

Numerical Analysis

Numerical Analysis Iterative methods

by Csaba Gáspár

Széchenyi István University

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Numerical Analysis

The fixed point theorem and its applications

Banach's fixed point theorem

Suppose that the mapping $F: \mathbf{R}^N \to \mathbf{R}^N$ is a **contraction**, i.e. there exists a constant $0 \le q < 1$ such that for arbitrary $x, y \in \mathbf{R}^N$, the following inequality holds:

 $||F(x) - F(y)|| \le q \cdot ||x - y||$. Then the equation x = F(x)

$$x^{(n+1)} := F(x^{(n)}) \qquad (n = 0, 1, 2, ...)$$



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The fixed point theorem and its applications

Banach's fixed point theorem

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 $||F(x) - F(y)|| \le q \cdot ||x - y||$. Then the equation x = F(x)has a unique solution $x^* \in \mathbf{R}^N$, (which is called the **fixed point** of F). Moreover, for arbitrary vector $x_0 \in \mathbb{R}^N$, the

$$x^{(n+1)} := F(x^{(n)})$$
 $(n = 0, 1, 2, ...)$

$$||x^{(n)} - x^*|| \le q^n \cdot ||x^{(0)} - x^*||.$$



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Banach's fixed point theorem

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 $||F(x) - F(y)|| \le q \cdot ||x - y||$. Then the equation x = F(x) has a unique solution $x^* \in \mathbf{R}^N$, (which is called the **fixed point** of F). Moreover, for arbitrary vector $x_0 \in \mathbf{R}^N$, the vector sequence defined by the recursion

$$x^{(n+1)} := F(x^{(n)})$$
 $(n = 0, 1, 2, ...)$

converges to the fixed point x^* .

The error of the nth element:

$$||x^{(n)} - x^*|| \le q^n \cdot ||x^{(0)} - x^*||.$$



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Let $B \in \mathbf{M}_{N \times N}$ be a given matrix, and let $f \in \mathbf{R}^N$ be a given vector. Consider the algebraic linear system

$$x = Bx + f$$

If any of the matrix norms of B induced by a vector norm is less than 1, then the above system of equations has a unique solution x^* , namely, for arbitrary starting vector, $x^{(0)}$, the vector sequence defined by the recursion

$$x^{(n+1)} := Bx^{(n)} + f$$
 $(n = 0, 1, 2, ...)$

converges to the (unique) solution x^* .

The error of the nth term can be estimated by:

$$|x^{(n)} - x^*|| \le ||B||^n \cdot ||x^{(0)} - x^*||.$$



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 $(n = 0, 1, 2, ...)$

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The error of the nth term can be estimated by:

$$||x^{(n)} - x^*|| < ||B||^n \cdot ||x^{(0)} - x^*||.$$



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Another (a priori) error estimation:

$$||x^{(n)} - x^*|| \le \frac{||B||^n}{1 - ||B||} \cdot ||x^{(1)} - x^{(0)}||.$$

And an a posteriori error estimation:

$$|x^{(n)} - x^*|| \le \frac{||B||}{1 - ||B||} \cdot ||x^{(n)} - x^{(n-1)}||.$$



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Fixed point iteration

Define $B:=\left(\begin{array}{ccc} 0.00 & 0.50 & 0.25 \\ 0.50 & 0.00 & 0.25 \\ 0.50 & 0.25 & 0.00 \end{array} \right)$, $f:=\left(\begin{array}{c} 0.25 \\ 0.25 \\ 0.25 \end{array} \right)$, and

consider the system of equations x = Bx + f The exact

$$x = Bx + f$$
 The example $x = Bx + f$

solution:
$$x^* = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$
.



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 $\text{Define }B:=\left(\begin{array}{ccc}0.00&0.50&0.25\\0.50&0.00&0.25\\0.50&0.25&0.00\end{array}\right),\quad f:=\left(\begin{array}{c}0.25\\0.25\\0.25\end{array}\right)\text{, and}$

consider the system of equations x = Bx + f The exact

solution:
$$x^* = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$
.

The column sum norm of B equals to 1, but the row sum norm is 0.75. Thus, the fixed point theorem is applicable.



