

Conjugate Gradient Method for System of Linear Algebraic Equations

Salah Gazi Shareef^{1,*}, Diman Abdulqader Sulaiman²

¹ Department of Mathematic, Faculty of Science, University of Zakho, Zakho, Kurdistan Region, Iraq

Email address: dimanabdulqader90@gmail.com

Email address: salah.gazi2014@gmail.com

Abstract

The Conjugate Gradient Method is an iterative technique for solving large sparse systems of linear equations. As a linear algebra and matrix manipulation technique, it is a useful tool in approximating solutions to linearized partial differential equations. The fundamental concepts are introduced and utilized as the foundation for the derivation of the Conjugate Gradient Method.

Keywords: Conjugate Gradient Method, System of Linear Algebraic Equations, Optimization problems.

1. Introduction

The Conjugate Gradient Method is an iterative technique for solving large sparse systems of linear equations [1–3]. As a linear algebra and matrix manipulation technique, it is a useful tool in approximating solutions to linearized partial differential equations. The fundamental concepts are introduced and utilized as the foundation for the derivation of the Conjugate Gradient Method [4–6]. Alongside the fundamental concepts, an intuitive geometric understanding of the Conjugate Gradient Method's details are included to add clarity [7], [8]. A detailed and rigorous analysis of the theorems which prove the Conjugate Gradient algorithm are presented. Extensions of the Conjugate Gradient Method through preconditioning the system in order to improve the efficiency of the Conjugate Gradient Method are discussed [2], [5], [9–11].

Consider the problem of finding the vector x that minimizes the scalar function

$F(x) = \frac{1}{2}x^T A - b^T x$, where the matrix A is symmetric and positive definite because $f(x)$

is minimized when its gradient $\nabla f = Ax - b$ is zero, we see that minimization is equivalent to solving $Ax = b$

Gradient method accomplishes the minimization by iteration, starting with an initial vector x_0 .

Each iterative cycle k computes a refined solution $x_{k+1} = x_k + \alpha_k d_k$, the step length α_k is chosen so that x_{k+1} minimizes $f(x_{k+1})$ in the search direction d_k that is x_{k+1} must satisfy.

$$d_{k+1}^T A d_k = 0$$

$$Ax=b$$

$$A(x_k + \alpha_k d_k) = b(1)$$

$$Ax_k + \alpha_k A d_k = b$$

$$\alpha_k A d_k = b - Ax_k$$

Introducing the residual $r_k = b - Ax_k$

Eq. (1) becomes $\alpha_k A d_k = r_k$.

Permute multiplying both sides by d_k and solving for α_k , we obtain

$$\alpha_k d_k^T A d_k = d_k^T r_k$$

$$\alpha_k = \frac{d_k^T r_k}{d_k^T A d_k}$$

We are still with the problem of determining the search direction d_k .

Intuition tells us to choose $d_k = -\nabla f = r_k$, since this is the direction of the largest negative change in $f(x)$. [1-2], [4-5], [7]

$$d_{k+1} = r_{k+1} + \beta_k d_k$$

2. New Conjugate Gradient for System of Linear Equations Coefficient 1 (α_k^{new1})

To find a new conjugate gradient for system of linear equations Coefficient 1 we will use the quadratic form:

Let $F(x) = \frac{1}{2}(x - x^*)^T A(x - x^*)$ be a quadratic function

$$\text{and } F(x_{k+1}) = \frac{1}{2}(x_{k+1} - x^*)^T A(x_{k+1} - x^*)$$

Where $x_{k+1} = x_k + \alpha_k d_k$,

$$\text{Then, } F(x_{k+1}) = \frac{1}{2}(x_k + \alpha_k d_k - x^*)^T A(x_k + \alpha_k d_k - x^*)$$

$$\begin{aligned}
 &= \frac{1}{2} (x_k^T A + \alpha_k d_k^T A - x^{*T} A)^T (x_k + \alpha_k d_k - x^*) \\
 &= \frac{1}{2} (x_k^T A x_k + \alpha_k x_k^T A d_k - x_k^T A x^* + \alpha_k d_k^T A x_k + \alpha_k^2 d_k^T A d_k - \alpha_k d_k^T A x^* - \\
 &\quad x^{*T} A x_k - \alpha_k x^{*T} A d_k + x^{*T} A x^*) \\
 \nabla f &= \frac{1}{2} (x_k^T A d_k + d_k^T A x_k + 2\alpha_k d_k^T A d_k - d_k^T A x^* - x^{*T} A d_k) \\
 \nabla f &= \frac{1}{2} (2x_k^T A d_k + 2\alpha_k d_k^T A d_k - 2x^{*T} A d_k) \\
 \nabla f &= x_k^T A d_k + \alpha_k d_k^T A d_k - x^{*T} A d_k
 \end{aligned}$$

