept to generate single-/multi-shell sampling scheme in dMRI. These two methods outperforms the state-of-the-art methods based on electrostatic energy in [2] and SC in [3]. Please note that the rotational invariance of the estimated fiber direction is also improved by the schemes generated by IMOC+CNLO, although we did not show the experimental result in this abstract due to the limited space.

Reference: [1] Jones DK, Optimal strategies for measuring diffusion in anisotropic systems by magnetic resonance imaging, MRM 1999. [2] Caruyer E, Design of multishell sampling schemes with uniform coverage in diffusion MRI, MRM 2013. [3] Cheng J, Designing single- and multiple-shell sampling schemes for diffusion MRI using spherical code, MICCAI 2014. [4] Steven G. Johnson, The NLopt nonlinear-optimization package, http://ab-initio.mit.edu/nlopt. [5] Cook PA, Camino: Open-Source Diffusion-MRI Reconstruction and Processing, ISMRM 2006.