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Effective Condition Number for Numerical Partial Differential Equations (Second Edition)

Li Zi-Cai (李子才) Huang Hung-Tsai (黄宏财)
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(偏微分方程数值解的有效条件数（第二版))

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This book is dedicated to our families.

Preface to the Series in Information and Computational Science

Since the 1970s, Science Press has published more than thirty volumes in its series Monographs in Computational Methods. This series was established and led by the late academician, Feng Kang, the founding director of the Computing Center of the Chinese Academy of Sciences. The monograph series has provided timely information of the frontier directions and latest research results in computational mathematics. It has had great impact on young scientists and the entire research community, and has played a very important role in the development of computational mathematics in China.

To cope with these new scientific developments, the Ministry of Education of the People's Republic of China in 1998 combined several subjects, such as computational mathematics, numerical algorithms, information science, and operations research and optimal control, into a new discipline called Information and Computational Science. As a result, Science Press also reorganized the editorial board of the monograph series and changed its name to Series in Information and Computational Science. The first editorial board meeting was held in Beijing in September 2004, and it discussed the new objectives, and the directions and contents of the new monograph series.

The aim of the new series is to present the state of the art in Information and Computational Science to senior undergraduate and graduate students, as well as to scientists working in these fields. Hence, the series will provide concrete and systematic expositions of the advances in information and computational science, encompassing also related interdisciplinary developments.

I would like to thank the previous editorial board members and assistants, and all the mathematicians who have contributed significantly to the monograph series on Computational Methods. As a result of their contributions the monograph series achieved an outstanding reputation in the community. I sincerely wish that we will extend this support to the new Series in Information and Computational Science, so that the new series can equally enhance the scientific development in information and computational science in this century.

Shi Zhongci

2005.7

Preface to the Second Edition

There exist many books on numerical methods for linear algebra, and for partial differential equations (PDE), separately. However, few seem to combine linear algebra with numerical PDE. There are also numerous books on error analysis of numerical PDE, but only a few focus on the stability issue (e.g., Higham [106]). The stability analysis of numerical methods is typically addressed by the condition number, proposed by Wilkinson [272] in 1963. In this book, an effective condition number is used to explore the stability of numerical PDE. The effective condition number is a sharper estimation of stability than the traditional condition number; hence it is more advantageous. In fact, the effective condition number was first studied by Rice [225] in 1981; however, it has largely escaped notice of the linear algebra community (see [14]) In this book, a systematic stability analysis is explored for numerical PDE, based on the effective condition number.

The first edition of *Effective Condition Number for Numerical Partial Differential Equations* was published by Science Press, Beijing, 2013, and then by Alpha Science International Ltd, UK, 2014 [177]. In this second edition, some errors discovered after the publication of the previous edition have been corrected. In addition, new progresses are reported as Chapters 6, 10 and 14. The length of the book increases by about 30%.

The three new chapters are briefly described as follows. In Chapter 6, a systematic stability analysis for the MFS is established to demonstrate the merits of the effective condition number, and to fill the gap between computation and theory. The MFS is a new trend of numerical PDE; an international conference series was initiated in 2007. The severe instability of the MFS is a crucial issue, but the optimal convergence can be achieved (see Li [149]). In this chapter, a new approach is proposed to derive the sharp asymptotes of Cond and Cond eff. Since the condition number of the MFS is large and even huge, the effective condition number is a much better estimate of numerical stability.

In Chapter 10, the singularity in boundary layers, which is more important than the boundary singularity discussed in Chapter 9, is analyzed. The effective condition number is applied to boundary layers by the FDM using different local refinements.

In Chapter 14, for the generalized Sylvester equation resulting from the linear control systems, the effective condition number is also employed.

Li Zi-Cai
Huang Hung-Tsai
Wei Yi-min
Cheng Alexander H.-D.
October 2015

Preface

For numerical methods, the stability is a crucial issue in the sense that the unstable numerical methods are useless in practical applications. The Lax's principle [90] for initial problems states that under the consistent condition, the convergence and the stability are equivalent to each other. When the truncation errors are derived, which are not very difficult, the errors of the numerical solutions can be obtained. However, the final numerical solutions also include rounding errors, which are related to stability. Since for the given algorithms of partial differential equations (PDE), the stability proof is often difficult and challenging, error analysis provides an easier pathway to answer the stability question.

Let us consider the finite element method (FEM) for elliptic boundary value problems. The uniformly V_h elliptic inequality is important for a priori error estimates [47], and it also implies stability, because the solutions of elliptic problems are not very sensitive to the perturbation of the data involved. The linear algebraic equations obtained from the FEM can be solved by the direct methods such as Gaussian elimination, or iterative methods such as the conjugate gradient methods, or the multigrid methods. Since all computations are completed in computer, the rounding errors are inevitable. Since the double precision has only 16 significant decimal digits, the final numerical solutions must have the extra errors from rounding errors. Even when certain software, such as the computer algebra software Mathematica, is used with more working digits, it is also finite. The more working digits are used, the more CPU time and the more computer storage are needed. Hence, the perturbation errors, such as rounding errors, are important to numerical methods for PDE.

