

MAP 2210 – Aplicações de Álgebra Linear

1º Semestre - 2020

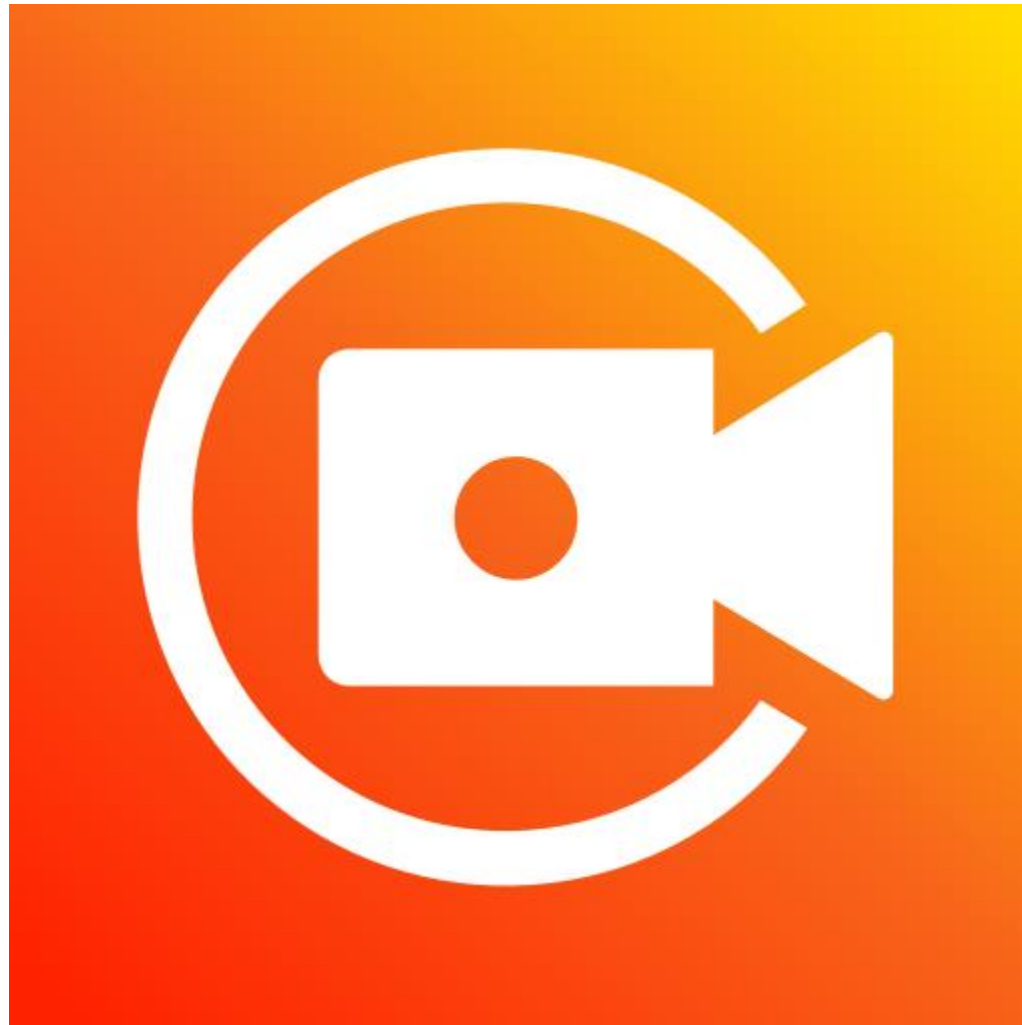
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Objetivos

Formação básica de álgebra linear aplicada a problemas numéricos.
Resolução de problemas em microcomputadores usando linguagens e/ou software adequados fora do horário de aula.

