

Greedy NNLS: Fiber Orientation Distribution From Non-Negatively Constrained Sparse Recovery

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Target Audience: Clinicians and scientists wishing to map WM fibers using a robust Fiber Orientation Distribution (FOD) from minimal DTI like acquisitions.

Purpose: The FOD¹ is a robust model for mapping crossing WM fibers. However, its angular resolution depends on the spherical harmonic (SH) basis order, which can imply a large number of acquisitions: 45, 66, 91 for orders 8, 10, 12. Further, it is necessary to compute the maxima of the SH-FOD to derive the fiber directions¹. To kill the two proverbial birds with a single stone, a non-negatively constrained sparse recovery was proposed for estimating FODs using Non-Negative Least-Squares (NNLS)² and was used to estimate 24th order FOD tensors from 32 acquisitions.

Here, we experimentally validate and discuss the merits of the NNLS for the constrained sparse recovery of the FOD and compare it with classical l1-minimization. We confirm results from literature³ to show that NNLS converges to highly sparse solutions which are correctly constrained, while classical l1-minimization is less sparse, contains negative solutions and is unstable with noisy data. Finally, we discuss the NNLS algorithm and attribute the sparsity to its design, which mirrors the design of Orthogonal Matching Pursuit (OMP). We conclude that it is the NNLS's iterative greedy scheme, also the characteristic of OMP, which results in the recovery of a sparse support for the NNLS solution.

Methods: In [2], a single fiber orientation (delta) function was modelled as a rank-1 tensor of order $2n$, $C = \lambda c^{(\times)2n}$, the FOD as a decomposable tensor parameterized as the sum of r (unknown) rank-1 tensors²: $F = \sum C_i$, and the response function $R(\mathbf{q}, \mathbf{u})$, as a Watson kernel estimated from voxels with high FA (>0.8). The problem of FOD estimation was posed as a constrained LS problem: **(Eq-1)** $\min_{\mathbf{w}} \|\mathbf{B}\mathbf{w} - \mathbf{s}\|_2^2$ st. $\mathbf{w} \geq 0$, with \mathbf{w} a 321-D-vector corresponding to an initial estimate of $r_0=321$. Finally, **Eq-1**, was solved with an additional sparsity constraint on \mathbf{w} to also estimate the correct number of fibers r . This was accomplished by using NNLS.

However, sparsity problems are in general solved using methods such as l1-minimization^{6,7,3} or OMP⁵ variants. Here we compare l1-minimization⁷, which guarantees sparsity but not non-negativity, for the FOD estimation, with the NNLS approach, which offers non-negativity and experimentally also sparsity^{2,3}. In keeping with [3,7], we formulate three problems out of **Eq-1**: **(P1)** $\min_{\mathbf{w}} \|\mathbf{w}\|_1$ st. $\mathbf{B}\mathbf{w} = \mathbf{s}$; **(P2)** $\min_{\mathbf{w}} \|\mathbf{w}\|_1$ st. $\|\mathbf{B}\mathbf{w} - \mathbf{s}\|_2 \leq \epsilon$ (to account for noise); and **(P3)** **Eq-1** solved by NNLS. **(P1)** & **(P2)** use l1-minimization but do not account for $\mathbf{w} \geq 0$, whereas **(P3)** accounts for $\mathbf{w} \geq 0$ but not sparsity explicitly. We test on synthetic data generated from a bi-tensor model², with the single fiber's FA=0.8, $b=1500s/mm^2$ and 32 acquisitions. We consider both noise-free signal and signal corrupted by Rician noise with SNR=20 (and 50 tests).

Results: We vary the crossing angles from 90°-0° but only present results for 45°. We estimate 24th order FOD tensors and present the “raw” sparsity of \mathbf{w} from the three problems without any heuristic cleaning².