Consider the overdetermined linear algebraic equations resulting from numerical PDE,

$$\boldsymbol{F}\boldsymbol{x} = \boldsymbol{b}, \tag{0.0.1}$$

where $\boldsymbol{F} \in \mathbf{R}^{m\times n}, m \geqslant n$, and $\boldsymbol{x} \in \mathbf{R}^n$ and $\boldsymbol{b} \in \mathbf{R}^m$ are the unknown and the known vectors, respectively. The traditional condition number in the 2-norm is defined by

$$\text{Cond} = \frac{\sigma_{\max}}{\sigma_{\min}}, \tag{0.0.2}$$

where $\sigma_{\max}$ and $\sigma_{\min}$ are the maximal and the minimal singular values, respectively.

The new effective condition number in this book is defined by

$$\text{Cond\_eff} = \frac{\|\boldsymbol{b}\|}{\sigma_{\min}\|\boldsymbol{x}\|}, \tag{0.0.3}$$

where $\|\boldsymbol{x}\|$ is the 2-norm. When there exist the perturbation of $\boldsymbol{b}$ and $\boldsymbol{F}$, the practical computation for (0.0.1) is carried out by

$$\boldsymbol{F}(\boldsymbol{x} + \Delta\boldsymbol{x}) = \boldsymbol{b} + \Delta\boldsymbol{b}, \tag{0.0.4}$$

$$(\boldsymbol{F} + \Delta\boldsymbol{F})(\boldsymbol{x} + \Delta\boldsymbol{x}) = \boldsymbol{b} + \Delta\boldsymbol{b}, \tag{0.0.5}$$

where $\Delta\boldsymbol{F} \in \mathbf{R}^{m\times n}$ $(m \geqslant n)$, $\Delta\boldsymbol{x} \in \mathbf{R}^n$ and $\Delta\boldsymbol{b} \in \mathbf{R}^m$. Suppose that $\Delta\boldsymbol{F}$ is small so that $\text{rank}(\boldsymbol{F}) = \text{rank}(\boldsymbol{F} + \Delta\boldsymbol{F}) = n$. For (0.0.4) (i.e., $\Delta\boldsymbol{F} = \boldsymbol{0}$), there exist the bounds of relative errors,

$$\frac{\|\Delta\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leqslant \text{Cond} \times \frac{\|\Delta\boldsymbol{b}\|}{\|\boldsymbol{b}\|}, \quad \frac{\|\Delta\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leqslant \text{Cond\_eff} \times \frac{\|\Delta\boldsymbol{b}\|}{\|\boldsymbol{b}\|}. \tag{0.0.6}$$

Equations (0.0.6) indicate the errors from the perturbation, e.g., from the rounding errors. More specifically, the relative errors of the solution $\boldsymbol{x}$ may be enlarged from the rounding errors by a factor of Cond, and Cond has often been used to provide a stability analysis of numerical methods (see Wilkinson [272]). In fact, since the upper bound Cond in (0.0.6) is the worst case, it rarely happens in most PDE problems. The Cond_eff in (0.0.3) is smaller, or even much smaller than the Cond in (0.0.2). Then the error bound of $\boldsymbol{x}$ can be improved by Cond_eff and shown in (0.0.6). Such a conclusion has been proved by the analysis and computation in this entire book. Since the algorithms of (0.0.3) are so simple, easy and straightforward in computation, the Cond_eff is strongly recommended, to replace the Cond. This is one objective of this book.

The idea of effective condition number was first studied in Rice [225] and Chan and Foulser [29], and the formula (0.0.3) of Cond_eff was first used in Christiansen and Saranen [44]. Only a few papers [29, 43, 44, 63] follow this trend for stability analysis. Recently, we have carried out a systematic study on effective condition number of various numerical methods for PDE and the boundary integral equation (BIE). Interestingly, the Cond_eff is significantly smaller than the Cond for numerical methods of PDE, but only fairly smaller than the Cond for numerical methods of BIE [116]. Comparing (0.0.3) with (0.0.2), the minimal singular value $\sigma_{\min}$ is crucial for both Cond_eff and Cond, but the maximal singular value $\sigma_{\max}$ is necessary only to Cond. Hence when $\sigma_{\max}$ is large, the Cond is large, but the Cond_eff may remain small. This happens for the finite element method (FEM), the finite difference method (FDM), the Trefftz method (TM) and the spectral method (SM) for elliptic boundary value problems. In particular, when the maximal boundary length h

of grids and elements is small in FDM and FEM, the traditional condition number Cond is large (or even huge for local refinements of partitions). However, the effective condition number is small, to display a good stability of numerical methods. This is particularly important to the local refinements used in FDM and FEM for singularity problems in Li [144], explored in Chapters 9−11.