NÃO ESQUEÇA DE INICIAR A GRAVAÇÃO



MAP 2210 – Aplicações de Álgebra Linear

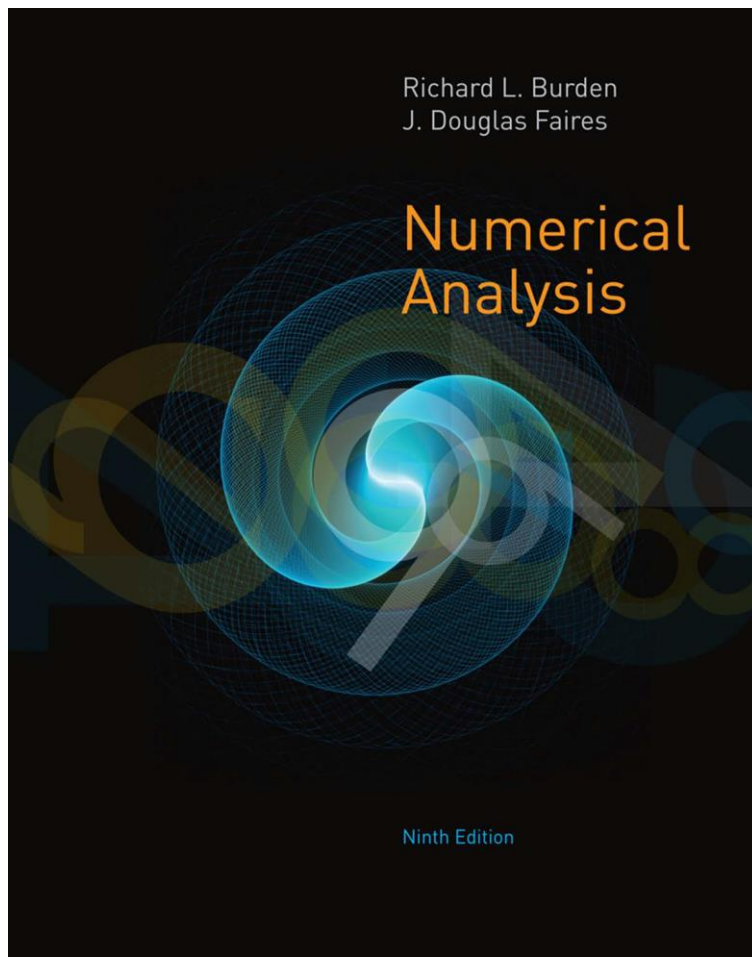
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Numerical Analysis

NINTH EDITION

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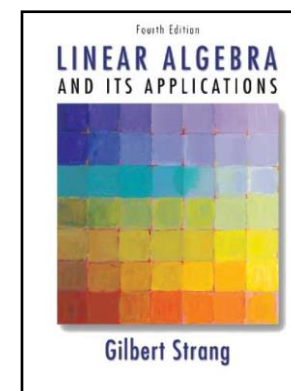
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7.6 The Conjugate Gradient Method

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

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^t \mathbf{y}, \quad (7.26)$$

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.

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} ,

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

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

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

so

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

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 $g(\mathbf{x})$ 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 $k = 1, 2, 3, \dots$, 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 $\mathbf{x} = (x_1, x_2, \dots, x_n)^t$. Thus,

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

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

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

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 $\{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}\}$ that satisfy

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

This is called an ***A-orthogonality condition***, and the set of vectors $\{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}\}$ 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 $\{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}\}$ 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 $k = 1, 2, \dots, n$. Then, assuming exact arithmetic, $A\mathbf{x}^{(n)} = \mathbf{b}$. ■

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

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

Subtracting \mathbf{b} from this result yields

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

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

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

The A -orthogonality property gives, for each k ,

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

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 ,

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

so

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

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 $\{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}\}$.
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

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

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

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

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

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

and

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

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

Before discussing how to determine the A -orthogonal set, we will continue the development. The use of an A -orthogonal set $\{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}\}$ of direction vectors gives what is called a *conjugate direction* method. The following theorem shows the orthogonality of the residual vectors $\mathbf{r}^{(k)}$ and the direction vectors $\mathbf{v}^{(j)}$. A proof of this result using mathematical induction is considered in Exercise 14.

Theorem 7.33

The residual vectors $\mathbf{r}^{(k)}$, where $k = 1, 2, \dots, n$, for a conjugate direction method, satisfy the equations

$$\langle \mathbf{r}^{(k)}, \mathbf{v}^{(j)} \rangle = 0, \quad \text{for each } j = 1, 2, \dots, k.$$



The conjugate gradient method of Hestenes and Stiefel chooses the search directions $\{\mathbf{v}^{(k)}\}$ during the iterative process so that the residual vectors $\{\mathbf{r}^{(k)}\}$ are mutually orthogonal. To construct the direction vectors $\{\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \dots\}$ and the approximations $\{\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \dots\}$, we start with an initial approximation $\mathbf{x}^{(0)}$ and use the steepest descent direction $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$ as the first search direction $\mathbf{v}^{(1)}$.

