Iterative methods for solving linear systems

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EPFL

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Plan

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Iterative methods

(Sec. 6.3 of the book)

Solve the linear system $A\mathbf{x} = \mathbf{b}$, $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$ using an iterative method consists in building a series of vectors $\mathbf{x}^{(k)}$, $k \geq 0$, in $\mathbb{R}^n$ that converge at the exact solution $\mathbf{x}$, i.e.:

$$\lim_{k\to\infty} \mathbf{x}^{(k)} = \mathbf{x}$$

for any initial vector $\mathbf{x}^{(0)} \in \mathbb{R}^n$.

We can consider the following recurrence relation:

$$\mathbf{x}^{(k+1)} = B\mathbf{x}^{(k)} + \mathbf{g}, \quad k \geq 0 \tag{1}$$

where $B \in \mathbb{R}^{n\times n}$ is a well chosen matrix (depending on A) and $\mathbf{g}$ is a vector (that depends on A and $\mathbf{b}$), satisfying the strong consistency condition:

$$\mathbf{x} = B\mathbf{x} + \mathbf{g}. \tag{2}$$

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$$\mathbf{x} = B\mathbf{x} + \mathbf{g}. \tag{2}$$

The general scheme

Given $\mathbf{x} = A^{-1}\mathbf{b}$, we get $\mathbf{g} = (I - B)A^{-1}\mathbf{b}$; the iterative method is therefore completely defined by the matrix B, known as *iteration matrix*.
By defining the error at step k as

$$\boxed{\mathbf{e}^{(k)} := \mathbf{x} - \mathbf{x}^{(k)}, \text{ for } k = 0, 1, \ldots}$$

we obtain the following recurrence relation:

$$\boxed{\mathbf{e}^{(k+1)} = B\mathbf{e}^{(k)} \quad \text{and thus} \quad \mathbf{e}^{(k+1)} = B^{k+1}\mathbf{e}^{(0)}, \quad k = 0, 1, \ldots.}$$

because:

$$\mathbf{e}^{(k+1)} = \mathbf{x} - \mathbf{x}^{(k+1)} = (B\mathbf{x} + \mathbf{g}) - \left(B\mathbf{x}^{(k)} + \mathbf{g}\right) = B\left(\mathbf{x} - \mathbf{x}^{(k)}\right) = B\mathbf{e}^{(k)}$$

Convergence

Proposition

If the iteration matrix $B \in \mathbb{R}^{n\times n}$ of the iterative method (1) *is symmetric and positive definite (SPD), we have:*

$$\|\mathbf{e}^{(k)}\| \leq (\rho(B))^k \|\mathbf{e}^{(0)}\|,$$

for $k = 0, 1, \ldots,$ with $\rho(B)$ being the spectral radius of B.

Convergence (continued)

We can show that $\lim_{k\to\infty} \mathbf{e}^{(k)} = \mathbf{0}$ for all $\mathbf{e}^{(0)}$ (and thus for all $\mathbf{x}^{(0)}$) if and only if $\lim_{k\to\infty} B^k = \mathbf{0}$, which occurs for

$$\boxed{\rho(B) < 1,}$$

where $\rho(B)$ is the *spectral radius* of the matrix B, defined by

$$\boxed{\rho(B) = \max |\lambda_i(B)|}$$

and $\lambda_i(B)$ are the eigenvalues of the matrix B.

The smaller the value of $\rho(B)$, the less iterations are needed to reduce the initial error of a given factor.

Plan

Construction of an iterative method

Splitting methods

A general way of setting up an iterative method is based on the decomposition of the matrix A:

$$A = P - (P - A)$$

where P is an invertible matrix called *preconditioner* of A.
Hence,

$$A\mathbf{x} = \mathbf{b} \quad \Leftrightarrow \quad P\mathbf{x} = (P - A)\mathbf{x} + \mathbf{b}$$

which is of the form (2), obtaining

$$B = P^{-1}(P - A) = I - P^{-1}A \quad \text{and} \quad \mathbf{g} = P^{-1}\mathbf{b}.$$

Splitting methods (continued)

We can define the corresponding iterative method

$$P(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = \mathbf{r}^{(k)} \qquad k \geq 0$$

where $\mathbf{r}^{(k)}$ represents the *residual* at the iteration k: $\boxed{\mathbf{r}^{(k)} = \mathbf{b} - A\mathbf{x}^{(k)}}$

We can generalize this method as follows:

$$P(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = \alpha_k \mathbf{r}^{(k)} \qquad k \geq 0 \tag{3}$$

where $\alpha_k \neq 0$ is a parameter that improves the convergence of the series $\mathbf{x}^{(k)}$.

