

## The uncertainty principle in numerical linear algebra

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### Abstract.

In current paper we present comparative analysis of methodological and computational aspects of traditional methods for solving basic linear algebra problems. It is shown that the "critical components" method, also, referred to as "the uncertainty principle in linear algebra", introduced in [1] and later developed in papers referenced in [2-4], has an advantage over fundamental concepts, lying beneath such well-known methods as regularization, singular decomposition and the iterative QR-decomposition with deflation.

Analogies are drawn between the uncertainty relations in linear algebra and in quantum mechanics. We discuss the role of the established uncertainty relations in generating new numerical methods for finding effective stable approximations to the solutions of ill-posed linear algebra problems.

First of all about the title. The paper could be stated as "The minimum uncertainty principle in linear algebra", which would suit the contents better, but original title is also appropriate so we leave it as it is not to create any inconvenience to the organizing committee. We will soon expand more on the meaning we put into the "uncertainty principle", whereas now let us mention the following.

Quantum mechanics is a mathematical theory describing the states of small objects of nature (elementary particles). It operates with such fundamental constants as  $h$  - Planck constant and  $m$  - mass of the particle, where  $h \ll 1$  and  $m \ll 1$  in suitable units. Computational mathematics also deals with fundamental machine constants, such as  $\epsilon_0 > 0$  - minimal positive machine generated number,  $\epsilon_1 > 0$  - relative error of putting numbers in computer memory,  $\epsilon_\infty > 0$  - maximal computer generated number different from infinity. Computer operates only with rational real numbers for which  $0 < \epsilon_0 \ll \epsilon_1 \ll 1 \ll \epsilon_\infty < \infty$ .

In quantum mechanics there is a well-known Heisenberg uncertainty principle:  $\Delta x \Delta v \geq h/m$ . Speaking probabilistic language it means the following. If  $f_1(x) \Delta x$  is the probability of finding the particle between  $x$  and  $x \pm \Delta x$ , and  $f_2(v) \Delta v$  is the probability for it to have velocity between  $v$  and  $v \pm \Delta v$ , then  $\Delta x$  and  $\Delta v$  satisfy the above relation. One of the main corollaries quantum mechanics draws from the Heisenberg principle is that one cannot simultaneously make both  $\Delta x$  and  $\Delta v$  arbitrary small if the right-hand side of the inequality is fixed. This principle points out the uncertainty that has to exist when we make any attempt to describe the objects of such nature. It seems that probabilistic (and not deterministic) model is the maximum we can count on in this situation.

Analyzing the set up of the problem for solving ill-posed systems of linear equations (see [1-3])

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$$AZ = F, \quad \det A \neq 0, \quad (1)$$

we noticed that all existing methods, including regularization, can be conceptually described by the following scheme. If  $\|A^{-1}\| \|A\| \gg 1$ , each method finds its own generalized inverse matrix  $\bar{A}^{-1}$ , such that  $\bar{Z} = \bar{A}^{-1}F$ . In fact, it is (often silently) implied here that there exists the preimage, i. e., the matrix  $\bar{A}$  such that

$$\bar{A}\bar{Z} = \bar{F}, \quad \bar{A} - A = \Delta_{\bar{A}}, \quad Z - \bar{Z} = \Delta_{\bar{Z}}, \quad \Delta F = F - \bar{F} \quad (2)$$

If  $\alpha_0$  is the parameter of given algorithm, and

$$\delta_F = \frac{\|\Delta F\|}{\|F\|}, \quad \delta_{\bar{A}} = \frac{\|\Delta_{\bar{A}}\|}{\|A\|} \quad (3)$$

are the a priori estimates for the vector  $F$  and the coefficient matrix, correspondingly, then  $\bar{Z} = Z(\alpha_0, \delta_F, \delta_{\bar{A}})$  found this way to be named the approximation to the solution of system (1) stable to small perturbation of input data (3).

