MAP 2220 – FUNDAMENTOS DE ANÁLISE NUMÉRICA

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Prof. Dr. Luis Carlos de Castro Santos

lsantos@ime.usp.br/lccs13@yahoo.com

7 Iterative Techniques in Matrix Algebra 431

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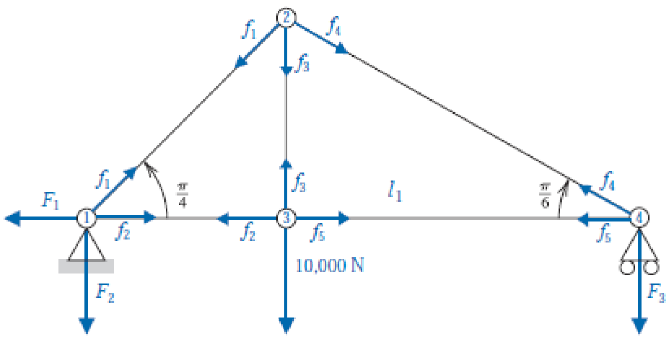


$$\equiv \begin{bmatrix} -1 & 0 & 0 & \frac{\sqrt{2}}{2} & 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & \frac{\sqrt{2}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & -1 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -\frac{\sqrt{2}}{2} & 0 & 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & -1 \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 10{,}000 \\ 0 \\ 0 \end{bmatrix}.$$

Jacobi's Method

$$x_i^{(k)} = \frac{1}{a_{ii}}\left[\sum_{\substack{j=1\\ j\neq i}}^{n}\left(-a_{ij}x_j^{(k-1)}\right) + b_i\right], \qquad \text{for } i = 1, 2, \ldots, n.$$

$\mathbf{x}^{(k)} = T_j\mathbf{x}^{(k-1)} + \mathbf{c}_j.$ $\quad T_j = D^{-1}(L+U)$ and $\mathbf{c}_j = D^{-1}\mathbf{b}$

The Gauss-Seidel Method

$$x_i^{(k)} = \frac{1}{a_{ii}}\left[-\sum_{j=1}^{i-1}(a_{ij}x_j^{(k)}) - \sum_{j=i+1}^{n}(a_{ij}x_j^{(k-1)}) + b_i\right],$$

$\mathbf{x}^{(k)} = T_g\mathbf{x}^{(k-1)} + \mathbf{c}_g.$ $\quad T_g = (D-L)^{-1}U$ and $\mathbf{c}_g = (D-L)^{-1}\mathbf{b}$,

SOR, for Successive Over-Relaxation,

$$x_i^{(k)} = (1-\omega)x_i^{(k-1)} + \frac{\omega}{a_{ii}}\left[b_i - \sum_{j=1}^{i-1}a_{ij}x_j^{(k)} - \sum_{j=i+1}^{n}a_{ij}x_j^{(k-1)}\right]$$

$\mathbf{x}^{(k)} = T_\omega\mathbf{x}^{(k-1)} + \mathbf{c}_\omega.$ $\qquad T_\omega = (D-\omega L)^{-1}[(1-\omega)D + \omega U]$ and $\mathbf{c}_\omega = \omega(D-\omega L)^{-1}\mathbf{b}.$

7.5 Error Bounds and Iterative Refinement

It seems intuitively reasonable that if $\tilde{\mathbf{x}}$ is an approximation to the solution $\mathbf{x}$ of $A\mathbf{x} = \mathbf{b}$ and the residual vector $\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}}$ has the property that $\|\mathbf{r}\|$ is small, then $\|\mathbf{x} - \tilde{\mathbf{x}}\|$ would be small as well. This is often the case, but certain systems, which occur frequently in practice, fail to have this property.

Example 1 The linear system $A\mathbf{x} = \mathbf{b}$ given by

$$\begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 3.0001 \end{bmatrix}$$

has the unique solution $\mathbf{x} = (1, 1)^t$. Determine the residual vector for the poor approximation $\tilde{\mathbf{x}} = (3, -0.0001)^t$.

Solution We have

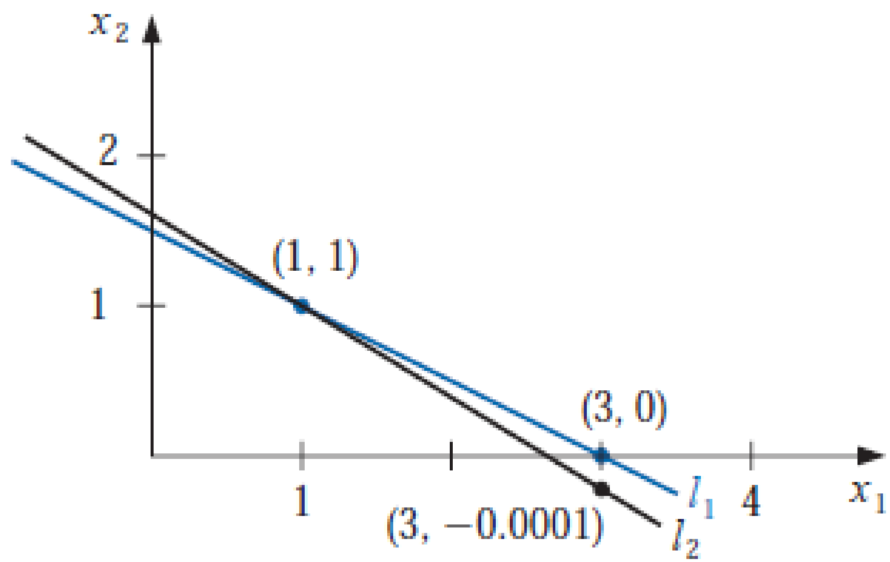
$$\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}} = \begin{bmatrix} 3 \\ 3.0001 \end{bmatrix} - \begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix} \begin{bmatrix} 3 \\ -0.0001 \end{bmatrix} = \begin{bmatrix} 0.0002 \\ 0 \end{bmatrix},$$

so $\|\mathbf{r}\|_\infty = 0.0002$. Although the norm of the residual vector is small, the approximation $\tilde{\mathbf{x}} = (3, -0.0001)^t$ is obviously quite poor; in fact, $\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty = 2$. ■

