Numerical Analysis
Iterative methods

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The fixed point theorem for multivariate functions

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 $x = F(x)$ 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

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

converges to the fixed point x^*.

The error of the nth element:

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

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Application to linear systems of equations

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

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

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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Application to linear systems of equations

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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Application to linear systems of equations, example

Define $B := \begin{pmatrix} 0.00 & 0.50 & 0.25 \\ 0.50 & 0.00 & 0.25 \\ 0.50 & 0.25 & 0.00 \end{pmatrix}$, $f := \begin{pmatrix} 0.25 \\ 0.25 \\ 0.25 \end{pmatrix}$, and consider the system of equations $\boxed{x = Bx + f}$ 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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Let the starting approximation be as follows:

$$x^{(0)} := \begin{pmatrix} 1.0000 \\ 2.0000 \\ -3.0000 \end{pmatrix}.$$

Then the first 7 terms:

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Let the starting approximation be as follows:

$$x^{(0)} := \begin{pmatrix} 1.0000 \\ 2.0000 \\ -3.0000 \end{pmatrix}.$$

Then the first 7 terms:

$$x^{(1)} := \begin{pmatrix} 0.5000 \\ 0.0000 \\ 1.2500 \end{pmatrix}$$

Application to linear systems of equations, example

Let the starting approximation be as follows:

$$x^{(0)} := \begin{pmatrix} 1.0000 \\ 2.0000 \\ -3.0000 \end{pmatrix}.$$

Then the first 7 terms:

$$x^{(2)} := \begin{pmatrix} 0.5625 \\ 0.8125 \\ 0.5000 \end{pmatrix}$$

Application to linear systems of equations, example

Let the starting approximation be as follows:

$$x^{(0)} := \begin{pmatrix} 1.0000 \\ 2.0000 \\ -3.0000 \end{pmatrix}.$$

Then the first 7 terms:

$$x^{(3)} := \begin{pmatrix} 0.7813 \\ 0.6563 \\ 0.7344 \end{pmatrix}$$

Application to linear systems of equations, example

Let the starting approximation be as follows:

$$x^{(0)} := \begin{pmatrix} 1.0000 \\ 2.0000 \\ -3.0000 \end{pmatrix}.$$

Then the first 7 terms:

$$x^{(4)} := \begin{pmatrix} 0.7617 \\ 0.8242 \\ 0.8047 \end{pmatrix}$$

Application to linear systems of equations, example

Let the starting approximation be as follows:

$$x^{(0)} := \begin{pmatrix} 1.0000 \\ 2.0000 \\ -3.0000 \end{pmatrix}.$$

Then the first 7 terms:

$$x^{(5)} := \begin{pmatrix} 0.8633 \\ 0.8320 \\ 0.8369 \end{pmatrix}$$

Application to linear systems of equations, example

Let the starting approximation be as follows:

$$x^{(0)} := \begin{pmatrix} 1.0000 \\ 2.0000 \\ -3.0000 \end{pmatrix}.$$

Then the first 7 terms:

$$x^{(6)} := \begin{pmatrix} 0.8752 \\ 0.8909 \\ 0.8896 \end{pmatrix}$$

Application to linear systems of equations, example

Let the starting approximation be as follows:

$$x^{(0)} := \begin{pmatrix} 1.0000 \\ 2.0000 \\ -3.0000 \end{pmatrix}.$$

Then the first 7 terms:

$$x^{(7)} := \begin{pmatrix} 0.9178 \\ 0.9100 \\ 0.9103 \end{pmatrix}$$

Application to linear systems of equations

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

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

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Application to linear systems of equations

Sometimes it may be dangerous...

Application to linear systems of equations

Define $B := \begin{pmatrix} 0.5 & 100 & 0 & 0 \\ 0 & 0.5 & 100 & 0 \\ 0 & 0 & 0.5 & 100 \\ 0 & 0 & 0 & 0.5 \end{pmatrix}$, and consider the system of equations $\boxed{x = Bx}$. The exact solutions is: $x^* = \mathbf{0}$.

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

Application to linear systems of equations

Define $B := \begin{pmatrix} 0.5 & 100 & 0 & 0 \\ 0 & 0.5 & 100 & 0 \\ 0 & 0 & 0.5 & 100 \\ 0 & 0 & 0 & 0.5 \end{pmatrix}$, and consider the system of equations $\boxed{x = Bx}$. The exact solutions is: $x^* = \mathbf{0}$.

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Define $B := \begin{pmatrix} 0.5 & 100 & 0 & 0 \\ 0 & 0.5 & 100 & 0 \\ 0 & 0 & 0.5 & 100 \\ 0 & 0 & 0 & 0.5 \end{pmatrix}$, and consider the system of equations $\boxed{x = Bx}$. The exact solutions is: $x^* = \mathbf{0}$.

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Application to linear systems of equations

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

Then the first 7 terms:

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:

$$x^{(1)} := \begin{pmatrix} 0 \\ 0 \\ 100.0 \\ 0.5 \end{pmatrix}$$

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

Application to linear systems of equations

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

Then the first 7 terms:

$$x^{(2)} := \begin{pmatrix} 0 \\ 10000 \\ 100 \\ 0 \end{pmatrix}$$

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Application to linear systems of equations

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

Then the first 7 terms:

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

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

Application to linear systems of equations

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

Then the first 7 terms:

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

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Application to linear systems of equations

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

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

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

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Application to linear systems of equations

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

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

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

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:

$$Ax = b$$

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:

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

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

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The Richardson iteration

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.

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

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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.

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

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The Jacobi iteration

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:

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

Rearranging the equations:

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

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This gives us the following iteration (**Jacobi iteration**):

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

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

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

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

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The Jacobi iteration

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:

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

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The Seidel iteration

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 written (similarly to the Jacobi iteration):

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

whence (**Seidel iteration**):

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

The Seidel iteration

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 written (similarly to the Jacobi iteration):

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The Seidel iteration

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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The variational principle

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

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

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Energetic functional

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

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

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 F are called **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.

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

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

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The gradient method

The gradient method

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

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

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

$$Ax = b$$

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 $n = 0, 1, 2...$:

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

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

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The conjugate gradient method

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