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Image regularization by nonnegatively constrained Conjugate Gradient

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ABSTRACT

In the image reconstruction context the nonnegativity of the computed solution is often required. Conjugate Gradient (CG), used as a reliable regularization tool, may give solutions with negative entries, particularly when large nearly zero plateaus are present. The active constraints set, detected by projection onto the nonnegative orthant, turns out to be largely incomplete leading to poor effects on the accuracy of the reconstructed image. In this paper an inner-outer method based on CG is proposed to compute nonnegative reconstructed images with a strategy which enlarges subsequently the active constraints set. This method appears to be especially suitable for the reconstruction of images having large nearly zero backgrounds. The numerical experimentation validates the effectiveness of the proposed method when compared to other strategies for nonnegative reconstruction.

1. Introduction

A Fredholm integral equation of the first kind

$$g(s) = \int \widehat{K}(s,t) f(t)\, dt \tag{1}$$

is often used for modeling the image formation process, where $f(t)$ and $g(s)$ represent a real object and its image, respectively. The kernel $\widehat{K}(s,t)$, called the *point spread function* (PSF) and assumed to be square integrable, represents the imaging system and is responsible for the blurring of the image. In practical applications the *blurred image* $g(s)$ is not available, being replaced by a finite set $\mathbf{g}$ of measured quantities, and is degraded by the noise which affects the process of image recording. Hence the problem of restoring $f(t)$ from $\mathbf{g}$ is an ill-posed problem. The linear system obtained by the discretization of (1) inherits this feature, in the sense that the resulting matrix is severely ill-conditioned, and regularization methods must be used to solve it [2,14,24]. This kind of problem arises for example in the reconstruction of astronomical images taken by a telescope and of medical and microscopy images.

One of the main features of the problem is the nonnegativity of the functions involved in (1). When discretized, the equation leads to a linear problem whose solution is constrained to be nonnegative. Iterative methods applied as regularization techniques may give solutions with negative entries. A projection onto the nonnegative orthant may have poor effects

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on the accuracy of the reconstructed image. In this paper an inner-outer method based on CG is proposed to compute nonnegative reconstructed images with a strategy which enlarges subsequently the active constraints set. This method appears to be especially suitable for images having large zero backgrounds. For this type of problems, one naturally wonders if the zeros of the original image are correctly reconstructed. As a matter of fact, an algorithm can fail by putting to zero nonzero values of the original image (false positive) or by giving nonzero values in correspondence to zero values of the original image (false negative). This behavior will be analyzed using the well-known measures of Information Retrieval, namely the F_1 score [22], which takes into account both types of errors.

The outline of the paper is the following: first, in Section 2 the problem under consideration is introduced and in Section 3 some strategies for nonnegative regularization present in the literature are recalled. In Section 4 our proposed inner-outer algorithm is motivated and described. In Section 5 the results of a numerical experimentation which compares the performance of our algorithm with those of four chosen methods are presented and discussed.

Notation: Throughout the paper, $\|\boldsymbol{v}\|$ denotes the Euclidean norm of the vector $\boldsymbol{v}$, i.e. $\|\boldsymbol{v}\|^2 = \boldsymbol{v}^T\boldsymbol{v}$. The elementwise multiplication and division between two vectors are denoted by $\odot$ and $\oslash$.

2. The problem

Let $\widehat{\boldsymbol{b}} = A\widehat{\boldsymbol{x}}$ be the discretized version of Eq. (1). In image reconstruction problems the N-vector $\widehat{\boldsymbol{x}}$ stores columnwise the pixels of an $n \times n$ original object, with $N = n^2$, and $\widehat{\boldsymbol{b}}$ analogously stores the blurred image. The imaging system is represented by a large not necessarily square matrix A, often severely ill-conditioned with singular values decaying to zero without significant gap to indicate numerical rank. The matrix A might not be explicitly available, as long as the products $A\boldsymbol{x}$ and $A^T\boldsymbol{x}$ are computable for any vector $\boldsymbol{x}$. A common special case is the one which occurs when the PSF is bandlimited space invariant, i.e. invariant with respect to translations and with a bounded support, and A is a square 2-level Toeplitz matrix with a limited bandwidth. Moreover, it may happen that the image has sufficiently large zero background along the boundary, so that periodic boundary conditions can be safely imposed. In this case A becomes a 2-level circulant matrix and the matrix-by-vector product can be computed by low cost Fourier transforms. This is the structure we assume for our numerical examples, but the proposed algorithm can be applied equally well to general matrices A.