The difficulty in Example 1 is explained quite simply by noting that the solution to the system represents the intersection of the lines

$$l_1: \quad x_1 + 2x_2 = 3 \quad \text{and} \quad l_2: \quad 1.0001x_1 + 2x_2 = 3.0001.$$

The point $(3, -0.0001)$ lies on l_2, and the lines are nearly parallel. This implies that $(3, -0.0001)$ also lies close to l_1, even though it differs significantly from the solution of the system, given by the intersection point $(1, 1)$. (See Figure 7.7.)



Example 1 was clearly constructed to show the difficulties that can—and, in fact, do—arise. Had the lines not been nearly coincident, we would expect a small residual vector to imply an accurate approximation.

In the general situation, we cannot rely on the geometry of the system to give an indication of when problems might occur. We can, however, obtain this information by considering the norms of the matrix A and its inverse.

Theorem 7.27 Suppose that $\tilde{\mathbf{x}}$ is an approximation to the solution of $A\mathbf{x} = \mathbf{b}$, A is a nonsingular matrix, and $\mathbf{r}$ is the residual vector for $\tilde{\mathbf{x}}$. Then for any natural norm,

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| \leq \|\mathbf{r}\| \cdot \|A^{-1}\|$$

and if $\mathbf{x} \neq \mathbf{0}$ and $\mathbf{b} \neq \mathbf{0}$,

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \|A\| \cdot \|A^{-1}\| \frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}. \tag{7.20}$$

■

Proof Since $\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}} = A\mathbf{x} - A\tilde{\mathbf{x}}$ and A is nonsingular, we have $\mathbf{x} - \tilde{\mathbf{x}} = A^{-1}\mathbf{r}$. Theorem 7.11 on page 440 implies that

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| = \|A^{-1}\mathbf{r}\| \leq \|A^{-1}\| \cdot \|\mathbf{r}\|.$$

Moreover, since $\mathbf{b} = A\mathbf{x}$, we have $\|\mathbf{b}\| \leq \|A\| \cdot \|\mathbf{x}\|$. So $1/\|\mathbf{x}\| \leq \|A\|/\|\mathbf{b}\|$ and

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq \frac{\|A\| \cdot \|A^{-1}\|}{\|\mathbf{b}\|}\|\mathbf{r}\|.$$

■ ■ ■

Condition Numbers

The inequalities in Theorem 7.27 imply that $\|A^{-1}\|$ and $\|A\| \cdot \|A^{-1}\|$ provide an indication of the connection between the residual vector and the accuracy of the approximation. In general, the relative error $\|\mathbf{x}-\tilde{\mathbf{x}}\|/\|\mathbf{x}\|$ is of most interest, and, by Inequality (7.20), this error is bounded by the product of $\|A\| \cdot \|A^{-1}\|$ with the relative residual for this approximation, $\|\mathbf{r}\|/\|\mathbf{b}\|$. Any convenient norm can be used for this approximation; the only requirement is that it be used consistently throughout.

Definition 7.28 The **condition number** of the nonsingular matrix A relative to a norm $\|\cdot\|$ is

$$K(A) = \|A\| \cdot \|A^{-1}\|.$$

With this notation, the inequalities in Theorem 7.27 become

$$\|\mathbf{x} - \tilde{\mathbf{x}}\| \le K(A)\frac{\|\mathbf{r}\|}{\|A\|}$$

and

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\|\mathbf{x}\|} \le K(A)\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}.$$

For any nonsingular matrix A and natural norm $\|\cdot\|$,

$$1 = \|I\| = \|A \cdot A^{-1}\| \le \|A\| \cdot \|A^{-1}\| = K(A).$$

A matrix A is **well-conditioned** if $K(A)$ is close to 1, and is **ill-conditioned** when $K(A)$ is significantly greater than 1. Conditioning in this context refers to the relative security that a small residual vector implies a correspondingly accurate approximate solution.

Example 2 Determine the condition number for the matrix

$$A = \begin{bmatrix} 1 & 2 \\ 1.0001 & 2 \end{bmatrix}.$$

Solution We saw in Example 1 that the very poor approximation $(3, -0.0001)^t$ to the exact solution $(1, 1)^t$ had a residual vector with small norm, so we should expect the condition number of A to be large. We have $\|A\|_\infty = \max\{|1| + |2|, |1.001| + |2|\} = 3.0001$, which would not be considered large. However,

$$A^{-1} = \begin{bmatrix} -10000 & 10000 \\ 5000.5 & -5000 \end{bmatrix}, \quad \text{so} \quad \|A^{-1}\|_\infty = 20000,$$

and for the infinity norm, $K(A) = (20000)(3.0001) = 60002$. The size of the condition number for this example should certainly keep us from making hasty accuracy decisions based on the residual of an approximation. ■

Although the condition number of a matrix depends totally on the norms of the matrix and its inverse, the calculation of the inverse is subject to roundoff error and is dependent on the accuracy with which the calculations are performed. If the operations involve arithmetic with t digits of accuracy, the approximate condition number for the matrix A is the norm of the matrix times the norm of the approximation to the inverse of A, which is obtained using t-digit arithmetic. In fact, this condition number also depends on the method used to calculate the inverse of A. In addition, because of the number of calculations needed to compute the inverse, we need to be able to estimate the condition number without directly determining the inverse.

