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Geometric Approach to Symmetric Positive Definite Linear Systems

Xinyuan Wu*

School of Mathematics, Nanjing University, Nanjing 210093, P.R. China.

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Abstract. This paper compares the performance of the conjugate gradient method and geometric approach in the case of symmetric positive definite (SPD) linear systems. This approach is based on the geometric theory of ODEs which was effectively initiated by Poncaré and Liapunov. The simplest and most obvious advantage of the geometric approach over the conjugate gradient method (the MATLAB code `pcg`) is that this approach can find the inverse of the underlying positive definite matrix and the solution. We present various numerical examples, which demonstrate the superiority of the geometric approach. For SPD linear systems, this approach provides much higher accuracy than the conjugate gradient method. In particular, since it is a one-stop procedure, it can avoid the growth of accumulated round-off errors to some extent.

AMS subject classifications: 15A06, 15A09, 15A16, 65F05, 65F22, 65F60, 65F99

Key words: Geometric approach, linear algebraic system, direct method, conjugate gradient method, matrix inversion.

1. Introduction

In the development and design of numerical algorithms, established methods are constantly being inspected, and the numerical comparison of methods is a never-ending process through which we learn the essence and nature of computational mathematics. In a recent paper [35], the author proposed an exponential approach to highly ill-conditioned linear algebraic systems

$$Ax = b, \tag{1.1}$$

where A is a $d \times d$ symmetric positive definite matrix and $b \in \mathbb{R}^d$ an arbitrary nonzero vector. It should be noted that the main theme of that paper was the numerical treatment of linear algebraic systems with highly ill-conditioned matrices. There is no such an assumption in

*Corresponding author. *Email address:* `xywu@nju.edu.cn` (X.Y. Wu)

this paper. Accordingly, the so-called exponential approach is referred to as the geometric approach because of the geometric theory of ordinary differential equations. The main contribution of this paper is the analysis of the geometric properties and the error estimation of the approach mentioned.

It is convenient to express the unique solution of (1.1) by $x^* = A^{-1}b$. Note that for the Eqs. (1.1), the conjugate gradient methods have been developed by Lanczos [23], Hestenes [18], Hestenes and Stiefel [19], Stiefel [32], and Reid [29, 30]. These methods are most important popular algorithms for solving Eqs. (1.1) arising in applications. The conjugate gradient method for nonlinear problems was first suggested by Fletcher and Reeves [14] and theoretically analysed by Daniel [10, 11]. The conjugate gradient method for nonlinear elliptic boundary value problems over irregular regions was proposed by Bartels *el al.* [2]. Moreover, nonlinear conjugate gradient methods have also been well developed [1].

It is known that the subject of numerical mathematics is the development of numerical methods for efficient approximations of the solutions to mathematically expressed problems. The efficiency of the method depends on both the accuracy required and the easiness of its implementation. Therefore, it is natural to ask whether the geometric approach shows improved computational performance and/or better properties than conjugate gradient methods for (1.1)? This paper gives the affirmative answer and that is also the main focus of the present paper.

Clearly, the so-called exponential approach in [35] also can be thought as a geometric rule, since it was derived by using the geometric theory of ordinary differential equations and the closed form solution of a dynamic system associated with the linear algebraic system (1.1). As a matter of fact, the exponential approach is a direct method which is expressed in an exponential rule. This makes it possible that one could not help thinking of Cramer's rule which is useless for any practical application as we have known. Fortunately, however, the geometric approach is completely different from Cramer's rule, and can be effectively carried out in terms of the MATLAB code of matrix exponential which has been well developed — cf. [5, 31].

Although, the exponential approach was proposed specially for highly ill-conditioned linear algebraic systems in [35], there are not enough numerical examples to demonstrate the superiority of the method over the MATLAB solver of the conjugate gradient method. Besides, the geometric properties of this approach also have to be analysed in detail. In particular, the paper mentioned does not consider such an important aspect as the error estimates and we think that there should be more numerical experiments to compare the geometric approach and the conjugate gradient method are needed. The aim of the present paper is to fill these gaps. We show the mathematical significance, geometric properties and error analysis of the geometric approach in detail. Besides, we demonstrate the advantages of this approach in comparison with the conjugate gradient method.

This paper is organised as follows. We summarise the geometric approach in Section 2. A detailed structured algorithm without program is stated in Section 3. In Section 4 we present an error estimate of the geometric approach for the SPD linear system (1.1). A variety of numerical experiments in Section 5 further demonstrate the superiority of the geometric approach for the SPD linear system (1.1). The final section draws some conclusions.