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TITLE: INVERSE PROBLEMS SVD AND PSEUDO SVD

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INVERSE PROBLEMS SVD AND PSEUDO SVD

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Running head: NEED

Abstract. Physical experiments often give rise to integral equations of the first kind. If the detection equipment can be adjusted that fact can lead to a kernel function that depends on one or more parameters. We address the general question of how to choose those parameters in such a way as to make the integral operator as well-conditioned as possible, thus optimizing the experiment. Attention is focused on the condition number of the discretized kernel and on its principal singular vector. Several examples are given and some preliminary general results are obtained.

1. Introduction. In many areas of diagnostic physics linear integral equations of the first kind arise:

$$g(x) = \int_a^b K(x,y)f(y)dy \tag{1.1}$$

In (1.1) $K(x,y)$ represents the response of a detector (or a set of detectors) g is the measured data (usually containing experimental error) and f is the "signal" which is to be found.

Often there are experimental techniques which make possible the construction of "families" of detectors. For instance, different foil thicknesses may be employed, different mirror angles may be used, chemical compositions may be varied, specific diodes may be chosen, etc. Thus $K(x,y)$ while it must, in order to perform the experiment, have certain properties, can depend on a variety of parameters. In practice, these parameters are often chosen arbitrarily, or by some "time-honored rules-of-thumb." Our goal here is to try to devise mathematical methods by which to select such parameters in order to make the experiment as efficient as possible.

In many practical situations a prediction $F_p(y)$ of the signal $F(y)$ is available. This estimate is based on the basic physics involved, past experiences, and often, the skill and insight of the experimenter. It is reasonable to use this prediction in making the choice of detector parameters.

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Usually (1.1) is solved approximately by replacing it with a matrix equation

$$\mathbf{g} = \mathbf{K}\mathbf{F} \tag{1.2}$$

obtained by some discretation scheme [ ]. In (1.2) $\mathbf{K}$ may be $M \times N$, with $\mathbf{F}$ an N vector and $\mathbf{g}$ an M vector. We shall concentrate on (1.2).

A general rule is that the condition number C of $\mathbf{K}$ should be as small as possible. This minimizes the effect of experimental errors in $\mathbf{g}$. Thus a valuable parameter should be selected so as to minimize C.

2. A Practical Example. Consider the kernel

$$K(x,y) = \begin{cases} 0 \ , & 0 \le y \le \gamma(x) - \left(\dfrac{\alpha(x)}{\beta(x)}\right)^{1/2} \ , \\ \alpha(x) - \beta(x)(y-\gamma(x))^2 \ , & \gamma(x) - \left(\dfrac{\alpha(x)}{\beta(x)}\right)^{1/2} \le y \le \gamma(x) \ , \\ \delta(x)\exp(-\eta(x)(y-\gamma(x)) \ , & \gamma(x) \le y \le 1 \ . \end{cases} \tag{2.3}$$

Here each of the functions $\alpha, \beta, \gamma, \delta, \nu$ is constant over a given interval $x_i \le x < x_{i+1}$, $i = 1,2,3,4,5$. Thus

$$\alpha(x) = \alpha_i \ , \quad x_i \le x < x_{i+1} \ ,$$

etc. The α_i, β_i, γ_i, δ_i, η_i constitute the parameter set, subject to many physical constraints. We thus wish to minimize the condition number of the associated matrix $\mathbf{K}$ by varying the parameter set.

The kernel $K(x,y)$ in (2.1) arises in certain x-ray spectroscopy experiments. Obviously, the problem of minimizing C is a formidable one. However, it may be argued that the analysis may be more easily carried out mathematically than by building many pieces of equipment. Such a study is undertaken in [ ]. It is found that often these experiments are designed in a fairly optimal way, indicating that many years of experience have led to reasonable "rules of thumb."

3. The Singular Value Decomposition Approach. It is known [ ] that $\mathbf{K}$ may be written as

$$\mathbf{K} = \mathbf{U}\Sigma\mathbf{V}^{\mathrm{T}} \tag{3.4}$$

where $\mathbf{U}$ and $\mathbf{V}$ are unitary matrices and Σ is a diagonal matrix. Equation (3.1) is the so called singular value decomposition of $\mathbf{K}$. The columns $\mathbf{u}_i$ and $\mathbf{v}_i$ of $\mathbf{U}$ and $\mathbf{V}$ are the singular vectors of $\mathbf{K}$ and the elements σ_i of Σ are its singular values. If (1.2) has a solution $\mathbf{F}$ then that solution is given by

$$\mathbf{F} = \Sigma_{\mathrm{i=1}}^{\mathrm{M}} \frac{\mathbf{g}, \mathbf{u}_\mathrm{i}}{\sigma_\mathrm{i}} \mathbf{v}_\mathrm{i} \tag{3.5}$$

where (,) is the usual scalar product.