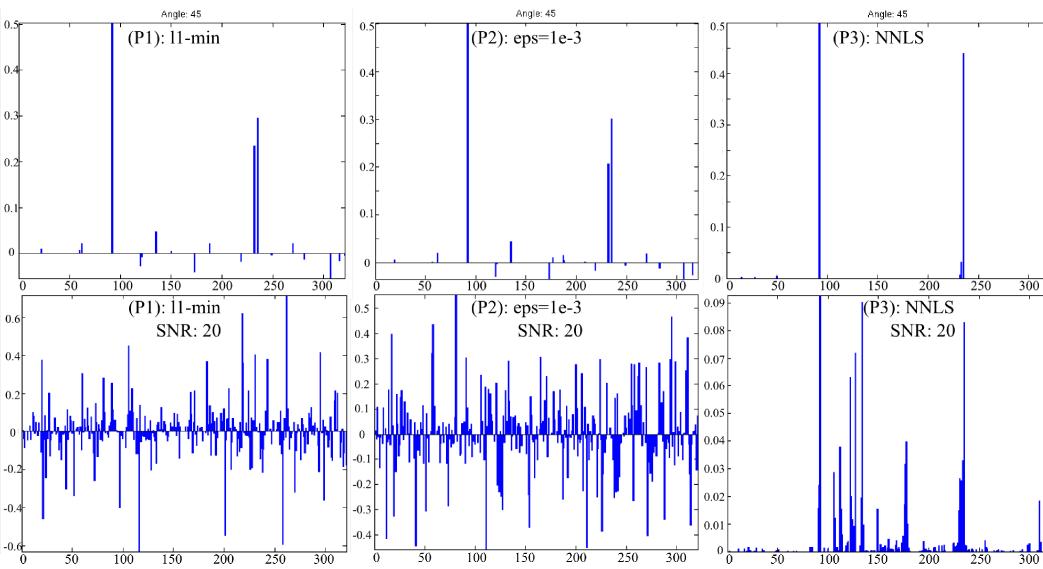


Fig. 1: (The x-axis represents the 321-coordinates of \mathbf{w} , the y-axis the value of w_i). The first row presents the results on noise-free signal. **(P1)** & **(P2)** generate, as expected, near identical, sparse solutions containing negative weights, although these are almost insignificant. However, **(P3)** generates a non-negatively constrained solution, which is considerably sparser. This is in agreement with [3]. In each case there are clearly two “main” weights in \mathbf{w} which correspond to the two fibers crossing at 45°. The second row presents the results on the signal corrupted by noise and the sparsity displayed in this row is the average of 50 tests. In this case the classical l1-minimization is at a clear disadvantage. Both **(P1)** & **(P2)** generate non-sparse solutions with significant negative weights. It is also hard to distinguish any “main” weights in \mathbf{w} in both cases. **(P3)** on the other hand is clearly more robust to noise. It still generates non-negatively constrained solutions that remain considerably sparse and it is still possible to distinguish two major weights in spite of the effects of noise. Clearly NNLS is the method of choice in this case.



Fig. 2: 24th order FOD tensors estimated from the noise-free signal with varying crossing angles from 90°-0° in steps of 3°. Crossings are detected till 23°.

Discussion: In **Fig. 1**, the sparsity demonstrated by NNLS in its solutions is surprising since NNLS does not explicitly account for it. This begs an explanation and a closer inspection of the NNLS algorithm. **Eq-1**, at its face value, contains 321 non-negativity (inequality) constraints and one could think of solving it naively using constrained optimization. However, the NNLS algorithm⁴ uses an active set strategy which proceeds iteratively, incrementally solving the LS functional of **Eq-1** by grabbing the greediest support at each step while respecting the corresponding inequality constraint. It begins with the initial solution $\mathbf{w}_0 = \mathbf{0}$, and all (321) constraints being active. Then in each iteration it greedily searches for a support in the active set that minimizes the LS functional the most and makes this constraint passive. However, since this could result in one or more constraint violations in the passive set, it then iterates through the passive set to find the best compromise which satisfies the constraints and updates the active and passive set of constraints.

This iterative greedy strategy of NNLS closely mirrors the greedy strategy of the OMP algorithm⁵. In fact, OMP as a heuristic algorithm has been successfully used in literature to recover solutions constrained to be sparse, because it begins with a $\mathbf{0}$ vector solution and iteratively proceeds to incrementally add the greediest support in each iteration that best minimizes its functional. This iterative greedy strategy results in a sparse solution.

Not surprisingly, therefore, the NNLS also results in a sparse solution – the only difference between NNLS and OMP being that OMP does not constrain its support to be non-negative. NNLS, therefore, heuristically results in a sparse solution that is also non-negative.

Conclusion: We experimentally compared the NNLS to classical l1-minimization for the estimation of FOD formulated as a non-negatively constrained sparse recovery problem². In agreement with the literature³, we found NNLS superior to l1-minimization in sparsity and robustness to noise. Finally we attributed the sparsity of NNLS to its iterative greedy design⁴. This mirrors the design of OMP and its variants⁵, which are historically proven heuristic methods popularly used for sparse recovery.

References: [1] Tournier et al. *NeuroImage* 35:1459–1472 (2007); [2] Ghosh et al. *ISBI* 254—257 (2013); [3] Jian & Vemuri *TMI* 26:1464—1471 (2007); [4] Lawson & Hanson (*Solving Least Squares Problems*), Prentice-Hall (1974); [5] Blumensath & Davies (*On the difference between orthogonal matching pursuit and orthogonal least squares*). *Tech. Rep. U. of Edinburgh*, (2007); [6] Landman et al. *NeuroImage* 59(3):2175—2186 (2012). [7] Candes & Romberg (www.l1-magic.org).