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$$\text{Define }B:=\left(\begin{array}{ccc}0.00 & 0.50 & 0.25\\0.50 & 0.00 & 0.25\\0.50 & 0.25 & 0.00\end{array}\right),\quad f:=\left(\begin{array}{c}0.25\\0.25\\0.25\end{array}\right)\text{, and}$$

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Fixed point iteration

Let the starting approximation be as follows:

$$x^{(0)} := \left(\begin{array}{c} 1.0000 \\ 2.0000 \\ -3.0000 \end{array} \right).$$



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Let the starting approximation be as follows:

$$x^{(0)} := \left(\begin{array}{c} 1.0000 \\ 2.0000 \\ -3.0000 \end{array} \right).$$

$$x^{(1)} := \left(\begin{array}{c} 0.5000\\ 0.0000\\ 1.2500 \end{array}\right)$$



Numerical Analysis

Fixed point iteration

Let the starting approximation be as follows:

$$x^{(0)} := \left(\begin{array}{c} 1.0000 \\ 2.0000 \\ -3.0000 \end{array} \right).$$

$$x^{(2)} := \left(\begin{array}{c} 0.5625\\ 0.8125\\ 0.5000 \end{array}\right)$$



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Let the starting approximation be as follows:

$$x^{(0)} := \left(\begin{array}{c} 1.0000 \\ 2.0000 \\ -3.0000 \end{array} \right).$$

$$x^{(3)} := \left(\begin{array}{c} 0.7813\\ 0.6563\\ 0.7344 \end{array}\right)$$



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Fixed point iteration

Let the starting approximation be as follows:

$$x^{(0)} := \left(\begin{array}{c} 1.0000 \\ 2.0000 \\ -3.0000 \end{array} \right).$$

$$x^{(4)} := \left(\begin{array}{c} 0.7617\\ 0.8242\\ 0.8047 \end{array}\right)$$



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Fixed point iteration

Let the starting approximation be as follows:

$$x^{(0)} := \left(\begin{array}{c} 1.0000 \\ 2.0000 \\ -3.0000 \end{array} \right).$$

$$x^{(5)} := \left(\begin{array}{c} 0.8633\\ 0.8320\\ 0.8369 \end{array}\right)$$



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Let the starting approximation be as follows:

$$x^{(0)} := \left(\begin{array}{c} 1.0000 \\ 2.0000 \\ -3.0000 \end{array} \right).$$

$$x^{(6)} := \left(\begin{array}{c} 0.8752\\ 0.8909\\ 0.8896 \end{array}\right)$$



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Fixed point iteration

Let the starting approximation be as follows:

$$x^{(0)} := \left(\begin{array}{c} 1.0000 \\ 2.0000 \\ -3.0000 \end{array} \right).$$

$$x^{(7)} := \left(\begin{array}{c} 0.9178\\ 0.9100\\ 0.9103 \end{array}\right)$$



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Let $B \in \mathbf{M}_{N \times N}$ be a matrix and let $f \in \mathbf{R}^N$ be a vector and consider the linear system of equations:

$$x = Bx + f$$

For convergence, the condition ||B|| < 1 is sufficient but not necessary...

If the absolute values of all eigenvalues of B are less than 1, then the above equation has a unique solution x^* , and for arbitrary starting vector $x^{(0)}$, the recursively defined sequence

$$x^{(n+1)} := Bx^{(n)} + f$$
 $(n = 0, 1, 2, ...)$

converges to the (unique) solution x^*



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method The conjugate gradient method Let $B \in \mathbf{M}_{N \times N}$ be a matrix and let $f \in \mathbf{R}^N$ be a vector and consider the linear system of equations:

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The conjugate gradient metho Sometimes it may be dangerous...



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Fixed point iteration

Define
$$B:=\left(egin{array}{cccc} 0.5 & 100 & 0 & 0 \\ 0 & 0.5 & 100 & 0 \\ 0 & 0 & 0.5 & 100 \\ 0 & 0 & 0 & 0.5 \end{array} \right)$$
, and consider the

system of equations x = Bx. The exact solutions is: $x^* = 0$.



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system of equations x = Bx. The exact solutions is: $x^* = 0$.