Equation (3.2) immediately indicates problems which can arise when g contains experimental error. If any of the σ_i are small (it is customary to order them by decreasing magnitude) the term

$$(g, u_i)/\sigma_i \tag{3.6}$$

is "mainly" error, and F will be seriously in error. (Note that if σ_i is "small" the condition number C will be large.) A common way of *partially* overcoming the difficulty is to truncate the series in (3.2) and simply ignore these troublesome σ_i values.

Equation (3.2) also suggests how use of the predicted signal $f_p(y)$—now the predicted vector $\mathbf{F_p}$—can be made. Observe that because $\mathbf{F_p}$ represents a signal it is non-negative. For convenience we suppose $\|\mathbf{F_p}\| = 1$. If $\mathbf{v_1} = \mathbf{F_p}$, and if $\mathbf{F_p}$ is a good prediction (than) the terms in (3.2) with $i > 1$ should contribute little to the sum. Thus the series truncation will be more valid. Our goal, then, is to try to adjust K, by judicious choice of the detector parameters, so as to obtain $\mathbf{v_1} = \mathbf{F_p}$.

4. Adjustment of the "Magnitude" of K. In practice it frequently happens that the "magnitude" or "height" of the detector is the parameter most easily adjusted. In the notation of (1.1) we replace $K(x, y)$ by $\phi(x)K(x, y)$ where ϕ is non-negative but otherwise (reasonably) arbitrary. In the matrix formulation we replace K by ϕK where ϕ is a non-negative diagonal matrix. K is here assumed $N \times N$.

We now ask that $\mathbf{F_p}$ be the first right singular vector of $\hat{\mathbf{K}} = \mathbf{phiK}$. It can be shown that [ ] in general

$$\mathbf{K^T K^S v_i} = \sigma_i \mathbf{v_i} \ . \tag{4.7}$$

Thus we desire

$$\hat{\mathbf{K}}^T \hat{\mathbf{K}} \mathbf{F_p} = \hat{\sigma}_i \mathbf{F_p} \ . \tag{4.8}$$

It will soon become obvious that we can select $\hat{\sigma}_1 = 1$ by adjusting ϕ. We rewrite (4.2):

$$(\phi \mathbf{K})^T \phi \mathbf{K} \mathbf{F}_p = \mathbf{K^T} \phi^2 \mathbf{K F_p} = \mathbf{F_p} \ . \tag{4.9}$$

Notice that $\mathbf{KF}_p$ is a known vector W. Thus

$$\mathbf{K^T S} = \mathbf{F_p} \ , \tag{4.10}$$

where

$$\mathbf{S} = \phi^2 \mathbf{W} \ . \tag{4.11}$$

Equation (4.5) can be solved for S. (Observe that there are no data errors involved.) Because K is associated with a detector its elements are non-negative. Hence

$\mathbf{W}$ is non-negative. If $\mathbf{S}$ is also non-negative then the elements of the diagonal matrix ϕ^2 are non-negative, and the matrix $\hat{\mathbf{K}} = \phi\mathbf{K}$ has the requisite property. That is, its first right singular vector is $\mathbf{F_p}$.

Of course, if ϕ^2 is *not* non-negative $\hat{\mathbf{K}}$ becomes complex and the physical meaning (e.g., changing the detector "height" is lost. In such an instance the device fails. Other detector parameters must be investigated.

5. Two Examples. EXAMPLE 1. Assume that

$$K_{ij} = \begin{cases} 0 , & j < i \\ \int_j^{j+1} e^{-x}dx = e^{-j} - e^{-(j+1)} , & j \geq i , \end{cases} \tag{5.12}$$

$$j = 1, 2, ..., 10 .$$

Suppose

$$F_{pi} = \frac{15}{\pi^4} \int_i^{i+1} \frac{px^3}{e^x - 1} dx \quad , i = \tag{5.13}$$

Using the approach described in the previous section we find the entries ϕ_{ii} of ϕ as presented in the first column of Table 1. Because they are all non-negative we can form $\hat{\mathbf{K}}$ as the matrix with entries

$$\hat{K}_{ij} = \phi_{ii} K_{ij} . \tag{5.14}$$

The physical experiment can now be performed with the detector(s) represented by $\hat{\mathbf{K}}$. The expected signal $\mathbf{F_p}$ is, of course, unchanged. it is unaffected by any modification in the detection equipment. The data $\hat{\mathbf{g}}$ will *not* be the same as if the original detector(s) (represented by $\mathbf{K}$) were used.

