Simultaneously resolve haemodynamic response function and activation response by rank-constrained optimization

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Target Audience: Neuroscience, fMRI, numerical algorithm design

Purpose: Simultaneously resolve haemodynamic response function (HRF) and activation response. Introduction of a fast algorithm for exactly solving rank-constrained optimization problems.

Researchers are moving towards neurodegenerative patients, children, and infants whose HRFs deviate from canonical form (1-4). Using canonical HRF for analysis cannot, therefore, yield optimal results. A goal of this work is to resolve HRF concurrently with activation analysis. Our proposed method is the first directly minimizing rank of an indefinite matrix by convergent iteration. Further, the Matlab implementation is fast (Table 1) and recovers response magnitudes and HRF coefficients near perfectly.

Methods: Following the formulation in (5), let $y = X\,\mathrm{vec}(h\beta^{\mathrm{T}}) + P\omega + \varepsilon$ be an observed fMRI time series where X is the design matrix, h is the HRF, β is a vector of response coefficients, P is a matrix of confounds (drift, motion), ε is a noise vector, and vec is the matrix vectorization operator (Fig 1). To simplify calculation, we assume data is precorrected for drift and motion **(**a simple task using software like FSL (6)**)** and that noise ε is uncorrelated **(**correlated cardiac and respiratory noise can easily be incorporated into design matrix X if physiological monitoring was in place during scanning**)**. The task, as in (5), is to solve an optimization problem $\underset{h,\beta}{\arg\min}\ \|y - X\,\mathrm{vec}(h\beta^{\mathrm{T}})\|^2$ which is made difficult by the products of variables. Rectangular matrix $h\beta^{\mathrm{T}}$ is rank 1 because a scaled replica of h comprises each column.

We express h as a linear combination of basis functions, i.e., $h = Q\alpha$. Basis functions used in this study are the canonical HRF and its first five derivatives. (Other basis options include FIR and Wavelet.) The optimization problem is transformed as Eqn 1. Vectorization operator vec (Fig 1) and its inverse are linear and uniquely invertible. The constraint $G \succcurlyeq 0$ means positive semidefinite. $\mathrm{rank}(G) = 1$ implies $\mathrm{rank}(H) = 1$ which is the only nonconvex constraint. The key to solving this semidefinite rank 1 problem is by transforming it to an equivalent sequence of convex optimization problems as in Eqn 2 (7,ch.4). Direction matrix W is a constant updated in each iteration (Fig 2). At optimality, $H = h\beta^{\mathrm{T}}$. Once optimal H is found, h and β can be resolved by singular value decomposition.

The proposed algorithm was tested by Matlab simulation on a 1.8GHz Duo CPU 4GB PC. Table 1 lists various test parameters. Each test was run 1000 times. During each run, weights α of the basis functions, event onset time, and activation response (β) were randomly chosen.

$$\begin{aligned}&\underset{H,Y,Z}{\text{find}} && H\\ &\text{subject to} && X\,\mathrm{vec}(H) = y\\ &&& G = \begin{bmatrix} Y & H\\ H^{\mathrm{T}} & Z\end{bmatrix}\\ &&& \mathrm{rank}(G) = 1\\ &&& G \succcurlyeq 0\end{aligned}$$

Eqn 1

$$\begin{aligned}&\underset{H,Y,Z}{\text{minimize}} && \mathrm{trace}(W^{\mathrm{T}}G)\\ &\text{subject to} && X\,\mathrm{vec}(H) = y\\ &&& G = \begin{bmatrix} Y & H\\ H^{\mathrm{T}} & Z\end{bmatrix}\\ &&& G \succcurlyeq 0\end{aligned}$$

Eqn 2

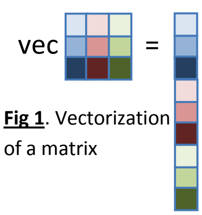

Fig 1. Vectorization of a matrix

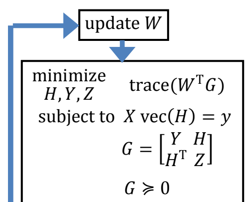

Fig 2. Flow chart of rank minimization method.

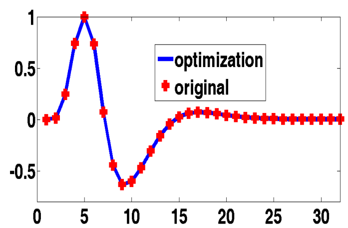

Fig 3. Rank-1 minimization recovers original HRF.

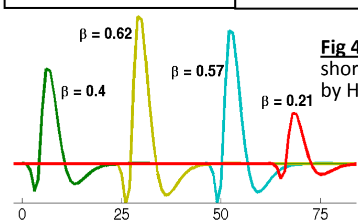

Fig 4. Response to each short stimulus is smoothed by HRF and weighted by β.

Table1: Average W iterations for 1000 simulations.

Length of h, Length of y, Number of impulsive events in stimuli	32, 256, 20	32, 512, 20	32, 512, 60	40, 320, 40
Average number of iterations of W	2	1	2	2

Results: Table 1 gives the average number of W iterations when solving each rank minimization problem. Figure 3 shows a typical result with length(h)=32. The result labeled '`optimization`' illustrates near perfect recovery of the original HRF (up to a scaling factor). In all runs, we achieved over 99.9% accuracy in recovering h and β.

Discussion: We presented a one-step process to simultaneously resolve HRF and quantify activation by rank minimization. This is a hard problem because a rank constraint is nonconvex (Eqn 1). We were able to directly solve it by substituting a direction matrix W for the rank constraint. For each iteration, W is fixed and then $\mathrm{trace}(W^{\mathrm{T}}G)$ is minimized. Matrix W is updated per iteration as in (7,ch.4) so that $\mathrm{trace}(W^{\mathrm{T}}G)$ converges to 0 (a global optimality condition). We reduced the required number of iterations (accelerated convergence) by extrapolation of direction vector W if found to be traveling in a linear direction.

Conclusion: We presented an optimization technique that quantifies subjects' response to fMRI stimuli and resolves their HRF during the same process. This technique holds great promise in studies involving a population whose HRF is different from the canonical design which is best suited for healthy adults. The novelty of our technique is that we solve a rank constrained (nonconvex) problem by reformulating it as a sequence of convex problems. We were able to accelerate computation speed to an average of 1 to 2 iterations per problem while resolving HRF with almost perfect accuracy.

References 1. Glover, Neuroimage 9(4):416–429. 2. Amemiya et al, Neuroimage 61(3):579-90. 3. Jacobs et al, Neuroimage 40(2):601–614. 4. Masterton et al, Neuroimage 51(1):252-60. 5. Pedregosa et al, 3rd Int Workshop Pattern Recognition Neuroimaging, May 2013. 6. fmrib.ox.ac.uk/fsl 7. Dattorro, *Convex Optimization and Euclidean Distance Geometry*.