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Solution of a complex least squares problem with constrained phase

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ABSTRACT

The least squares solution of a complex linear equation is in general a complex vector with independent real and imaginary parts. In certain applications in magnetic resonance imaging, a solution is desired such that each element has the same phase. A direct method for obtaining the least squares solution to the phase constrained problem is described.

1. Introduction

Consider the following linear equation given in the following equation:

$$\mathbf{Ax} = \mathbf{b} \tag{1}$$

where $\mathbf{A}$ is a complex $m \times n$ matrix, $\mathbf{b}$ is a complex m-vector and $\mathbf{x}$ is a complex n-vector. The minimum norm least squares solution to Eq. (1) has $2n$ parameters: the real and imaginary parts of $\mathbf{x}$, which may also be represented in polar form as the amplitude and phase. However in certain applications, it is reasonable to expect the phase paramenter for all elements of the solution to be the same and thus a phase constrained solution is desired.

This is a nonlinear optimization problem and has been studied previously using iterative Gauss–Newton search [1]. The present study derives an alternate, direct method for solving the phase constrained problem in which the minimum norm least squares solution is obtained such that the phase of every element of $\mathbf{x}$ is identical.

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2. Direct method

A solution of the desired form is assumed, $\mathbf{x}_{real}e^{i\phi}$, which comprises a real n-vector $\mathbf{x}_{real}$ and a real scalar ϕ. Eq. (1) is then re-written as in the following equation:

$$\mathbf{A}\mathbf{x}_{real}e^{i\phi} = \mathbf{b} \tag{2}$$

The goal is to minimize the sum of squares of the residual $\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{x}_{real}e^{i\phi}$ over $\mathbf{x}_{real}$ and ϕ. Using separable least squares [2] to isolate the linear terms, $\mathbf{x}_{real}$ can be obtained for any ϕ by equating $d(\mathbf{r}^{\mathrm{H}}\mathbf{r})/d\mathbf{x}_{real}$ to zero. This leads to the expression $\mathbf{M}\mathbf{x}_{real} = Re(\mathbf{A}^{\mathrm{H}}\mathbf{b}e^{-i\phi})$, where $\mathbf{M} \equiv Re(\mathbf{A}^{\mathrm{H}}\mathbf{A})$. The pseudoinverse $\mathbf{M}^{\dagger}$ yields the minimum norm least squares solution:

$$\hat{\mathbf{x}}_{real} = \mathbf{M}^{\dagger}Re(\mathbf{A}^{\mathrm{H}}\mathbf{b}e^{-i\phi}) \tag{3}$$

Note that the rank and condition number of $\mathbf{M}$ are not necessarily the same as those of $\mathbf{A}^{\mathrm{H}}\mathbf{A}$; in particular, $\mathbf{M}$ can have full rank even when $\mathbf{A}^{\mathrm{H}}\mathbf{A}$ does not.

Now the residual can be expressed as function of ϕ only and it remains to minimize $\mathbf{r}^{\mathrm{H}}\mathbf{r}$ over ϕ.

$$\mathbf{r} = \mathbf{b} - \mathbf{A}\mathbf{M}^{\dagger}Re(\mathbf{A}^{\mathrm{H}}\mathbf{b}e^{-i\phi})e^{i\phi} \tag{4}$$

Making use of the identities $\mathbf{A}^{\mathrm{H}}\mathbf{A} = \mathbf{M} + iIm(\mathbf{A}^{\mathrm{H}}\mathbf{A})$ and $\mathbf{M}^{\dagger}\mathbf{M}\mathbf{M}^{\dagger} = \mathbf{M}^{\dagger}$ and dropping imaginary terms (since $\mathbf{r}^{\mathrm{H}}\mathbf{r}$ is real):

$$\mathbf{r}^{\mathrm{H}}\mathbf{r} = \mathbf{b}^{\mathrm{H}}\mathbf{b} - Re(\mathbf{A}^{\mathrm{H}}\mathbf{b}e^{-i\phi})^{\mathrm{T}}\mathbf{M}^{\dagger}Re(\mathbf{A}^{\mathrm{H}}\mathbf{b}e^{-i\phi}) \tag{5}$$

Equating $d(\mathbf{r}^{\mathrm{H}}\mathbf{r})/d\phi$ to zero yields the condition for obtaining a minimum.