Each eigenvalue of B equals to 0.5, thus, the above theorem is applicable.



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Each eigenvalue of ${\cal B}$ equals to 0.5, thus, the above theorem is applicable.



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Fixed point iteration

Let the starting approximation be:
$$x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$
.



Numerical Analysis

Fixed point iteration

Let the starting approximation be:
$$x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$
.

$$x^{(1)} := \left(\begin{array}{c} 0\\0\\100.0\\0.5 \end{array}\right)$$



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Let the starting approximation be: $x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

Then the first 7 terms:

$$x^{(2)} := \left(\begin{array}{c} 0\\10000\\100\\0\end{array}\right)$$

For larger matrices which have the same structure, this necessarily causes overflow.



Numerical Analysis

Fixed point

iteration

Let the starting approximation be:
$$x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$
.

$$x^{(3)} := \begin{pmatrix} 1000000 \\ 15000 \\ 100 \\ 0 \end{pmatrix}$$



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Let the starting approximation be: $x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

Then the first 7 terms:

$$x^{(4)} := \begin{pmatrix} 2000000 \\ 15000 \\ 100 \\ 0 \end{pmatrix}$$

For larger matrices which have the same structure, this necessarily causes overflow.



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Let the starting approximation be:
$$x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$
.

Then the first 7 terms:

$$x^{(5)} := \begin{pmatrix} 2500000 \\ 12500 \\ 0 \\ 0 \end{pmatrix}$$

For larger matrices which have the same structure, this necessarily causes overflow.



Application to linear systems of equations

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Let the starting approximation be: $x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$.

Then the first 7 terms:

$$x^{(6)} := \begin{pmatrix} 2500000 \\ 9400 \\ 0 \\ 0 \end{pmatrix}$$

For larger matrices which have the same structure, this necessarily causes overflow.



Application to linear systems of equations

Numerical Analysis

Fixed point iteration

Let the starting approximation be:
$$x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$
.

Then the first 7 terms:

$$x^{(7)} := \begin{pmatrix} 2187500 \\ 6600 \\ 0 \\ 0 \end{pmatrix}$$



Application to linear systems of equations

Numerical Analysis

Fixed point iteration

Let the starting approximation be:
$$x^{(0)} := \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$
.

Then the first 7 terms:

$$x^{(7)} := \begin{pmatrix} 2187500 \\ 6600 \\ 0 \\ 0 \end{pmatrix}$$

For larger matrices which have the same structure, this necessarily causes overflow.



Numerical Analysis

The Richardson iteration

Let $A \in \mathbf{M}_{N \times N}$ be a self-adjoint, positive definite matrix. Let $b \in \mathbf{R}^N$ be a vector and consider the linear system of equations:

$$Ax = b$$

$$x = x - \omega \cdot (Ax - b) = (I - \omega A)x + \omega b$$

$$x^{(n+1)} := (I - \omega A)x^{(n)} + \omega b$$

$$(n = 0, 1, 2, ...)$$



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Let $A \in \mathbf{M}_{N \times N}$ be a **self-adjoint, positive definite** matrix. Let $b \in \mathbf{R}^N$ be a vector and consider the linear system of equations:

$$Ax = b$$

which is equivalent to the system of equations

$$x = x - \omega \cdot (Ax - b) = (I - \omega A)x + \omega b$$

(where $\omega > 0$ is a temporarily arbitrary parameter).

Applying the fixed point iteration:

$$x^{(n+1)} := (I - \omega A)x^{(n)} + \omega b$$

$$= x^{(n)} - \omega(Ax^{(n)} - b)$$

$$(n = 0, 1, 2, \dots)$$



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$$= x^{(n)} - \omega(Ax^{(n)} - b)$$

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$$x^{(n+1)} := (I - \omega A)x^{(n)} + \omega b$$
 $= x^{(n)} - \omega (Ax^{(n)} - b)$

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Let $A \in \mathbf{M}_{N \times N}$ be a self-adjoint, positive definite matrix.

Convergence theorem

For each parameter $0<\omega<\frac{2}{||A||}$, (where ||A|| is an arbitrary matrix norm induced by a vector norm):

$$\rho(I - \omega A) < 1,$$

consequently, the Richardson iteration is convergent.