In practical problems vector $\widehat{\boldsymbol{b}}$ is not exactly known, because it is contaminated by measurement inaccuracies or discretization. Hence only a noisy image $\boldsymbol{b} = \widehat{\boldsymbol{b}} + \boldsymbol{\eta}$ is available, where the noise level is measured by

$$\eta = \frac{\|\boldsymbol{b} - \widehat{\boldsymbol{b}}\|}{\|\widehat{\boldsymbol{b}}\|}, \tag{2}$$

and in some cases can be roughly estimated. The system to be solved is thus

$$A\boldsymbol{x} = \boldsymbol{b}. \tag{3}$$

In this paper we consider the case where the entries of the noise vector $\boldsymbol{\eta}$ are normally distributed with zero mean and normalized in such a way that η ranges in a given interval.

The ith component of the vectors $\widehat{\boldsymbol{x}}$, $\widehat{\boldsymbol{b}}$ and $\boldsymbol{b}$ represents respectively the light intensity or the radiation emitted by the ith pixel of the object, arriving at the ith pixel of the blurred image and recorded in the ith pixel of the noisy image. The component a_{ij} of matrix A measures the fraction of the light or of the rays emitted by the ith pixel of the object which arrives at the jth pixel of the image. Because of the ill-conditioning of A and of the presence of the noise, the solution $A^\dagger\boldsymbol{b}$ of (3), where $A\dagger$ is the Moore–Penrose generalized inverse, may be quite different from the original image $\widehat{\boldsymbol{x}}$.

All the quantities involved in the problem, i.e. A, $\widehat{\boldsymbol{x}}$, $\widehat{\boldsymbol{b}}$ and $\boldsymbol{b}$, are assumed componentwise nonnegative. Actually, when simulated test problems are considered for the experimentation, negative entries of $\boldsymbol{b}$ could arise corresponding to very small nonnegative entries of $\widehat{\boldsymbol{b}}$. In this case the vector $\boldsymbol{b}$ is further projected onto the nonnegative orthant. Anyway, it is reasonable to expect the approximation of $\widehat{\boldsymbol{x}}$ obtained by solving (3) to be nonnegative. The constrained *least squares* approximation to the solution $\widehat{\boldsymbol{x}}$ is given by

$$\boldsymbol{x}_{ls} = \underset{\boldsymbol{x} \geq \boldsymbol{0}}{\operatorname{argmin}}\ \phi(\boldsymbol{x}), \quad \text{where} \quad \phi(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{b} - A\boldsymbol{x}\|^2. \tag{4}$$

The gradient of $\phi(\boldsymbol{x})$ is $\text{grad}_x\,\phi(\boldsymbol{x}) = A^TA\boldsymbol{x} - A^T\boldsymbol{b} = -A^T\boldsymbol{r}$, where $\boldsymbol{r} = \boldsymbol{b} - A\boldsymbol{x}$ is the residual vector. The function $\phi(\boldsymbol{x})$ is convex and its minimum points are found by solving the system $\text{grad}_x\,\phi(\boldsymbol{x}) = 0$, i.e. the so-called *normal equations*

$$A^TA\boldsymbol{x} = A^T\boldsymbol{b}. \tag{5}$$

Due to the large dimension of system (5) and to the presence of the noise $\boldsymbol{\eta}$, a regularization method must be employed, coupled with suitable strategies for enforcing nonnegativity. Iterative methods enjoying the semiconvergence property are often used. According to this property, an integer K exists for which the error attains a minimum. After the Kth iteration, the computed vectors $\boldsymbol{x}_k$ are progressively contaminated by the noise and move away from $\widehat{\boldsymbol{x}}$ toward $A^\dagger\boldsymbol{b}$ which can be largely different from $A^\dagger\widehat{\boldsymbol{b}}$. A good terminating procedure is hence needed to detect the correct index K where to stop the iteration.

In the following we assume that both $A\boldsymbol{x} \neq \boldsymbol{0}$ and $A^T\boldsymbol{x} \neq \boldsymbol{0}$ for any $\boldsymbol{x} \geq \boldsymbol{0}$ with $\boldsymbol{x} \neq \boldsymbol{0}$, and that $A\boldsymbol{e} > \boldsymbol{0}$ and $A^T\boldsymbol{e} > \boldsymbol{0}$, where $\boldsymbol{e}$ is the vector of all ones (i.e. the sums by rows and columns of A are all nonzero).