Assume that the conjugate directions $\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(k-1)}$ and the approximations $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(k-1)}$ have been computed with

$$\mathbf{x}^{(k-1)} = \mathbf{x}^{(k-2)} + t_{k-1}\mathbf{v}^{(k-1)},$$

where

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

If $\mathbf{x}^{(k-1)}$ is the solution to $A\mathbf{x} = \mathbf{b}$, we are done. Otherwise, $\mathbf{r}^{(k-1)} = \mathbf{b} - A\mathbf{x}^{(k-1)} \neq \mathbf{0}$ and Theorem 7.33 implies that $\langle \mathbf{r}^{(k-1)}, \mathbf{v}^{(i)} \rangle = 0$, for each $i = 1, 2, \dots, k-1$.

We use $\mathbf{r}^{(k-1)}$ to generate $\mathbf{v}^{(k)}$ by setting

$$\mathbf{v}^{(k)} = \mathbf{r}^{(k-1)} + s_{k-1}\mathbf{v}^{(k-1)}.$$

We want to choose s_{k-1} so that

$$\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k)} \rangle = 0.$$

Since

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

and

$$\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k)} \rangle = \langle \mathbf{v}^{(k-1)}, A\mathbf{r}^{(k-1)} \rangle + s_{k-1}\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k-1)} \rangle,$$

we will have $\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k)} \rangle = 0$ when

$$s_{k-1} = -\frac{\langle \mathbf{v}^{(k-1)}, A\mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k-1)}, A\mathbf{v}^{(k-1)} \rangle}.$$

It can also be shown that with this choice of s_{k-1} we have $\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(i)} \rangle = 0$, for each $i = 1, 2, \dots, k-2$ (see [Lu], p. 245). Thus $\{\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(k)}\}$ is an A -orthogonal set.

Having chosen $\mathbf{v}^{(k)}$, we compute

$$\begin{aligned} t_k &= \frac{\langle \mathbf{v}^{(k)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} = \frac{\langle \mathbf{r}^{(k-1)} + s_{k-1}\mathbf{v}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} \\ &= \frac{\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle} + s_{k-1} \frac{\langle \mathbf{v}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle}. \end{aligned}$$

By Theorem 7.33, $\langle \mathbf{v}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle = 0$, so

$$t_k = \frac{\langle \mathbf{r}^{(k-1)}, \mathbf{r}^{(k-1)} \rangle}{\langle \mathbf{v}^{(k)}, A\mathbf{v}^{(k)} \rangle}. \quad (7.30)$$

Thus

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

To compute $\mathbf{r}^{(k)}$, we multiply by A and subtract \mathbf{b} to obtain

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

or

$$\mathbf{r}^{(k)} = \mathbf{r}^{(k-1)} - t_k A\mathbf{v}^{(k)}.$$

This gives

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

Further, from Eq. (7.30),

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

so

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

In summary, we have

$$\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}; \quad \mathbf{v}^{(1)} = \mathbf{r}^{(0)};$$

and, for $k = 1, 2, \dots, n$,

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

and

$$\mathbf{v}^{(k+1)} = \mathbf{r}^{(k)} + s_k \mathbf{v}^{(k)}. \tag{7.31}$$

Conjugate Gradient Method

MAP2210

Dados $x(0)$, b , A , N

$r = b - Ax$

$v = r$

$\alpha = \langle v, v \rangle = \langle r, r \rangle$

$k = 1$

Enquanto $k \leq N$

$u = A.v$

$t = \alpha / \langle v, u \rangle$

$x = x + t.v$

$r = r - t.u$

$\beta = \langle r, r \rangle$

se $\beta < \text{TOL}$ saída x, r

$s = \beta / \alpha$

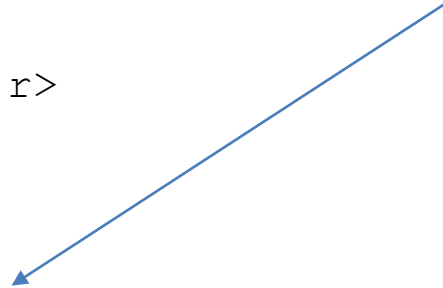
$v = r + s.v$

$\alpha = \beta$

$k = k + 1$

Se $k > N$ saída x, r, k

multiplicação matrix-vetor
pode ser customizada para
matrizes esparsas



Example 2

The linear system $Ax = b$ given by

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

has solution $(3, 4, -5)^t$. Use the conjugate gradient method with $x^{(0)} = (0, 0, 0)^t$