If we assume that the approximate solution to the linear system $A\mathbf{x} = \mathbf{b}$ is being determined using t-digit arithmetic and Gaussian elimination, it can be shown (see [FM], pp. 45–47) that the residual vector $\mathbf{r}$ for the approximation $\tilde{\mathbf{x}}$ has

$$\|\mathbf{r}\| \approx 10^{-t}\|A\| \cdot \|\tilde{\mathbf{x}}\|. \tag{7.21}$$

From this approximation, an estimate for the effective condition number in t-digit arithmetic can be obtained without the need to invert the matrix A. In actuality, this approximation assumes that all the arithmetic operations in the Gaussian elimination technique are performed using t-digit arithmetic but that the operations needed to determine the residual are done in double-precision (that is, $2t$-digit) arithmetic. This technique does not add significantly to the computational effort and eliminates much of the loss of accuracy involved with the subtraction of the nearly equal numbers that occur in the calculation of the residual.

The approximation for the t-digit condition number $K(A)$ comes from consideration of the linear system

$$A\mathbf{y} = \mathbf{r}.$$

The solution to this system can be readily approximated because the multipliers for the Gaussian elimination method have already been calculated. So A can be factored in the form P^tLU as described in Section 5 of Chapter 6. In fact $\tilde{\mathbf{y}}$, the approximate solution of $A\mathbf{y} = \mathbf{r}$, satisfies

$$\tilde{\mathbf{y}} \approx A^{-1}\mathbf{r} = A^{-1}(\mathbf{b} - A\tilde{\mathbf{x}}) = A^{-1}\mathbf{b} - A^{-1}A\tilde{\mathbf{x}} = \mathbf{x} - \tilde{\mathbf{x}}; \tag{7.22}$$

and

$$\mathbf{x} \approx \tilde{\mathbf{x}} + \tilde{\mathbf{y}}.$$

So $\tilde{\mathbf{y}}$ is an estimate of the error produced when $\tilde{\mathbf{x}}$ approximates the solution $\mathbf{x}$ to the original system. Equations (7.21) and (7.22) imply that

$$\|\tilde{\mathbf{y}}\| \approx \|\mathbf{x}-\tilde{\mathbf{x}}\| = \|A^{-1}\mathbf{r}\| \leq \|A^{-1}\| \cdot \|\mathbf{r}\| \approx \|A^{-1}\| \left(10^{-t}\|A\| \cdot \|\tilde{\mathbf{x}}\|\right) = 10^{-t}\|\tilde{\mathbf{x}}\| K(A).$$

This gives an approximation for the condition number involved with solving the system $A\mathbf{x} = \mathbf{b}$ using Gaussian elimination and the t-digit type of arithmetic just described:

$$K(A) \approx \frac{\|\tilde{\mathbf{y}}\|}{\|\tilde{\mathbf{x}}\|} 10^t. \tag{7.23}$$

Illustration The linear system given by

$$\begin{bmatrix} 3.3330 & 15920 & -10.333 \\ 2.2220 & 16.710 & 9.6120 \\ 1.5611 & 5.1791 & 1.6852 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 15913 \\ 28.544 \\ 8.4254 \end{bmatrix}$$

has the exact solution $\mathbf{x} = (1, 1, 1)^t$.

Using Gaussian elimination and five-digit rounding arithmetic leads successively to the augmented matrices

$$\begin{bmatrix} 3.3330 & 15920 & -10.333 & 15913 \\ 0 & -10596 & 16.501 & 10580 \\ 0 & -7451.4 & 6.5250 & -7444.9 \end{bmatrix}$$

and

$$\begin{bmatrix} 3.3330 & 15920 & -10.333 & 15913 \\ 0 & -10596 & 16.501 & -10580 \\ 0 & 0 & -5.0790 & -4.7000 \end{bmatrix}.$$

The approximate solution to this system is

$$\tilde{\mathbf{x}} = (1.2001, 0.99991, 0.92538)^t.$$

The residual vector corresponding to $\tilde{\mathbf{x}}$ is computed in double precision to be

$$\mathbf{r} = \mathbf{b} - A\tilde{\mathbf{x}}$$

$$= \begin{bmatrix} 15913 \\ 28.544 \\ 8.4254 \end{bmatrix} - \begin{bmatrix} 3.3330 & 15920 & -10.333 \\ 2.2220 & 16.710 & 9.6120 \\ 1.5611 & 5.1791 & 1.6852 \end{bmatrix} \begin{bmatrix} 1.2001 \\ 0.99991 \\ 0.92538 \end{bmatrix}$$

$$= \begin{bmatrix} 15913 \\ 28.544 \\ 8.4254 \end{bmatrix} - \begin{bmatrix} 15913.00518 \\ 28.26987086 \\ 8.611560367 \end{bmatrix} = \begin{bmatrix} -0.00518 \\ 0.27412914 \\ -0.186160367 \end{bmatrix},$$

so

$$\|\mathbf{r}\|_\infty = 0.27413.$$

The estimate for the condition number given in the preceding discussion is obtained by first solving the system $A\mathbf{y} = \mathbf{r}$ for $\tilde{\mathbf{y}}$:

$$\begin{bmatrix} 3.3330 & 15920 & -10.333 \\ 2.2220 & 16.710 & 9.6120 \\ 1.5611 & 5.1791 & 1.6852 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} -0.00518 \\ 0.27413 \\ -0.18616 \end{bmatrix}.$$