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Splitting methods (continued)

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$$P(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = P\mathbf{z}^{(k)} = \mathbf{r}^{(k)} \qquad k \geq 0,\ \mathbf{z}^{(k)} = \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}$$

The preconditioned residual $\mathbf{z}^{(k)} \in \mathbb{R}^n$ is the solution of the linear system:

$$P\mathbf{z}^{(k)} = \mathbf{r}^{(k)} \quad \text{for } k = 0, 1, \ldots,$$

with $P \in \mathbb{R}^{n \times n}$ being the nonsingular preconditioning matrix.
We observe that:

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

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Preconditioned iterative method

Algorithm 6.3: Preconditioned Iterative Method

1: **Given** $\mathbf{x}^{(0)} \in \mathbb{R}^n$, set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$;
2: **for** $k = 0, 1, \ldots,$ until a stopping criterion is satisfied **do**
3: Solve the linear system $P\mathbf{z}^{(k)} = \mathbf{r}^{(k)}$;
4: Set $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \mathbf{z}^{(k)}$;
5: Set $\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - A\mathbf{z}^{(k)}$;
6: **end for**

Stopping criterion

- At the first $k \geq 0$ for which

$$\|\mathbf{r}^{(k)}\| < \text{tol} \quad \text{or} \quad \frac{\|\mathbf{r}^{(k)}\|}{\|\mathbf{r}^{(0)}\|} < \text{tol},$$

  for some tolerance tol
- Also limit the maximum number of iterations by some $k_{\max}$ that is "sufficiently large"

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Preconditioned iterative method: remarks

- Each iteration requires solving the linear system $P\mathbf{z}^{(k)} = \mathbf{r}^{(k)}$
- P chosen such that the cost of solving $P\mathbf{z}^{(k)} = \mathbf{r}^{(k)}$ is small enough
  For example a diagonal or triangular P matrix would comply with this criterion.
- For convergence of the iterative method, aim at obtaining $\rho(B) < 1$, where $B = I - P^{-1}$

Plan

Jacobi method

If the elements of the diagonal of A are non zero, we can write

$$P_J = D = diag(a_{11}, a_{22}, \ldots, a_{nn})$$

D with the diagonal part of A being:

$$D_{ij} = \begin{cases} 0 & \text{si } i \neq j \\ a_{ij} & \text{si } i = j. \end{cases}$$

The Jacobi method corresponds to this choice with $\alpha_k = 1$ for all k.
We deduce:

$$D\mathbf{x}^{(k+1)} = \mathbf{b} - (A - D)\mathbf{x}^{(k)} \qquad k \geq 0.$$

By components:

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1, j\neq i}^{n} a_{ij} x_j^{(k)} \right), \quad i = 1, \ldots, n. \tag{4}$$

The Jacobi method can be written under the general form

$$\mathbf{x}^{(k+1)} = B\mathbf{x}^{(k)} + \mathbf{g},$$

with

$$B = B_J = D^{-1}(D - A) = I - D^{-1}A, \qquad \mathbf{g} = \mathbf{g}_J = D^{-1}\mathbf{b}.$$

Gauss-Seidel method

This method is defined as follows:

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

This method corresponds to (1) with $P_{GS} = D - E$ and $\alpha_k = 1$ $(\forall k \geq 0)$ where E is the lower triangular matrix

$$\begin{cases} E_{ij} = -a_{ij} & \text{si } i > j \\ E_{ij} = 0 & \text{si } i \leq j \end{cases}$$

(lower triangular part of A without the diagonal and with it's element's sign inverted).
That is we solve at each iteration:

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

We can write this method under the form (3), with the iteration matrix $B = B_{GS}$ given by

$$\boxed{B_{GS} = (D - E)^{-1}(D - E - A)}$$

and

$$\mathbf{g}_{GS} = (D - E)^{-1}\mathbf{b}.$$

Example

Given the matrix

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{pmatrix}.$$

We have then

$$D = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 \\ 0 & 0 & 11 & 0 \\ 0 & 0 & 0 & 16 \end{pmatrix};$$

Thus, the iteration matrix for the Jacobi method is

$$B_J = D^{-1}(D-A) = I - D^{-1}A = \begin{pmatrix} 0 & -2 & -3 & -4 \\ -5/6 & 0 & -7/6 & -4/3 \\ -9/11 & -10/11 & 0 & -12/11 \\ -13/16 & -14/16 & -15/16 & 0 \end{pmatrix}.$$

Example

For defining the matrix A and extracting its diagonal D and its lower triangular part E (without the diagonal and the sign inverted) with Matlab, we use the commands

```
>> A = [1,2,3,4;5,6,7,8;9,10,11,12;13,14,15,16];
>> D = diag(diag(A));
>> E = - tril(A,-1);
```

These allow us, for exemple, to compute the iteration matrix B_{GS} for the Gauss-Seidel method in the following way:

```
>> B_GS = (D-E)\(D-E-A);
```

We find:

$$B_{GS} = \begin{pmatrix} 0.0000 & -2.0000 & -3.0000 & -4.000 \\ 0.0000 & 1.6667 & 1.3333 & 2.0000 \\ 0.0000 & 0.1212 & 1.2424 & 0.3636 \\ 0.0000 & 0.0530 & 0.1061 & 1.1591 \end{pmatrix}.$$

Convergence

We have the following convergence results:

- (Prop 6.9) If A is nonsingular and strictly diagonally dominant by row, i.e.,

$$|a_{ii}| > \sum_{j=1,\ldots,n; j\neq i} |a_{ij}|, \quad i = 1, \ldots, n,$$

  then Jacobi and Gauss-Seidel methods converge.