We must to compute the $\alpha_k^{new 1}$, and we can write $\nabla f = 0$, then

$$\begin{aligned}
 0 &= x_k^T A d_k + \alpha_k d_k^T A d_k - x^{*T} A d_k \\
 \alpha_k d_k^T A d_k &= x^{*T} A d_k - x_k^T A d_k \\
 \alpha_k^{new 1} &= \frac{x^{*T} A d_k - x_k^T A d_k}{d_k^T A d_k}
 \end{aligned}$$

Becease $x^* = A^{-1}b \Rightarrow b = Ax^*$

$$\text{Then } \alpha_k^{new 1} = \frac{b^T d_k - x_k^T A d_k}{d_k^T A d_k}$$

$$\alpha_k^{new 1} = \frac{d_k^T (b - x_k^T A)}{d_k^T A d_k}$$

2.1. Algorithm of New Conjugate Gradient for System of Linear Equations Coefficient (1):-

Step(1):- choose x_0 (initial point), matrix A and vector b

Step(2):- $r_0 = b - Ax_0$

Step(3):- $d_0 = r_0$

Step(4):- Do with $k=0,1,2,\dots$

$$\alpha_k^{new 1} = \frac{d_k^T (b - x_k^T A)}{d_k^T A d_k}$$

$$x_{k+1} = x_k + \alpha_k d_k$$

$$r_{k+1} = b - Ax_{k+1}$$

If $|r_{k+1}| \leq \varepsilon$ exit loop (convergence criterion ; ε is the error tolerance)

$$\beta_k = \frac{-r_{k+1}^T A d_k}{d_k^T A d_k}$$

$$d_{k+1} = r_{k+1} + \beta_k d_k$$

Step(5):- End do

Example 2.2. Consider the system $\begin{bmatrix} 5 & -2 & 0 \\ -2 & 5 & 1 \\ 0 & 1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 20 \\ 10 \\ -10 \end{bmatrix}$, where $A =$

$\begin{bmatrix} 5 & -2 & 0 \\ -2 & 5 & 1 \\ 0 & 1 & 5 \end{bmatrix}$ is positive definite and symmetric for conjugate gradient method, first

set the starting point $x_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$, so

$$r_0 = b - Ax_0 = \begin{bmatrix} 20 \\ 10 \\ -10 \end{bmatrix} - \begin{bmatrix} 5 & -2 & 0 \\ -2 & 5 & 1 \\ 0 & 1 & 5 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 20 \\ 10 \\ -10 \end{bmatrix}$$

$$r_0 = d_0 = \begin{bmatrix} 20 \\ 10 \\ -10 \end{bmatrix}$$

$$Ad_0 = \begin{bmatrix} 5 & -2 & 0 \\ -2 & 5 & 1 \\ 0 & 1 & 5 \end{bmatrix} \begin{bmatrix} 20 \\ 10 \\ -10 \end{bmatrix} = \begin{bmatrix} 80 \\ 0 \\ -40 \end{bmatrix}$$

$$\alpha_0^{new 1} = \frac{d_0^T (b - x_0^T A)}{d_0^T A d_0} = \frac{400 + 100 + 100}{1600 + 400}$$

$$\alpha_0^{new 1} = 0.3$$

$$x_1 = x_0 + \alpha_0 d_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} + 0.3 \begin{bmatrix} 20 \\ 10 \\ -10 \end{bmatrix}$$

$$x_1 = \begin{bmatrix} 6 \\ 3 \\ -3 \end{bmatrix}$$

$$r_1 = b - Ax_1 = \begin{bmatrix} 20 \\ 10 \\ -10 \end{bmatrix} - \begin{bmatrix} 5 & -2 & 0 \\ -2 & 5 & 1 \\ 0 & 1 & 5 \end{bmatrix} \begin{bmatrix} 6 \\ 3 \\ -3 \end{bmatrix}$$

$$r_1 = \begin{bmatrix} -4 \\ 10 \\ 2 \end{bmatrix}$$

$$\beta_0 = \frac{-r_1^T A d_0}{d_0^T A d_0}$$

$$= \frac{320+80}{1600+400}$$

$$\beta_0 = 0.2$$

$$d_1 = r_1 + \beta_0 d_0 = \begin{bmatrix} -4 \\ 10 \\ 2 \end{bmatrix} + 0.2 \begin{bmatrix} 20 \\ 10 \\ -10 \end{bmatrix}$$