This implies that $\tilde{\mathbf{y}} = (-0.20008, 8.9987 \times 10^{-5}, 0.074607)^t$. Using the estimate in Eq. (7.23) gives

$$K(A) \approx \frac{\|\tilde{\mathbf{y}}\|_\infty}{\|\tilde{\mathbf{x}}\|_\infty} 10^5 = \frac{0.20008}{1.2001} 10^5 = 16672. \qquad (7.24)$$

To determine the *exact* condition number of A, we first must find A^{-1}. Using five-digit rounding arithmetic for the calculations gives the approximation:

$$A^{-1} \approx \begin{bmatrix} -1.1701 \times 10^{-4} & -1.4983 \times 10^{-1} & 8.5416 \times 10^{-1} \\ 6.2782 \times 10^{-5} & 1.2124 \times 10^{-4} & -3.0662 \times 10^{-4} \\ -8.6631 \times 10^{-5} & 1.3846 \times 10^{-1} & -1.9689 \times 10^{-1} \end{bmatrix}.$$

Theorem 7.11 on page 440 implies that $\|A^{-1}\|_\infty = 1.0041$ and $\|A\|_\infty = 15934$.

As a consequence, the ill-conditioned matrix A has

$$K(A) = (1.0041)(15934) = 15999.$$

The estimate in (7.24) is quite close to $K(A)$ and requires considerably less computational effort.

Since the actual solution $\mathbf{x} = (1, 1, 1)^t$ is known for this system, we can calculate both

$$\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty = 0.2001 \quad \text{and} \quad \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty}{\|\mathbf{x}\|_\infty} = \frac{0.2001}{1} = 0.2001.$$

The error bounds given in Theorem 7.27 for these values are

$$\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty \le K(A)\frac{\|\mathbf{r}\|_\infty}{\|A\|_\infty} = \frac{(15999)(0.27413)}{15934} = 0.27525$$

and

$$\frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|_\infty}{\|\mathbf{x}\|_\infty} \le K(A)\frac{\|\mathbf{r}\|_\infty}{\|\mathbf{b}\|_\infty} = \frac{(15999)(0.27413)}{15913} = 0.27561. \qquad \square$$

7.6 The Conjugate Gradient Method

The conjugate gradient method of Hestenes and Stiefel [HS] was originally developed as a direct method designed to solve an $n \times n$ positive definite linear system. As a direct method it is generally inferior to Gaussian elimination with pivoting. Both methods require n steps to determine a solution, and the steps of the conjugate gradient method are more computationally expensive than those of Gaussian elimination.

However, the conjugate gradient method is useful when employed as an iterative approximation method for solving large sparse systems with nonzero entries occurring in predictable patterns. These problems frequently arise in the solution of boundary-value problems. When the matrix has been preconditioned to make the calculations more effective, good results are obtained in only about $\sqrt{n}$ iterations. Employed in this way, the method is preferred over Gaussian elimination and the previously-discussed iterative methods.

Throughout this section we assume that the matrix A is positive definite. We will use the *inner product* notation

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^t \mathbf{y}, \tag{7.26}$$

where $\mathbf{x}$ and $\mathbf{y}$ are n-dimensional vectors. We will also need some additional standard results from linear algebra. A review of this material is found in Section 9.1.

The next result follows easily from the properties of transposes (see Exercise 12).

Theorem 7.30 For any vectors $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ and any real number α, we have

(a) $\langle \mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{y}, \mathbf{x} \rangle$;

(b) $\langle \alpha\mathbf{x}, \mathbf{y} \rangle = \langle \mathbf{x}, \alpha\mathbf{y} \rangle = \alpha\langle \mathbf{x}, \mathbf{y} \rangle$;

(c) $\langle \mathbf{x} + \mathbf{z}, \mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{z}, \mathbf{y} \rangle$;

(d) $\langle \mathbf{x}, \mathbf{x} \rangle \geq 0$;

(e) $\langle \mathbf{x}, \mathbf{x} \rangle = 0$ if and only if $\mathbf{x} = \mathbf{0}$. ■

When A is positive definite, $\langle \mathbf{x}, A\mathbf{x} \rangle = \mathbf{x}^t A\mathbf{x} > 0$ unless $\mathbf{x} = \mathbf{0}$. Also, since A is symmetric, we have $\mathbf{x}^t A\mathbf{y} = \mathbf{x}^t A^t\mathbf{y} = (A\mathbf{x})^t\mathbf{y}$, so in addition to the results in Theorem 7.30, we have for each $\mathbf{x}$ and $\mathbf{y}$,

$$\langle \mathbf{x}, A\mathbf{y} \rangle = (A\mathbf{x})^t\mathbf{y} = \mathbf{x}^t A^t\mathbf{y} = \mathbf{x}^t A\mathbf{y} = \langle A\mathbf{x}, \mathbf{y} \rangle. \tag{7.27}$$

The following result is a basic tool in the development of the conjugate gradient method.