It often happens that the methods, except for the critical components method, lead to unsatisfactory solutions of system (1), as shown in [3]. Analysis of the reasons for such behavior yields the following conclusion. All the methods, including critical component method ([3]), implicitly encounter the condition we call

**The uncertainty principle in linear algebra:**

$\mu(\bar{A})\beta(A) \geq \alpha$ , where

$$\mu(\bar{A}) = \|\delta_{\bar{A}}^{(1)}\| = \|(A^{-1}\bar{A} - E)\|, \quad \beta(A) = \frac{1}{\|(A^T A)^{-1}\|}, \quad (4)$$

$$\mu(\bar{A}) \ll 1, \quad \beta(A) \ll 1, \quad \alpha = \alpha(\epsilon_0, \epsilon_1, \delta_F, \delta_{\bar{A}}) \ll 1.$$

The equality in (4) occurs only for the optimal  $\alpha_0$ , which is almost impossible to achieve, whereas the uncertainty condition reacts with high changes in  $\bar{Z}$  on small perturbations of  $\alpha_0$ .

As in the case of quantum uncertainty relation, (4) produced a corollary, which formed the basis of the new effective method ([3, 4]) for solving ill-posed systems of linear equations. This result is formulated below as follows:

**Theorem 1** (Minimum uncertainty principle in linear algebra). *Consider a system of linear algebraic equations (1), where  $\det A \neq 0$ , and the perturbed system (2). Then (2) has a unique solution  $\bar{Z}^{(0)}$ , approximating exact solution  $Z$  and stable to small perturbations  $\delta_F, \delta_{\bar{A}}$ , if the following hold:*

$$\|(A\delta_{\bar{A}}^{(1)})F^{(1)}\| + \|(E - (E + \delta_{\bar{A}}^{(1)})^{-1})F^{(1)}\| = 2\delta_F, \quad (5)$$

$$\|\delta_{\bar{A}}^{(1)}\| \leq \text{cond}(A)\delta_{\bar{A}} < 1, \quad F^{(1)} = \frac{F}{\|F\|}, \quad (6)$$

$$(\epsilon_0 + \epsilon_1) \leq \delta_F \leq \delta_F^{\text{ap}}, \quad (7)$$

where  $\delta_F^{\text{ap}}$  is the a priori estimate of  $\delta_F$  taking into account  $\delta_{\bar{A}}$  and  $\delta_F$ .

Here  $\bar{Z}^0$  satisfies:

$$\|\bar{Z}^{(0)}\| = \inf_{\{\bar{Z}\}} \|Z\|, \quad \delta_{\bar{Z}^{(0)}} = \inf_{\{\bar{Z}\}} \delta_{\bar{Z}}, \quad \delta_{\bar{F}^{(0)}} = \inf_{\{\bar{F}\}} \delta_{\bar{F}}. \quad (8)$$

We do not provide the proof of the theorem due to space limitations.

**Corollary 1.** *In the case of regularization minimum uncertainty principle (5)–(8) yields the following result for  $\alpha_{\text{op}}$  – optimal parameter of regularization:*

$$\alpha_{\text{op}} = \left( \frac{\lambda_m}{\lambda_1} \right) \left[ \delta_F + \frac{1}{2}(\lambda_1 - 1) \right],$$

if  $\lambda_1 + 2\delta_F > 1$ , where  $\epsilon_1 \leq \delta_F \leq \delta_F^{\text{op}}$  and  $\lambda_1, \lambda_m$  are maximal and minimal eigenvalues of  $A^T A$ , respectively.

**Corollary 2.** *The method of regularization and the critical component method are the corollary of the minimum uncertainty principle. Numerical methods of solving spectral problems developed based on [1] and systemized in [2] also follow from the Principle.*

In conclusion let us note that numerous experiments using new software package JINRLINPACK [4] developed with the help of the new concept showed its high effectiveness comparing to most known packages.

## References

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