Thus, if we define $\omega:=\frac{1}{||A||}$, then the iteration is convergent. ω should be defined in such a way that the convergence is as fast as possible.



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Solution of systems of equations by Richardson's iteration

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The optimal choice of the parameter

The spectral radius $\rho(I-\omega A)$ is the least (thus, the convergence is the fastest), when

$$\omega = \frac{2}{\lambda_{\max} + \lambda_{\min}}. \quad \text{In this case: } \rho(I - \omega A) = \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}}$$

For the optimal choice of the parameter ω , one needs information about the eigenvalues of A.

If the quotient $\lambda_{\text{max}}/\lambda_{\text{min}}$ i.e. the condition number of A is great, then the convergence remains slow (even if the parameter is optimally chosen).



Solution of systems of equations by Richardson's iteration

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$$\omega = \frac{2}{\lambda_{\max} + \lambda_{\min}}. \quad \text{In this case: } \rho(I - \omega A) = \frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}}$$

For the optimal choice of the parameter ω , one needs information about the eigenvalues of A.

If the quotient $\lambda_{\rm max}/\lambda_{\rm min}$ i.e. the condition number of A is great, then the convergence remains slow (even if the parameter is optimally chosen).



Solution of systems of equations by Richardson's iteration

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Let $A \in \mathbf{M}_{N \times N}$ be a regular matrix. Let $b \in \mathbf{R}^N$ be a vector and consider the system of equations:

$$Ax = b$$

Componentwise:

$$\sum_{j=1}^{k-1} A_{kj} x_j + A_{kk} x_k + \sum_{j=k+1}^{N} A_{kj} x_j = b_k \quad (k = 1, 2, ..., N)$$

Rearranging the equations:

$$x_k = \frac{1}{A_{kk}} \left(-\sum_{j=1}^{k-1} A_{kj} x_j - \sum_{j=k+1}^{N} A_{kj} x_j + b_k \right) \quad (k = 1, 2, ..., N)$$



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This gives us the following iteration (Jacobi iteration):

$$x_k^{(n+1)} := \frac{1}{A_{kk}} \left(-\sum_{j=1}^{k-1} A_{kj} x_j^{(n)} - \sum_{j=k+1}^N A_{kj} x_j^{(n)} + b_k \right)$$

$$(k = 1, 2, ..., N, n = 0, 1, 2, ...)$$

Formally: decompose A into a sum of a lower triangular, a diagonal and an upper diagonal matrix: A = L + D + U. Ther the Jacobi iteration has the form:

$$x^{(n+1)} := D^{-1}(-(L+U)x^{(n)} + b)$$
 $(n = 0, 1, 2, ...)$



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The Jacobi iteration

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Convergence theorem

If the matrix A is diagonally dominant, i.e.

$$|A_{kk}| > \sum_{j \neq k} |A_{kj}|, \qquad (k = 1, 2, ..., N)$$

then the Jacobi iteration is convergent.

In this case, the row sum norm of $B := D^{-1}(-L - U)$ is less than 1, since:

$$\sum_{j=1}^{N} |B_{kj}| \le \frac{1}{|A_{kk}|} \sum_{j \ne k} |A_{kj}| < 1 \qquad (k = 1, 2, ..., N)$$



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$$x_k = \frac{1}{A_{kk}} \left(-\sum_{j=1}^{k-1} A_{kj} x_j - \sum_{j=k+1}^{N} A_{kj} x_j + b_k \right) \quad (k = 1, 2, ..., N)$$

whence (Seidel iteration):

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Formally: decompose A into a sum of a lower triangular, a diagonal and an upper diagonal matrix: A = L + D + U. Then the Seidel iteration has the form:

$$x^{(n+1)} := (L+D)^{-1}(-Ux^{(n)} + b) \qquad (n = 0, 1, 2, ...)$$

Convergence theorems

- 1) If the matrix A is **diagonally dominant**, then the Seidel iteration is convergent.
- 2) If the matrix A is self-adjoint and positive definite, then the Seidel iteration is convergent.