Theorem 7.31 The vector $\mathbf{x}^*$ is a solution to the positive definite linear system $A\mathbf{x} = \mathbf{b}$ if and only if $\mathbf{x}^*$ produces the minimal value of

$$g(\mathbf{x}) = \langle \mathbf{x}, A\mathbf{x} \rangle - 2\langle \mathbf{x}, \mathbf{b} \rangle.$$ ■

Proof Let $\mathbf{x}$ and $\mathbf{v} \neq \mathbf{0}$ be fixed vectors and t a real number variable. We have

$$\begin{aligned} g(\mathbf{x} + t\mathbf{v}) &= \langle \mathbf{x} + t\mathbf{v}, A\mathbf{x} + tA\mathbf{v} \rangle - 2\langle \mathbf{x} + t\mathbf{v}, \mathbf{b} \rangle \\ &= \langle \mathbf{x}, A\mathbf{x} \rangle + t\langle \mathbf{v}, A\mathbf{x} \rangle + t\langle \mathbf{x}, A\mathbf{v} \rangle + t^2\langle \mathbf{v}, A\mathbf{v} \rangle - 2\langle \mathbf{x}, \mathbf{b} \rangle - 2t\langle \mathbf{v}, \mathbf{b} \rangle \\ &= \langle \mathbf{x}, A\mathbf{x} \rangle - 2\langle \mathbf{x}, \mathbf{b} \rangle + 2t\langle \mathbf{v}, A\mathbf{x} \rangle - 2t\langle \mathbf{v}, \mathbf{b} \rangle + t^2\langle \mathbf{v}, A\mathbf{v} \rangle, \end{aligned}$$

so

$$g(\mathbf{x} + t\mathbf{v}) = g(\mathbf{x}) - 2t\langle \mathbf{v}, \mathbf{b} - A\mathbf{x} \rangle + t^2\langle \mathbf{v}, A\mathbf{v} \rangle. \tag{7.28}$$

With $\mathbf{x}$ and $\mathbf{v}$ fixed we can define the quadratic function h in t by

$$h(t) = g(\mathbf{x} + t\mathbf{v}).$$

Then h assumes a minimal value when $h'(t) = 0$, because its t^2 coefficient, $\langle \mathbf{v}, A\mathbf{v} \rangle$, is positive. Because

$$h'(t) = -2\langle \mathbf{v}, \mathbf{b} - A\mathbf{x} \rangle + 2t\langle \mathbf{v}, A\mathbf{v} \rangle,$$

the minimum occurs when

$$\hat{t} = \frac{\langle \mathbf{v}, \mathbf{b} - A\mathbf{x} \rangle}{\langle \mathbf{v}, A\mathbf{v} \rangle},$$

and, from Equation (7.28),

$$
\begin{aligned}
h(\hat{t}\,) &= g(\mathbf{x} + \hat{t}\mathbf{v}) \\
&= g(\mathbf{x}) - 2\hat{t}\langle \mathbf{v}, \mathbf{b} - A\mathbf{x}\rangle + \hat{t}^2\langle \mathbf{v}, A\mathbf{v}\rangle \\
&= g(\mathbf{x}) - 2\frac{\langle \mathbf{v}, \mathbf{b} - A\mathbf{x}\rangle}{\langle \mathbf{v}, A\mathbf{v}\rangle}\langle \mathbf{v}, \mathbf{b} - A\mathbf{x}\rangle + \left(\frac{\langle \mathbf{v}, \mathbf{b} - A\mathbf{x}\rangle}{\langle \mathbf{v}, A\mathbf{v}\rangle}\right)^2 \langle \mathbf{v}, A\mathbf{v}\rangle \\
&= g(\mathbf{x}) - \frac{\langle \mathbf{v}, \mathbf{b} - A\mathbf{x}\rangle^2}{\langle \mathbf{v}, A\mathbf{v}\rangle}.
\end{aligned}
$$

So for any vector $\mathbf{v} \neq \mathbf{0}$, we have $g(\mathbf{x} + \hat{t}\mathbf{v}) < g(\mathbf{x})$ unless $\langle \mathbf{v}, \mathbf{b} - A\mathbf{x}\rangle = 0$, in which case $g(\mathbf{x}) = g(\mathbf{x} + \hat{t}\mathbf{v})$. This is the basic result we need to prove Theorem 7.31.

Suppose $\mathbf{x}^*$ satisfies $A\mathbf{x}^* = \mathbf{b}$. Then $\langle \mathbf{v}, \mathbf{b} - A\mathbf{x}^*\rangle = 0$ for any vector $\mathbf{v}$, and $g(\mathbf{x})$ cannot be made any smaller than $g(\mathbf{x}^*)$. Thus, $\mathbf{x}^*$ minimizes g.

On the other hand, suppose that $\mathbf{x}^*$ is a vector that minimizes g. Then for any vector $\mathbf{v}$, we have $g(\mathbf{x}^* + \hat{t}\mathbf{v}) \geq g(\mathbf{x}^*)$. Thus, $\langle \mathbf{v}, \mathbf{b} - A\mathbf{x}^*\rangle = 0$. This implies that $\mathbf{b} - A\mathbf{x}^* = \mathbf{0}$ and, consequently, that $A\mathbf{x}^* = \mathbf{b}$. ■ ■ ■

To begin the conjugate gradient method, we choose $\mathbf{x}$, an approximate solution to $A\mathbf{x}^* = \mathbf{b}$, and $\mathbf{v} \neq \mathbf{0}$, which gives a *search direction* in which to move away from $\mathbf{x}$ to improve the approximation. Let $\mathbf{r} = \mathbf{b} - A\mathbf{x}$ be the residual vector associated with $\mathbf{x}$ and

$$t = \frac{\langle \mathbf{v}, \mathbf{b} - A\mathbf{x} \rangle}{\langle \mathbf{v}, A\mathbf{v} \rangle} = \frac{\langle \mathbf{v}, \mathbf{r} \rangle}{\langle \mathbf{v}, A\mathbf{v} \rangle}.$$

If $\mathbf{r} \neq \mathbf{0}$ and if $\mathbf{v}$ and $\mathbf{r}$ are not orthogonal, then $\mathbf{x} + t\mathbf{v}$ gives a smaller value for g than $g(\mathbf{x})$ and is presumably closer to $\mathbf{x}^*$ than is $\mathbf{x}$. This suggests the following method.