A	4	3	0		
	3	4	-1		
	0	-1	4		
b =	24	30	-24		
k=	0				
x =	0	0	0		
r =	24	30	-24		
v =	24	30	-24		
			alpha	<v,v> =	2052
k=	1				
u = Av	186	216	-126		
				<u,v> =	13968
			t =	alpha/<u,v>	0,14691
x = x + t*v	3,526	4,407	-3,526		
r = r - t*u	-3,325	-1,732	-5,490		
			beta =	<r,r> =	44,1902965
			s =	beta/alpha	0,02154
v = r + s*v	-2,808	-1,086	-6,007		
			alpha =	beta	44,2

 $||r||^2$


k=	2				
u = Av	-14,489	-6,761	-22,940		
				$\langle u, v \rangle =$	185,817
			t =	$\alpha / \langle u, v \rangle$	0,23782
x = x + t*v	2,858	4,149	-4,954		
r = r - t*u	0,121	-0,124	-0,034		
			beta =	$\langle r, r \rangle =$	0,03122766
			s =	β / α	0,00071
v = r + s*v	0,119	-0,125	-0,038		
			alpha =	beta	0,0
k=	3				
u = Av	0,101	-0,104	-0,029		
				$\langle u, v \rangle =$	0,02618391
			t =	$\alpha / \langle u, v \rangle$	1,19263
x = x + t*v	3,000	4,000	-5,000		
r = r - t*u	0,000	0,000	0,000		
			beta =	$\langle r, r \rangle =$	5,9634E-30
			s =	β / α	1,91E-28
v = r + s*v	0,000	0,000	0,000		
			alpha =	beta	0,0

 $\|r\|^2$


EXERCISE SET 7.6

5. Perform only two steps of the conjugate gradient method on each of the following linear systems. Compare the results in parts (b) and (c) to the results obtained in parts (b) and (c) of Exercise 1 of Section 7.3 and Exercise 1 of Section 7.4.

a.
$$\begin{aligned} 3x_1 - x_2 + x_3 &= 1, \\ -x_1 + 6x_2 + 2x_3 &= 0, \\ x_1 + 2x_2 + 7x_3 &= 4. \end{aligned}$$

b.
$$\begin{aligned} 10x_1 - x_2 &= 9, \\ -x_1 + 10x_2 - 2x_3 &= 7, \\ -2x_2 + 10x_3 &= 6. \end{aligned}$$

c.
$$\begin{aligned} 10x_1 + 5x_2 &= 6, \\ 5x_1 + 10x_2 - 4x_3 &= 25, \\ -4x_2 + 8x_3 - x_4 &= -11, \\ -x_3 + 5x_4 &= -11. \end{aligned}$$

d.
$$\begin{aligned} 4x_1 + x_2 - x_3 + x_4 &= -2, \\ x_1 + 4x_2 - x_3 - x_4 &= -1, \\ -x_1 - x_2 + 5x_3 + x_4 &= 0, \\ x_1 - x_2 + x_3 + 3x_4 &= 1. \end{aligned}$$

e.
$$\begin{aligned} 4x_1 + x_2 + x_3 + x_5 &= 6, \\ x_1 + 3x_2 + x_3 + x_4 &= 6, \\ x_1 + x_2 + 5x_3 - x_4 - x_5 &= 6, \\ x_2 - x_3 + 4x_4 &= 6, \\ x_1 - x_3 + 4x_5 &= 6. \end{aligned}$$

f.
$$\begin{aligned} 4x_1 - x_2 - x_4 &= 0, \\ -x_1 + 4x_2 - x_3 - x_5 &= 5, \\ -x_2 + 4x_3 - x_6 &= 0, \\ -x_1 + 4x_4 - x_5 &= 6, \\ -x_2 - x_4 + 4x_5 - x_6 &= -2, \\ -x_3 - x_5 + 4x_6 &= 6. \end{aligned}$$

Implementem o método em Python

Fim...

ALLA 12