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Let $A \in \mathbf{M}_{N \times N}$ be a self-adjoint and positive definite matrix. Let $b \in \mathbf{R}^N$ be a vector and consider the linear system of equations:

$$Ax = b$$

Denote by x^* the exact solution.

Energetic inner product and norm

Define

$$\langle x, y \rangle_A := \langle Ax, y \rangle$$

(energetic inner product) and

$$||x||_A := \sqrt{\langle x, x \rangle_A} = \sqrt{\langle Ax, x \rangle}$$

(energetic norm)



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Variational methods

Energetic functional

Denote by $F: \mathbf{R}^N \to \mathbf{R}$ the energetic functional:

$$F(x) := \langle Ax, x \rangle - 2\langle x, b \rangle = ||x||_A^2 - 2\langle x, x^* \rangle_A = ||x - x^*||_A^2 - ||x^*||_A^2$$



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Variational principle

There exists a unique vector x^* which minimizes the energetic functional F, and this equals to the unique solution of the equation Ax=b .

The methods based on the minimization of the functional ${\cal F}$ are called **variational methods**.



Numerical Analysis

Variational methods

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Minimization along a direction

Let $x \in \mathbf{R}^N$ be an approximate minimizing vector of F. Let $e \in \mathbf{R}^N$ be a given direction vector. Seek the minimizing vector of F along a line which passes through the point x and has the direction vector e, i.e. minimize the univariate function

$$f(t) := F(x + t \cdot e) = \langle Ax + t \cdot Ae, x + t \cdot e \rangle - 2\langle x + t \cdot e, b \rangle$$

The vector $\tilde{x} := x + t \cdot e$ is considered an improved minimizing vector of F.

$$f(t) = \langle Ax, x \rangle + 2t \langle Ax, e \rangle + t^2 \langle Ae, e \rangle - 2\langle x, b \rangle - 2t \langle b, e \rangle$$

= $F(x) + 2t \langle Ax - b, e \rangle + t^2 \langle Ae, e \rangle$, whence

 $t = -\frac{\langle Ax - b, e \rangle}{\langle Ae, e \rangle} \qquad \tilde{x} = x - \frac{\langle Ax - b, e \rangle}{\langle Ae, e \rangle} e$



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In each step, perform a minimization along the direction e:= $r^{(n)} := Ax^{(n)} - b \quad \text{(which is the direction of the steepest decrease of } F \text{ at the point } x^{(n)} \text{) i.e.}$

$$x^{(n+1)} := x^{(n)} - \frac{||r^{(n)}||^2}{\langle Ar^{(n)}, r^{(n)} \rangle} r^{(n)} \quad (n = 0, 1, 2, ...)$$

In each step of the gradient method, a Richardson type iteration is performed. The speed of convergence is not less than that of the Richardson iteration with the optimal parameter. However, here no information is needed about the eigenvalues of A.



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The conjugate gradient method

Let $x^{(0)}\in\mathbf{R}^N$ be an arbitrary starting approximation. Define $r^{(0)}:=Ax^{(0)}-b$, $d^{(0)}:=-r^{(0)}$, and for n=0,1,2...:

$$r^{(n)} := Ax^{(n)} - b$$

$$x^{(n+1)} := x^{(n)} - \frac{\langle r^{(n)}, d^{(n)} \rangle}{\langle Ad^{(n)}, d^{(n)} \rangle} \cdot d^{(n)}$$

$$r^{(n+1)} := Ax^{(n+1)} - b$$

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$$\begin{split} r^{(n)} &:= Ax^{(n)} - b \\ x^{(n+1)} &:= x^{(n)} - \frac{\langle r^{(n)}, d^{(n)} \rangle}{\langle Ad^{(n)}, d^{(n)} \rangle} \cdot d^{(n)} \\ r^{(n+1)} &:= Ax^{(n+1)} - b \\ d^{(n+1)} &:= -r^{(n+1)} + \frac{\langle Ar^{(n+1)}, d^{(n)} \rangle}{\langle Ad^{(n)}, d^{(n)} \rangle} \cdot d^{(n)} \end{split}$$



The conjugate gradient method

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If no round-off errors are generated, then the conjugate gradient method provides the exact solution after at most N iteration steps.