Let $\mathbf{x}^{(0)}$ be an initial approximation to $\mathbf{x}^*$, and let $\mathbf{v}^{(1)} \neq \mathbf{0}$ be an initial search direction. For $k = 1, 2, 3, \ldots,$ we compute

$$t_k = \frac{\langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle},$$

$$\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)}$$

and choose a new search direction $\mathbf{v}^{(k+1)}$. The object is to make this selection so that the sequence of approximations $\{\mathbf{x}^{(k)}\}$ converges rapidly to $\mathbf{x}^*$.

To choose the search directions, we view g as a function of the components of $\mathbf{x} = (x_1, x_2, \ldots, x_n)^t$. Thus,

$$g(x_1, x_2, \ldots, x_n) = \langle \mathbf{x}, A\mathbf{x} \rangle - 2\langle \mathbf{x}, \mathbf{b} \rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} x_i x_j - 2 \sum_{i=1}^{n} x_i b_i.$$

Taking partial derivatives with respect to the component variables x_k gives

$$\frac{\partial g}{\partial x_k}(\mathbf{x}) = 2\sum_{i=1}^{n} a_{ki}x_i - 2b_k,$$

which is the kth component of the vector $2(A\mathbf{x} - \mathbf{b})$. Therefore, the gradient of g is

$$\nabla g(\mathbf{x}) = \left(\frac{\partial g}{\partial x_1}(\mathbf{x}), \frac{\partial g}{\partial x_2}(\mathbf{x}), \ldots, \frac{\partial g}{\partial x_n}(\mathbf{x})\right)^t = 2(A\mathbf{x} - \mathbf{b}) = -2\mathbf{r},$$

where the vector $\mathbf{r}$ is the residual vector for $\mathbf{x}$.

From multivariable calculus, we know that the direction of greatest decrease in the value of $g(\mathbf{x})$ is the direction given by $-\nabla g(\mathbf{x})$; that is, in the direction of the residual $\mathbf{r}$. The method that chooses

$$\mathbf{v}^{(k+1)} = \mathbf{r}^{(k)} = \mathbf{b} - A\mathbf{x}^{(k)}$$

is called the *method of steepest descent*. Although we will see in Section 10.4 that this method has merit for nonlinear systems and optimization problems, it is not used for linear systems because of slow convergence.

An alternative approach uses a set of nonzero direction vectors $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$ that satisfy

$$\langle \mathbf{v}^{(i)}, A\mathbf{v}^{(j)} \rangle = 0, \quad \text{if} \quad i \neq j.$$

This is called an A-**orthogonality condition**, and the set of vectors $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$ is said to be A-**orthogonal**. It is not difficult to show that a set of A-orthogonal vectors associated with the positive definite matrix A is linearly independent. (See Exercise 13(a).) This set of search directions gives

$$t_k = \frac{\langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} = \frac{\langle \mathbf{v}^{(k)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle}$$

and $\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)}$.

The following theorem shows that this choice of search directions gives convergence in at most n-steps, so as a direct method it produces the exact solution, assuming that the arithmetic is exact.

Theorem 7.32 Let $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$ be an A-orthogonal set of nonzero vectors associated with the positive definite matrix A, and let $\mathbf{x}^{(0)}$ be arbitrary. Define

$$t_k = \frac{\langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} \quad \text{and} \quad \mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)},$$

for $k = 1, 2, \ldots, n$. Then, assuming exact arithmetic, $A\mathbf{x}^{(n)} = \mathbf{b}$. ■

Proof Since, for each $k = 1, 2, \ldots, n$, $\mathbf{x}^{(k)} = \mathbf{x}^{(k-1)} + t_k \mathbf{v}^{(k)}$, we have

$$\begin{aligned}
A\mathbf{x}^{(n)} &= A\mathbf{x}^{(n-1)} + t_n A\mathbf{v}^{(n)} \\
&= (A\mathbf{x}^{(n-2)} + t_{n-1} A\mathbf{v}^{(n-1)}) + t_n A\mathbf{v}^{(n)} \\
&\ \ \vdots \\
&= A\mathbf{x}^{(0)} + t_1 A\mathbf{v}^{(1)} + t_2 A\mathbf{v}^{(2)} + \cdots + t_n A\mathbf{v}^{(n)}.
\end{aligned}$$

Subtracting $\mathbf{b}$ from this result yields

$$A\mathbf{x}^{(n)} - \mathbf{b} = A\mathbf{x}^{(0)} - \mathbf{b} + t_1 A\mathbf{v}^{(1)} + t_2 A\mathbf{v}^{(2)} + \cdots + t_n A\mathbf{v}^{(n)}.$$

We now take the inner product of both sides with the vector $\mathbf{v}^{(k)}$ and use the properties of inner products and the fact that A is symmetric to obtain

$$\begin{aligned}
\langle A\mathbf{x}^{(n)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle &= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + t_1 \langle A\mathbf{v}^{(1)}, \mathbf{v}^{(k)} \rangle + \cdots + t_n \langle A\mathbf{v}^{(n)}, \mathbf{v}^{(k)} \rangle \\
&= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + t_1 \langle \mathbf{v}^{(1)}, A\mathbf{v}^{(k)} \rangle + \cdots + t_n \langle \mathbf{v}^{(n)}, A\mathbf{v}^{(k)} \rangle.
\end{aligned}$$