$$d_1 = \begin{bmatrix} 0 \\ 12 \\ 0 \end{bmatrix}$$

$$A d_1 = \begin{bmatrix} 5 & -2 & 0 \\ -2 & 5 & 1 \\ 0 & 1 & 5 \end{bmatrix} \begin{bmatrix} 0 \\ 12 \\ 0 \end{bmatrix} = \begin{bmatrix} -24 \\ 60 \\ 12 \end{bmatrix}$$

$$\alpha_0^{new\ 1} = \frac{d_1^T (b - x_1^T A)}{d_1^T A d_1} = \frac{120}{720}$$

$$\alpha_1 = 0.16666667$$

$$x_2 = x_1 + \alpha_1 d_1 = \begin{bmatrix} 6 \\ 3 \\ -3 \end{bmatrix} + 0.16666667 \begin{bmatrix} 0 \\ 12 \\ 0 \end{bmatrix} = \begin{bmatrix} 6 \\ 3 \\ -3 \end{bmatrix} + \begin{bmatrix} 0 \\ 2.00000004 \\ 0 \end{bmatrix}$$

$$x_2 = \begin{bmatrix} 6 \\ 5.00000004 \\ -3 \end{bmatrix}$$

The exact solution is $x_1 = 6, x_2 = 5$ and $x_3 = -3$.

Example 2.3. Solve the system of linear algebraic equations

$$\begin{bmatrix} 10 & -2 & -1 & -1 \\ -2 & 10 & -1 & -1 \\ -1 & -1 & 10 & -2 \\ -1 & -1 & -2 & 10 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 3 \\ 15 \\ 27 \\ -9 \end{bmatrix}$$

by Conjugate Gradient method with the initial point $x_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

First iteration:

$$\text{Now we compute the } r_0 = b - Ax_0 = \begin{bmatrix} 3 \\ 15 \\ 27 \\ -9 \end{bmatrix} - \begin{bmatrix} 10 & -2 & -1 & -1 \\ -2 & 10 & -1 & -1 \\ -1 & -1 & 10 & -2 \\ -1 & -1 & -2 & 10 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$r_0 = d_0 = \begin{bmatrix} 3 \\ 15 \\ 27 \\ -9 \end{bmatrix}$$

$$Ad_0 = \begin{bmatrix} 10 & -2 & -1 & -1 \\ -2 & 10 & -1 & -1 \\ -1 & -1 & 10 & -2 \\ -1 & -1 & -2 & 10 \end{bmatrix} \begin{bmatrix} 3 \\ 15 \\ 27 \\ -9 \end{bmatrix} = \begin{bmatrix} -18 \\ 126 \\ 270 \\ -162 \end{bmatrix}$$

$$b - x_0^T A = \begin{bmatrix} 3 \\ 15 \\ 27 \\ -9 \end{bmatrix}$$

$$\alpha_0^{new\ 1} = \frac{d_0^T (b - x_0^T A)}{d_0^T Ad_0} = \frac{1044}{10584}$$

$$\alpha_0^{new\ 1} = 0.09864$$

$$x_1 = x_0 + \alpha_0^{new\ 1} d_0 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + 0.09864 \begin{bmatrix} 3 \\ 15 \\ 27 \\ -9 \end{bmatrix}$$

$$x_1 = \begin{bmatrix} 0.29592 \\ 1.4796 \\ 2.66328 \\ -0.88776 \end{bmatrix}$$

second iteration:

$$r_1 = b - Ax_1 = \begin{bmatrix} 3 \\ 15 \\ 27 \\ -9 \end{bmatrix} - \begin{bmatrix} 10 & -2 & -1 & -1 \\ -2 & 10 & -1 & -1 \\ -1 & -1 & 10 & -2 \\ -1 & -1 & -2 & 10 \end{bmatrix} \begin{bmatrix} 0.29592 \\ 1.4796 \\ 2.66328 \\ -0.88776 \end{bmatrix}$$

$$r_1 = \begin{bmatrix} 4.77552 \\ 2.57136 \\ 0.3672 \\ 6.97968 \end{bmatrix}$$

$$\beta_0 = \frac{-r_1^T A d_0}{d_0^T A d_0}$$

$$= \frac{793.53216}{10584}$$

$$\beta_0 = 0.07497$$

$$d_1 = r_1 + \beta_0 d_0 = \begin{bmatrix} 4.77552 \\ 2.57136 \\ 0.3672 \\ 6.97968 \end{bmatrix} + 0.07497 \begin{bmatrix} 3 \\ 15 \\ 27 \\ -9 \end{bmatrix}$$

