Constrained Single Step Diffusion Tensor Reconstruction Using Cholesky Decomposition

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INTRODUCTION – The widely used method for estimating diffusion tensors from multi-shot & multi coil diffusion tensor data is a two step procedure : 1) Estimation of diffusion weighted images 2) Estimation of diffusion tensors from diffusion-weighted images using linear or non-linear least squares estimation. According to the diffusion model, the estimated tensors must be positive definite, which may not be true if high noise (low SNR) or high anisotropy is present [1]. Several methods have been proposed so far to guarantee the positive definiteness of the diffusion tensors. One way is to set the negative eigenvalues to zero or to a predefined value [2]. This is equivalent to projecting the tensor onto the subspace spanned by positive definite tensors. Other methods ensure positive definiteness by constraining the tensor to this subspace by transformation of parameter space [2-6]. In this study, we adopt the latter approach and use Cholesky decomposition to guarantee positive definiteness [2,4]. The novel mathematical framework presented here allows the reconstruction of diffusion tensors directly from the complex k-space data in a single step without the need for reconstructing the diffusion-weighted images first. It is shown that this method is effective in correcting rigid body motion on multi-shot & multi-coil DTI data, where, due to the rotational patient motion, each shot is potentially exposed to a different diffusion-encoding direction and coil sensitivities.

MATERIALS and METHODS – (a) *Image Reconstruction*: The signal equation for DTI is given by the following expression:

$$d(\mathbf{k}) = \sum_{\mathbf{r}} m(\mathbf{r}) e^{-\sum \mathbf{b} * \mathbf{D}(\mathbf{r})} s(\mathbf{r}) e^{-j\mathbf{k} \cdot \mathbf{r}} \quad (1)$$

where **r** represents image space point, **k** represents k-space point, $d(\mathbf{k})$ is the complex k-space data acquired for all k-space points, interleaves, diffusion encoding directions and coils, $m(\mathbf{r})$ is the non-diffusion weighted image, $\mathbf{s}(\mathbf{r})$ is the coil sensitivity, **b** is the diffusion encoding matrix and $\mathbf{D}(\mathbf{r})$ is the diffusion tensor. The "*" operation represents point by point multiplication of two matrices. In this study, instead of reconstructing the diffusion weighted images $m(\mathbf{r})\exp(-\sum \mathbf{b}^*\mathbf{D}(\mathbf{r}))$, we directly estimated **D** and $m(\mathbf{r})$ from d(**k**). For this, we defined a cost function and minimized the discrepancy between the acquired and reconstructed k-space data:

$$(\mathbf{D},m) = \underset{\mathbf{D}',m'}{\operatorname{arg\,min}} \left\| d\left(\mathbf{k}\right) - \sum_{\mathbf{r}} m'(\mathbf{r}) e^{-\sum \mathbf{b} * \mathbf{D}'(\mathbf{r})} s(\mathbf{r}) e^{-j\mathbf{k} \cdot \mathbf{r}} \right\|_{2}^{2}$$
(2)

As mentioned above, in order to obey the diffusion equation, the diffusion tensors **D** have to be positive definite. In order to guarantee this, we transform the parameter search space by re-writing the symmetric matrix **D** as the multiplication of a lower diagonal matrix and its transpose: $\mathbf{D}(\mathbf{r})=\mathbf{L}(\mathbf{r})\mathbf{L}(\mathbf{r})^{T}$, which is known as the Cholesky decomposition. Here, the diagonal entries of $\mathbf{L}(\mathbf{r})$ must be positive. What this operation does is to limit the search space for diffusion tensors to the subsace snamed by diffusion tensors that are positive.



Fig 1 – Color-coded FA maps and the locations of tensors that are not positive definite. In the case when motion correction was not applied, severe artifacts were visible (b). These were mostly removed by the application of method B (c). Accounting for the altered diffusion encoding direction with method C removed these artifacts. However, there were still a large amount of tensors that were not positive definite (h). Method D decreased the number of these non positive definite tensors significantly (i).

diffusion tensors to the subspace spanned by diffusion tensors that are positive definite. Thus, the new optimization problem becomes:

$$(\mathbf{L}, m) = \underset{\mathbf{L}', m'}{\arg\min} \left\| d\left(\mathbf{k}\right) - \sum_{\mathbf{r}} m'(\mathbf{r}) e^{-\sum \mathbf{b} \cdot \left(\mathbf{L}'(\mathbf{r}) \mathbf{L}'(\mathbf{r})^T\right)} s(\mathbf{r}) e^{-j\mathbf{k} \cdot \mathbf{r}} \right\|_{2}^{2} + \lambda \phi(\mathbf{L}'(\mathbf{r}))$$
(3)