The A-orthogonality property gives, for each k,

$$\langle A\mathbf{x}^{(n)} - \mathbf{b}, \mathbf{v}^{(k)}\rangle = \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)}\rangle + t_k\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)}\rangle. \tag{7.29}$$

However $t_k\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)}\rangle = \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(k-1)}\rangle$ so

$$\begin{aligned} t_k\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)}\rangle &= \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)} + A\mathbf{x}^{(0)} - A\mathbf{x}^{(1)} + \cdots - A\mathbf{x}^{(k-2)} + A\mathbf{x}^{(k-2)} - A\mathbf{x}^{(k-1)}\rangle \\ &= \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)}\rangle + \langle \mathbf{v}^{(k)}, A\mathbf{x}^{(0)} - A\mathbf{x}^{(1)}\rangle + \cdots + \langle \mathbf{v}^{(k)}, A\mathbf{x}^{(k-2)} - A\mathbf{x}^{(k-1)}\rangle. \end{aligned}$$

But for any i,

$$\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} + t_i\mathbf{v}^{(i)} \quad \text{and} \quad A\mathbf{x}^{(i)} = A\mathbf{x}^{(i-1)} + t_iA\mathbf{v}^{(i)},$$

so

$$A\mathbf{x}^{(i-1)} - A\mathbf{x}^{(i)} = -t_iA\mathbf{v}^{(i)}.$$

Thus

$$t_k\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)}\rangle = \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)}\rangle - t_1\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(1)}\rangle - \cdots - t_{k-1}\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k-1)}\rangle.$$

Because of the A-orthogonality, $\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(i)} \rangle = 0$, for $i \neq k$, so

$$\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle t_k = \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)} \rangle.$$

From Eq.(7.29),

$$\begin{aligned}
\langle A\mathbf{x}^{(n)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle &= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + \langle \mathbf{v}^{(k)}, \mathbf{b} - A\mathbf{x}^{(0)} \rangle \\
&= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle + \langle \mathbf{b} - A\mathbf{x}^{(0)}, \mathbf{v}^{(k)} \rangle \\
&= \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle - \langle A\mathbf{x}^{(0)} - \mathbf{b}, \mathbf{v}^{(k)} \rangle = 0.
\end{aligned}$$

Hence the vector $A\mathbf{x}^{(n)} - \mathbf{b}$ is orthogonal to the A-orthogonal set of vectors $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$. From this, it follows (see Exercise 13(b)) that $A\mathbf{x}^{(n)} - \mathbf{b} = \mathbf{0}$, so $A\mathbf{x}^{(n)} = \mathbf{b}$. ▪ ▪ ▪

Example 1 The linear system

$$
\begin{aligned}
4x_1 + 3x_2 \phantom{{}-x_3} &= 24,\\
3x_1 + 4x_2 - x_3 &= 30,\\
- x_2 + 4x_3 &= -24
\end{aligned}
$$

has the exact solution $\mathbf{x}^* = (3, 4, -5)^t$. Show that the procedure described in Theorem 7.32 with $\mathbf{x}^{(0)} = (0, 0, 0)^t$ produces this exact solution after three iterations.

Solution We established in Example 2 of Section 7.4 that the coefficient matrix

$$A = \begin{bmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix}.$$

of this system is positive definite. Let $\mathbf{v}^{(1)} = (1, 0, 0)^t$, $\mathbf{v}^{(2)} = (-3/4, 1, 0)^t$, and $\mathbf{v}^{(3)} = (-3/7, 4/7, 1)^t$. Then

$$\langle \mathbf{v}^{(1)}, A\mathbf{v}^{(2)} \rangle = \mathbf{v}^{(1)t} A\mathbf{v}^{(2)} = (1, 0, 0) \begin{bmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} -\frac{3}{4} \\ 1 \\ 0 \end{bmatrix} = 0,$$

$$\langle \mathbf{v}^{(1)}, A\mathbf{v}^{(3)} \rangle = (1, 0, 0) \begin{bmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} -\frac{3}{7} \\ \frac{4}{7} \\ 1 \end{bmatrix} = 0,$$

and

$$\langle \mathbf{v}^{(2)}, A\mathbf{v}^{(3)} \rangle = \left(-\frac{3}{4}, 1, 0 \right) \begin{bmatrix} 4 & 3 & 0 \\ 3 & 4 & -1 \\ 0 & -1 & 4 \end{bmatrix} \begin{bmatrix} -\frac{3}{7} \\ \frac{4}{7} \\ 1 \end{bmatrix} = 0.$$

Hence $\{\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \mathbf{v}^{(3)}\}$ is an A-orthogonal set.