$$d_1 = \begin{bmatrix} 5.00043 \\ 3.69591 \\ 2.39139 \\ 6.30495 \end{bmatrix}$$

$$d_1^T A d_1 = \begin{bmatrix} 5.00043 \\ 3.69591 \\ 2.39139 \\ 6.30495 \end{bmatrix}^T \begin{bmatrix} 10 & -2 & -1 & -1 \\ -2 & 10 & -1 & -1 \\ -1 & -1 & 10 & -2 \\ -1 & -1 & -2 & 10 \end{bmatrix} \begin{bmatrix} 5.00043 \\ 3.69591 \\ 2.39139 \\ 6.30495 \end{bmatrix} = 555.86432$$

$$d_1^T (b - x_1^T A) = 78.26782$$

$$\alpha_1^{new\ 1} = \frac{d_1^T (b - x_1^T A)}{d_1^T A d_1} = \frac{78.26782}{555.86432}$$

$$\alpha_1^{new\ 1} = 0.14080$$

$$x_2 = x_1 + \alpha_1^{new\ 1} d_1 = \begin{bmatrix} 0.29592 \\ 1.4796 \\ 2.66328 \\ -0.88776 \end{bmatrix} + 0.14080 \begin{bmatrix} 5.00043 \\ 3.69591 \\ 2.39139 \\ 6.30495 \end{bmatrix}$$

$$x_2 = \begin{bmatrix} 0.99998 \\ 1.99998 \\ 2.99999 \\ -0.00002 \end{bmatrix}$$

Then the exact solution is

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 0 \end{bmatrix}$$

3. New Conjugate Gradient for System of Linear Equations Coefficient 2 (α_k^{new2})

To find a new conjugate gradient for system of linear equations Coefficient (2) we will use the quadratic form:

Let $F(x) = \frac{1}{2}(x - x^*)^T A(x - x^*) + (x - x^*)b$ be a quadratic function

And $F(x_{k+1}) = \frac{1}{2}(x_{k+1} - x^*)^T A(x_{k+1} - x^*) + (x_{k+1} - x^*)b$

Because $x_{k+1} = x_k + \alpha_k d_k$, then

$$\begin{aligned} F(x) &= \frac{1}{2}(x_k + \alpha_k d_k - x^*)^T A(x_k + \alpha_k d_k - x^*) + (x_k + \alpha_k d_k - x^*)b \\ &= \frac{1}{2}(x_k^T A x_k + \alpha_k x_k^T A d_k - x_k^T A x^* + \alpha_k d_k^T A x_k + \alpha_k^2 d_k^T A d_k - \alpha_k d_k^T A x^* - \\ &\quad x^{*T} A x_k - \alpha_k x^{*T} A d_k + x^{*T} A x^*) + x_k^T b + \alpha_k d_k^T b - x^{*T} b \\ \nabla f &= \frac{1}{2}(x_k^T A d_k + d_k^T A x_k + 2\alpha_k d_k^T A d_k - d_k^T A x^* - x^{*T} A d_k) + d_k^T b \\ &= \frac{1}{2}(2x_k^T A d_k + 2\alpha_k d_k^T A d_k - 2x^{*T} A d_k) + d_k^T b \\ &= x_k^T A d_k + \alpha_k d_k^T A d_k - x^{*T} A d_k + d_k^T A x^* \\ \nabla f &= x_k^T A d_k + \alpha_k d_k^T A d_k \end{aligned}$$

We must to compute the α_k^{new2} , and we can write $\nabla f = 0$, then

$$\alpha_k d_k^T A d_k = -x_k^T A d_k$$

$$\alpha_k^{new2} = \frac{-x_k^T A d_k}{d_k^T A d_k}$$

Note: the initial point x_0 for α_k^{new2} not equal to zero

3.1. Algorithm of New Conjugate Gradient for System of Linear Equations Coefficient (2) :

Step(1):- choose x_0 (initial point) , matrix A and vector b

Step(2):- $r_0 = b - Ax_0$

Step(3):- $d_0 = r_0$

Step(4):- Do with $k=0,1,2,\dots$

$$\alpha_k^{new\ 2} = \frac{-x_k^T A d_k}{d_k^T A d_k}$$

$$x_{k+1} = x_k + \alpha_k d_k$$

$$r_{k+1} = b - A x_{k+1}$$

If $|r_{k+1}| \leq \varepsilon$ exit loop (convergence criterion ; ε is the error tolerance)

$$\beta_k = \frac{-r_{k+1}^T A d_k}{d_k^T A d_k}$$

$$d_{k+1} = r_{k+1} + \beta_k d_k$$

Step(5):- End do

Example 3.2. Consider the linear system $Ax=b$ given by $Ax = \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$ with the initial point $x_0 = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$, solve by the conjugate gradient method.