To demonstrate that the general approach can improve accuracy we assumed the *true* signal $\mathbf{F}$ to be given by $\mathbf{F_p} + \epsilon$ where

$$\epsilon_i = 6 \times 10^4 (11)(9 - 1) . \tag{5.15}$$

We then generated the corresponding data vectors $\mathbf{g}$ and $\hat{\mathbf{g}}$, added small amounts of random noise η and $\hat{\eta}$ to these data vectors, and retrieved the signal vector by solving $\mathbf{KF} = \mathbf{g} + \eta$ and $\hat{\mathbf{K}}\mathbf{F} = \hat{\mathbf{g}} + \hat{\eta}$. The results are shown in Table 2.

EXAMPLE 2. Let the matrix $\mathbf{K}$ be as in Example 1, but now assume a predicted signal whose first (five) components are the same as those of $\mathbf{F_p}$ in Example 1, but whose last four components are smaller:

$$F_p, i = 33.343 \int_i^{i+1} e^{-x^2/6} dx \quad , \quad i = 6, 7, 8, 9 . \tag{5.16}$$

when ϕ is computed in this case.

The elements are as shown in the second column of Table 1. Because several entries are negative the approach fails.

6. Preliminary Investigation of a Pseudo-Singular Value Decomposition. Ideally, the first column of V for some constructable K (that is, one corresponding to a set of acceptable parameters) would be F_p. (We always suppose $\| F_p \| = 1$.) This is usually too much to hope for. We ask if there are other orthogonal matrices P and Q and a diagonal matrix R such that

$$K = PRQ^T \tag{6.17}$$

where $q_1 = F_r$.

The answer is no; the decomposition (6.1) implies $P = U$ and $Q = V$. In an attempt to salvage something we try constructing P and Q in the following fashion.

Define q_1 by

$$Q_1 = F_p \tag{6.18}$$

and p by

$$KQ_1 = r_1 p_1 \ , \quad \| p_1 \| = 1 \ . \tag{6.19}$$

Observe that $r_1 p_1$ is the predicted data, which we anticipate will be nearly equal to q, the actual data.

Next, we construct a new vector q_2 such that

$$(q_1, q_2) = 0 \ , \quad \| q_2 \| = 1 \ , \tag{6.20}$$

and

$$(Kq_2, p_1) = 0 \tag{6.21}$$

Obviously there are many such vectors q_2; but there may be physical or mathematical reasons for a somewhat specific choice. We define p_2 and r_2 by

$$Kq_2 = r_2 p_2 \ , \quad \| p_2 \| = 1 \ . \tag{6.22}$$

The process can now be continued in a fairly obvious fashion until the number of components of q_i is less than the number orthogonality constraints. The vectors p_i and q_i are pseudo-singular vectors.

In the last analysis it is hoped that good approximations to F and g are

$$F \doteq \Sigma a_n q_n \ , \tag{6.23}$$

$$g \doteq \Sigma b_n p_n \ . \tag{6.24}$$

If this is the case

(6.25) $$KF = G$$

gives

(6.26) $$F \doteq \Sigma \frac{b_n}{r_n} q_n \ .$$

It is hoped that in practice only a very few terms in the sums are needed.

Some numerical experiments suggest that the number of sign changes in the components of q_i often increases faster than i. This emphasizes the desirability of very few terms in (6.6)-(6.8).

This approach is still in a very preliminary state, and much needs to be done. Simple examples suggest the method has promise.

7. Summary and Remarks. We have considered integral equations of the first kind which arise from experiments in diagnostic physics, and whose kernels depend upon parameters whose adjustment represents changes in the experimental setup. The ultimate goal has been to make the experiment as efficient as possible. Such mathematical studies can reduce the labor, time, and expense of actually adjusting—or even rebuilding—the experimental equipment.

We first examined an experiment in x-ray spectroscopy which leads to a kernel dependent on five parameters. Somewhat incomplete numerical studies were made in an effort to minimize the condition number of the matrix corresponding to the kernel. Thus our aim was to make the problem as well-conditioned as possible.

It was then observed that if the predicted signal (presumed to be a good estimate) in the experiment should happen to be equal to the principal singular vector of the matrix, the experiment should be close to optimal. We attempted to achieve this by multiplying each of the rows of the kernel matrix by a constant corresponding physically to changing the detector "height." The matter was studied only for square matrices, but the idea can probably be extended to the rectangular case. It was found that this device can sometimes be successful.

We then turned to the cases in which this simple approach fails and to defined pseudo-singular vectors and values, the first of these vectors being the predicted signal. The concept is not yet sufficiently developed to evaluate its level of success.

It is our belief that studies of this type can be of great value in the design of experiments. We hope that this initial humble effort will lead to further investigations of this kind.

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