$$-2Im(\mathbf{A}^{\mathrm{H}}\mathbf{b}e^{-i\phi})^{\mathrm{T}}\mathbf{M}^{\dagger}Re(\mathbf{A}^{\mathrm{H}}\mathbf{b}e^{-i\phi}) = 0 \tag{6}$$

Eq. (6) can be seen to be the imaginary part of $(\mathbf{A}^{\mathrm{H}}\mathbf{b})^{\mathrm{T}}\mathbf{M}^{\dagger}(\mathbf{A}^{\mathrm{H}}\mathbf{b})e^{-2i\phi}$. For the imaginary part of this expression to be zero, the overall phase must be zero which requires:

$$\hat{\phi} = \frac{1}{2}\angle(\mathbf{A}^{\mathrm{H}}\mathbf{b})^{\mathrm{T}}\mathbf{M}^{\dagger}(\mathbf{A}^{\mathrm{H}}\mathbf{b}) \tag{7}$$

The least squares solution to the phase constrained problem is thus $\hat{\mathbf{x}}_{real}e^{i\hat{\phi}}$ with the phase given by Eq. (7) and the real vector given by Eq. (3).

3. Application to magnetic resonance imaging

In magnetic resonance imaging, the separation of water and fat signals commonly makes use of the characteristic resonant frequencies of protons in water and fat molecules [3,4,5]. Differences in frequency come about because of electron shielding around the various functional groups (–OH, $-CH_2$, $-CH_3$, etc.), that cause protons to experience slightly different magnetic fields, typically several parts per million of the main field.

Data are sampled at three time points to observe the change in signal. The relevant matrix for this situation is given by Eq. (8), taking sampling times from Ref. [3] and the fat spectrum from Ref. [5].

$$\mathbf{A} = \begin{bmatrix} 1.000 & 0.881 - 0.443i \\ 1.000 & 0.119 + 0.895i \\ 1.000 & -0.701 - 0.381i \end{bmatrix} \tag{8}$$

Simulated data were generated for range of water and fat combinations with water + fat = 1 and phase 0. Gaussian random noise with standard deviation 0.1 was added to the real and imaginary parts. Estimates were calculated using unconstrained linear least squares and by phase constrained least squares. The means and standard deviations of the estimated parameters were computed from 10^6 trials. Table 1 indicates mean values are identical for both methods but the standard deviations are up to 41% higher when using the unconstrained method.

Table 1 Simulation results for the unconstrained and phase constrained estimation of water and fat based on Eq. (8). Results indicate mean values are identical for both methods while standard deviations are up to 41% higher in the unconstrained case.

Water fat	Mean (unconstrained)	Mean (constrained)	SD (unconstrained)	SD (constrained)	Ratio
1.0	$1.000 - 0.000i$	$1.000 - 0.000i$	0.0822	0.0820	1.002
0.0	$0.000 - 0.000i$	$-0.000 - 0.000i$	0.0914	0.0649	1.408
0.8	$0.800 + 0.000i$	$0.800 + 0.000i$	0.0822	0.0801	1.026
0.2	$0.200 - 0.000i$	$0.200 - 0.000i$	0.0914	0.0664	1.376
0.6	$0.600 - 0.000i$	$0.600 + 0.000i$	0.0822	0.0751	1.094
0.4	$0.400 - 0.000i$	$0.400 - 0.000i$	0.0914	0.0722	1.266
0.4	$0.400 - 0.000i$	$0.400 + 0.000i$	0.0822	0.0670	1.227
0.6	$0.600 - 0.000i$	$0.600 - 0.000i$	0.0914	0.0814	1.123
0.2	$0.200 + 0.000i$	$0.200 + 0.000i$	0.0822	0.0603	1.363
0.8	$0.800 + 0.000i$	$0.800 + 0.000i$	0.0914	0.0884	1.034
0.0	$0.000 - 0.000i$	$0.000 + 0.000i$	0.0822	0.0584	1.408
1.0	$1.000 + 0.000i$	$1.000 + 0.000i$	0.0914	0.0912	1.002

4. Conclusion

A direct method has been derived for solving a complex least squares problem with constrained phase. In application to water/fat separation in magnetic resonance imaging, the advantage over linear least squares is reduced standard deviation in the estimated parameters.

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