Our first step to compute the r_0 by the formula $r_0 = b - Ax$

$$r_0 = b - Ax_0 = \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 9 \\ 5 \end{bmatrix} = \begin{bmatrix} -8 \\ -3 \end{bmatrix}$$

$$r_0 = d_0$$

$$A d_0 = \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} -8 \\ -3 \end{bmatrix} = \begin{bmatrix} -35 \\ -17 \end{bmatrix}$$

$$\alpha_0^{new\ 2} = \frac{-x_0^T A d_0}{d_0^T A d_0} = \frac{87}{331}$$

$$\alpha_0^{new\ 2} = 0.2628$$

$$x_1 = x_0 + \alpha_0^{new 2} d_0 = \begin{bmatrix} 2 \\ 1 \end{bmatrix} + 0.2628 \begin{bmatrix} -8 \\ -3 \end{bmatrix}$$

$$x_1 = \begin{bmatrix} -0.1024 \\ 0.2116 \end{bmatrix}$$

$$r_1 = b - Ax_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} -0.1024 \\ 0.2116 \end{bmatrix}$$

$$r_1 = \begin{bmatrix} 1.198 \\ 1.4647 \end{bmatrix}$$

$$\beta_0 = \frac{-r_1^T Ad_0}{d_0^T Ad_0}$$

$$\text{Since } -r_1^T Ad_0 = 66.8792$$

$$\beta_0 = \frac{66.8792}{331}$$

$$\beta_0 = 0.20205$$

$$d_1 = r_1 + \beta_0 d_0 = \begin{bmatrix} 1.198 \\ 1.4647 \end{bmatrix} + 0.20205 \begin{bmatrix} -8 \\ -3 \end{bmatrix}$$

$$d_1 = \begin{bmatrix} -0.4184 \\ 0.86145 \end{bmatrix}$$

$$Ad_1 = \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} -0.4184 \\ 0.86145 \end{bmatrix} = \begin{bmatrix} -0.81215 \\ 2.16595 \end{bmatrix}$$

$$\alpha_1^{new 2} = \frac{-x_1^T Ad_1}{d_1^T Ad_1} = \frac{-0.54148}{2.20566}$$

$$\alpha_1^{new 2} = -0.2455$$

$$x_2 = x_1 + \alpha_1^{new 2} d_1 = \begin{bmatrix} -0.1024 \\ 0.2116 \end{bmatrix} + (-0.2455) \begin{bmatrix} -0.4184 \\ 0.86145 \end{bmatrix}$$

$$x_2 = \begin{bmatrix} -0.39651 \\ -0.1487 \end{bmatrix}$$

$$r_2 = b - Ax_2 = \begin{bmatrix} 1 \\ 2 \end{bmatrix} - \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} -0.39651 \\ -0.1487 \end{bmatrix}$$

$$r_2 = \begin{bmatrix} 2.73474 \\ 2.84261 \end{bmatrix}$$

$$\beta_1 = \frac{-r_2^T Ad_1}{d_1^T Ad_1}$$

$$-r_2^T Ad_1 = -3.93593$$

$$= \frac{-3.93593}{2.20566}$$

$$\beta_1 = -1.78447$$

$$d_2 = r_2 + \beta_1 d_1 = \begin{bmatrix} 2.73474 \\ 2.84261 \end{bmatrix} + (-1.78447) \begin{bmatrix} -0.4184 \\ 0.86145 \end{bmatrix}$$

$$d_2 = \begin{bmatrix} 3.48136 \\ 1.30538 \end{bmatrix}$$

$$Ad_2 = \begin{bmatrix} 4 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 3.48136 \\ 1.30538 \end{bmatrix} = \begin{bmatrix} 15.23082 \\ 7.39752 \end{bmatrix}$$

$$\alpha_2^{new\ 2} = \frac{-x_2^T Ad_2}{d_2^T Ad_2} = \frac{7.13918}{62.68052}$$

$$\alpha_2^{new\ 2} = 0.1139$$

$$x_3 = x_2 + \alpha_2^{new\ 2} d_2 = \begin{bmatrix} -0.39651 \\ -0.1487 \end{bmatrix} + 0.1139 \begin{bmatrix} 3.48136 \\ 1.30538 \end{bmatrix}$$

$$x_3 = \begin{bmatrix} 0.00002 \\ -0.00002 \end{bmatrix}$$

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