Applying the iterations described in Theorem 7.22 for A with $\mathbf{x}^{(0)} = (0,0,0)^t$ and $\mathbf{b} = (24,30,-24)^t$ gives

$$\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)} = \mathbf{b} = (24,30,-24)^t,$$

so

$$\langle \mathbf{v}^{(1)}, \mathbf{r}^{(0)} \rangle = \mathbf{v}^{(1)t}\mathbf{r}^{(0)} = 24, \quad \langle \mathbf{v}^{(1)}, A\mathbf{v}^{(1)} \rangle = 4, \quad \text{and} \quad t_0 = \frac{24}{4} = 6.$$

Hence

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + t_0\mathbf{v}^{(1)} = (0,0,0)^t + 6(1,0,0)^t = (6,0,0)^t.$$

Continuing, we have

$$\mathbf{r}^{(1)} = \mathbf{b} - A\mathbf{x}^{(1)} = (0,12,-24)^t; \quad t_1 = \frac{\langle \mathbf{v}^{(2)}, \mathbf{r}^{(1)} \rangle}{\langle \mathbf{v}^{(2)}, A\mathbf{v}^{(2)} \rangle} = \frac{12}{7/4} = \frac{48}{7};$$

$$\mathbf{x}^{(2)} = \mathbf{x}^{(1)} + t_1\mathbf{v}^{(2)} = (6,0,0)^t + \frac{48}{7}\left(-\frac{3}{4},1,0\right)^t = \left(\frac{6}{7},\frac{48}{7},0\right)^t;$$

$$\mathbf{r}^{(2)} = \mathbf{b} - A\mathbf{x}^{(2)} = \left(0,0,-\frac{120}{7}\right); \quad t_2 = \frac{\langle \mathbf{v}^{(3)}, \mathbf{r}^{(2)} \rangle}{\langle \mathbf{v}^{(3)}, A\mathbf{v}^{(3)} \rangle} = \frac{-120/7}{24/7} = -5;$$

$$\mathbf{x}^{(3)} = \mathbf{x}^{(2)} + t_2\mathbf{v}^{(3)} = \left(\frac{6}{7},\frac{48}{7},0\right)^t + (-5)\left(-\frac{3}{7},\frac{4}{7},1\right)^t = (3,4,-5)^t.$$

Since we applied the technique $n = 3$ times, this must be the actual solution. ■

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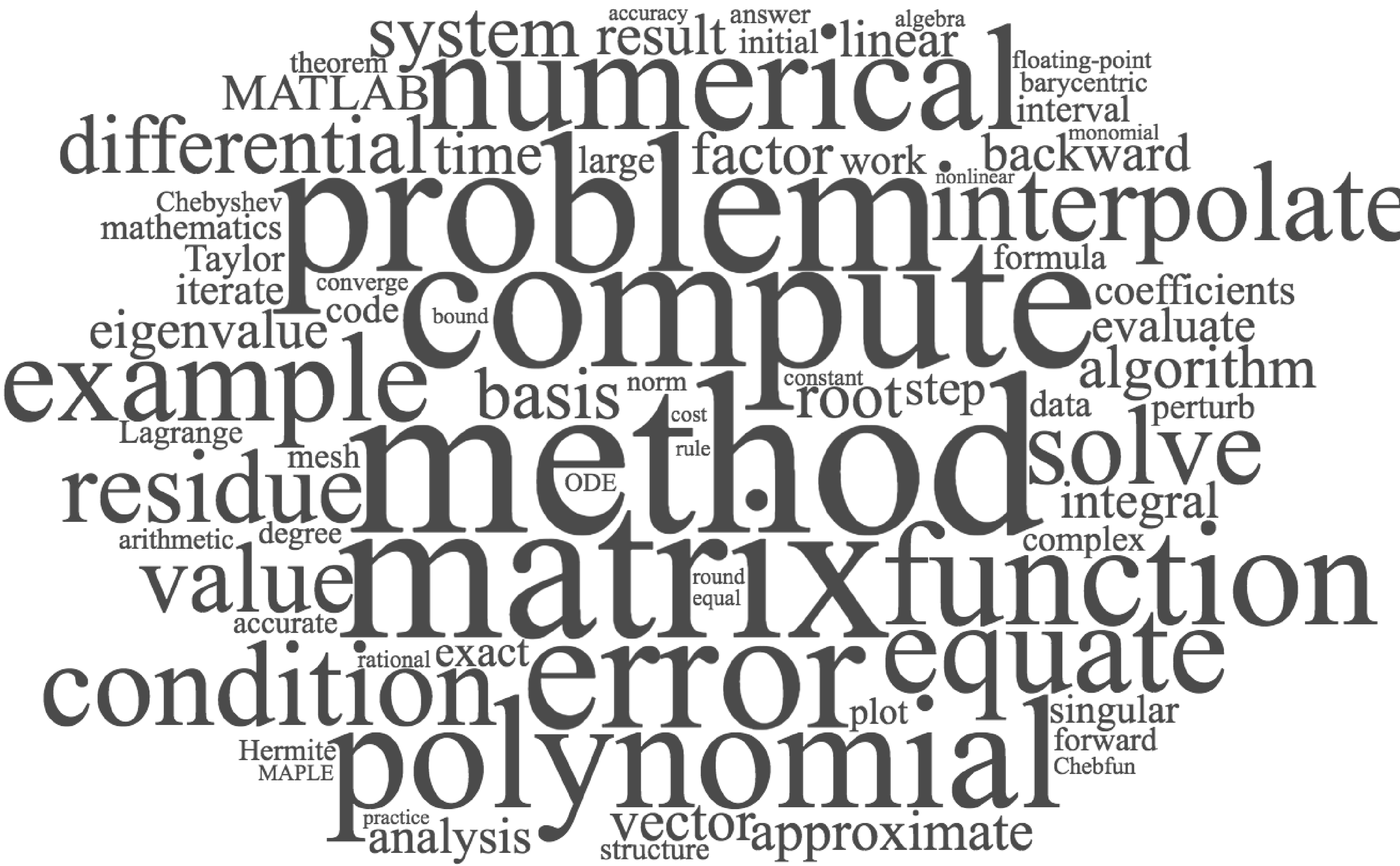
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