The last term on the right side is used to penalize negative diagonal entries in $\mathbf{L}'(\mathbf{r})$. In this study, we used a Non-Linear Conjugate Gradient (NLCG) approach to solve for (\mathbf{L} ,m). The Jacobian of this cost function is required for each iteration to determine search directions and perform 1D minimizations during NLCG optimization. A diagonal approximation to the Hessian is also calculated to speed up convergence. Analytical forms for the Jacobian and the diagonal Hessian can be evaluated efficiently using forward and inverse gridding operations. (*a*) *Phantom studies*: We used a computer phantom that contains two crossing rods and a circular ring (Fig 1). The diffusion is oriented along the rods and in the angular direction along the tangent of the ring. The eigenvalues were: $\lambda_1 = 1000 \times 10^6 \text{ mm}^2/\text{s}$. λ_2 and $\lambda_3 = 100 \times 10^6 \text{ mm}^2/\text{s}$. Synthetic k-space data were generated using 128 x 128 resolution, an interleaved spiral sequence with 4 interleaves and 6 diffusion encoding directions with b=800 s/mm². Simulations were carried out with simulated rotations of $\pm 20^0$ for each interleaf with probability of 0.5 each. Gaussian noise was added such that the SNR was 4. (*a*) *Post-processing*: Four methods were used to estimate **D** and *m* from k-space data: **A**) linear least squares estimation with motion correction; **C**) unconstrained NLCG with motion correction; **D**) constrained NLCG using Cholesky decomposition and motion correction. For method B, motion correction was accomplished by counter-rotating k-space trajectories, counter-rotating coil sensitivities and applying a linear phase to k-space data [7]. In addition to that, for methods C and D, the diffusion encoding matrix **b** was also rotated to account for the altered diffusion encoding direction. This change in the b-matrix from shot to shot was the main motivation for using a single step non-linear algorithm. In the presence of motion, $d(\mathbf{k})$, **b** and $s(\mathbf{r})$ in equation (3) are assumed to have been corrected for rot

RESULTS – Fig 1 shows the reconstructed color-coded FA maps (first row) and the locations of non positive definite tensors (second row) in each case. When there was no motion correction, the FA map showed serious motion artifacts (Fig 1b). Due to the high number of non positive definite tensors (Fig 1f), some of the FA values were above 1.0. After motion correction was applied using method B, the artifacts were significantly removed; however, some residual artifacts still remained because of the unaccounted change in diffusion encoding direction (Fig 1c). This is corrected by the application of method C. The tensor maps reconstructed with methods B and C show high number of non positive definite tensors (Fig 1g,h). The application of method D significantly reduced the number tensors that are not positive definite (Fig 1i). It should also be noticed that the FA map reconstructed with method D has slightly lower noise compared to the FA map reconstructed with method C. The mean angular deviation of the major eigenvectors from the true orientations was 14.1° for method B, 8.8° for method C and 9.1° for method D.

DISCUSSION – A novel non-linear single-step tensor estimation scheme that utilizes Cholesky decomposition to ensure the positive-definiteness of the diffusion tensors is introduced. The method is shown to be effective in obtaining accurate diffusion tensors in the presence of high noise. In case when rotational motion is present, significant improvements over the conventional tensor estimation schemes were obtained by simultaneously correcting for misregistration and change in diffusion-encoding direction between shots. Thus, the proposed method is especially useful for high resolution DTI scans where motion and noise are important issues. **References** [1] Skare et al, MRI, 18:659–669, 2000 [2] Koay et al, MRM, 55:930–936, 2006 [3] Batchelor et al, MRM, 53:221–225, 2005 [4] Wang et al, IEEE Trans. Med. Imag, 23,8:930-939 [5] D. Tschumperle et al, Lecture Notes in Computer Science, 2809:530–541, 2003. [6] Niethammer et al, IEEE EMBS, 2006 [7] Bammer et al, MRM, 57:90-102, 2007 **Acknowledgements** This work was supported in part by the NIH (2R01EB002711, 1R21EB006860), the Center of Advanced MR Technology at Stanford (P41RR09784), Lucas Foundation and Oak Foundation.