The previous study [29, 43, 225] for effective condition number was active until Banoczi et al. [14] in 1998, where a number of numerical examples of linear algebraic equations display insignificance of effective condition number. In fact, the Cond_eff is significant for numerical PDE, not for linear algebraic equations [164]. For the perturbations in (0.0.5), from Section 1.8 there exists the bound,

$$\frac{\|\Delta \boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leqslant \frac{\text{Cond\_eff}}{1-\delta}\left[\frac{1+\sqrt{5}}{2}\text{Cond} \times \frac{\|\Delta \boldsymbol{F}\|}{\|\boldsymbol{F}\|} + \frac{\|\Delta \boldsymbol{b}\|}{\|\boldsymbol{b}\|}\right], \tag{0.0.7}$$

where $\delta = \|\boldsymbol{F}^{\dagger}\|\|\Delta\boldsymbol{F}\| < 1$, and $\boldsymbol{F}^{\dagger}$ is the pseudo-inverse matrix of $\boldsymbol{F}$. In (0.0.7), the condition number is defined by $\text{Cond} = \|\boldsymbol{F}^{\dagger}\|\|\boldsymbol{F}\|$, and the effective condition number by $\text{Cond\_eff} = \|\boldsymbol{F}^{\dagger}\|\frac{\|\boldsymbol{b}\|}{\|\boldsymbol{x}\|}$. For linear algebraic equations, the rounding errors $\frac{\|\Delta \boldsymbol{b}\|}{\|\boldsymbol{b}\|}$ are smaller than the errors $\frac{\|\Delta \boldsymbol{F}\|}{\|\boldsymbol{F}\|}$ of solution methods, such as Gaussian elimination method, so that the condition number plays a dominant role in (0.0.7). However, for numerical PDE, the discretization and the truncation errors, $\frac{\|\Delta \boldsymbol{b}\|}{\|\boldsymbol{b}\|}$, are lager than $\frac{\|\Delta \boldsymbol{F}\|}{\|\boldsymbol{F}\|}$, so that the effective condition number plays a dominant role in (0.0.7).

Here, let us mention the most important references of condition number. The definition of the traditional condition number was given in Wilkinson [273], and then used in many books and papers, see Atkinson [3], Atkinson and Han [5], Christiansen [41], Cucker et al. [49], Geurts [77], Golub and van Loan [80], Laub [135], Parlett [218], Quarteroni and Valli [222], and Schwarz [230]. The condition number for eigenvalues was reported in Parlett [218] and Frayssé and Toumazou [74], and more discussions on condition number were given in Gulliksson and Wedin [87], Elsner et al. [67], Rice [224] and Rohn [226].

This book is a summary of our recent study of effective condition numbers, and the most significant results are selected from more than thirty papers, published in international journals in mathematics and engineering. There are a number of characteristics of this book. The effective condition number is a new criterion for numerical stability of numerical PDE, and this book covers the newest discoverers on this subject. The first characteristic is its novelty. Since the analysis of effective condition number involves two disciplines: linear algebra and partial differential the boundary singularities, the Cond_eff is much smaller than the Cond $= \mathcal{O}(h_{\min}^{-2})$.

Chapter 10: Singularly Perturbed Differential Equations by the Upwind Difference Scheme. The singularity in boundary layers in this chapter is more popular and important than the boundary singularity in Chapter 9. Different local refinements are employed, and the effective condition number is also advantageous over the condition number.

Chapter 11: Finite Element Method Using Local Mesh Refinements. For corner singularity of general PDE, the local mesh refinements are a must for FEM. The Cond_eff is independent of $h_{\min}$, and significantly smaller than the Cond.

Chapter 12: Hermite FEM for Biharmonic Equations. Effective condition number is applied to biharmonic equations by Hermite FEM, to show Cond_eff $= \mathcal{O}(1)$ for homogenous boundary conditions. In contrast, Cond $= \mathcal{O}(h^{-4})$.

Chapter 13: Truncated SVD and Tikhonov Regularization. The ill-conditioning of the truncated singular value decomposition (TSVD) and the Tikhonov regularization (TR) is studied by Cond and Cond_eff. The new computational formulas of Cond and Cond_eff are explored, and error bounds are derived. When the minimal singular value $\sigma_{\min}$ is infinitesimal, there exists a severe subtractive cancelation. This is the other stability. The Cond can be regarded as the global stability: Cond_eff plus the subtractive cancelation. This chapter provides a new stability analysis on the TSVD and the TR for numerical PDE.

Chapter 14: Small Sample Statistical Condition Estimation for the Generalized Sylvester Equation. In this chapter, the effective condition number has been applied to the generalized Sylvester equation resulting from the linear control systems. The effective condition number can be much smaller than the orthodox condition number. Based on the effective condition, the sharp perturbation bounds for the generalized Sylvester equation can be obtained.

Various problems by different numerical methods for different applications demonstrate the outstanding advantages of the effective condition number over the traditional condition number.

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Contents