- (Prop 6.10) If A is symmetric positive definite (SPD), then Gauss-Seidel method converges (Jacobi maybe not).

- (Prop 6.11) Let A be a tridiagonal nonsingular matrix whose diagonal elements are all non-zero. Then the Jacobi and the Gauss-Seidel methods are either both divergent or both convergent. In the latter case, $\rho(B_{GS}) = \rho(B_J)^2$, Gauss-Seidel converges faster.

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Plan

Preconditioned Richardson methods

(Sec. 6.3.4)

Consider the following iterative mehod:

$$\boxed{P(\mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}) = \alpha_k \mathbf{r}^{(k)}, \qquad k \geq 0.} \tag{5}$$

If $\alpha_k = \alpha$ (a constant) this method is called stationary preconditioned Richardson method; otherwise dynamic preconditioned Richardson method when α_k varies during the iterations.

The matrix P is called preconditioner of A.

Algorithm

Algorithm 6.4: Dynamic preconditioned Richardson method

1: **Given** $\mathbf{x}^{(0)} \in \mathbb{R}^n$, set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$;
2: **for** $k = 0, 1, \ldots,$ until a stopping criterion is satisfied **do**
3: Solve the linear system $P\mathbf{z}^{(k)} = \mathbf{r}^{(k)}$;
4: Choose α_k;
5: Set $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{z}^{(k)}$;
6: Set $\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha_k A\mathbf{z}^{(k)}$;
7: **end for**

Observe that:

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

Dynamic iteration matrix

The dynamic preconditioned Richardson method is defined as:

$$\mathbf{x}^{(k+1)} = B_k \mathbf{x}^{(k)} + \mathbf{g}_k,$$

where $k = 0, 1, 2, \ldots$.
The *dynamic iteration matrix* is given by:

$$B_k = I - \alpha_k P^{-1} A,$$

and the *iteration vector* is:

$$\mathbf{g}_k = \alpha_k P^{-1} \mathbf{b}.$$

- Since α_k varies with k, convergence properties change with the iteration number k
- Spectral radius of $\rho(B_k)$ changes, which must satisfy $\rho(B_k) < 1$ for the method to converge

Convergence of stationary preconditioned Richardson

Proposition (6.12)

If A and $P \in \mathbb{R}^{n\times n}$ are nonsingular, then stationary preconditioned Richardson method converges to $\mathbf{x} \in \mathbb{R}^n$ for all $\mathbf{x}^{(0)} \in \mathbb{R}^n$ if and only if

$$\alpha \left|\lambda_i(P^{-1}A)\right|^2 < 2\, Re\left(\lambda_i(P^{-1}A)\right), \text{ for all } i = 1, \ldots, n,$$

with $\alpha \neq 0$, where $\{\lambda_i(P^{-1}A)\}_{i=1}^n$ are eigenvalues of $P^{-1}A$.

Corollary (6.13)

If A and $P \in \mathbb{R}^{n\times n}$ are nonsingular with all eigenvalues $\{\lambda_i(P^{-1}A)\}_{i=1}^n$ real, then the stationary preconditioned Richardson method converges to $\mathbf{x} \in \mathbb{R}^n$ for all $\mathbf{x}^{(0)} \in \mathbb{R}^n$ if and only if

$$0 < \alpha\lambda_i(P^{-1}A) < 2, \text{ for all } i = 1, \ldots, n.$$

Convergence of stationary preconditioned Richardson

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$$0 < \alpha\lambda_i(P^{-1}A) < 2, \text{ for all } i = 1, \ldots, n.$$

Choices of α_k

If A and P are symmetric positive definite, then there are two optimal criteria to choose α_k:

1. *Stationary case*:

$$\alpha_k = \alpha_{opt} = \frac{2}{\lambda_{min} + \lambda_{max}}, \qquad k \geq 0,$$

   where λ_{min} and λ_{max} represent the larger and the smaller eigenvalue of the matrix $P^{-1}A$.

2. *Dynamic case*:

$$\alpha_k = \frac{(\mathbf{z}^{(k)})^T \mathbf{r}^{(k)}}{(\mathbf{z}^{(k)})^T A \mathbf{z}^{(k)}}, \qquad k \geq 0,$$

   where $\mathbf{z}^{(k)} = P^{-1}\mathbf{r}^{(k)}$ is the preconditioned residual.
   This method is also called preconditioned gradient method.

Case $P = I$

If $P = I$ and A is symmetric definite positive, we get the folowing methods:

- Stationary Richardson if we choose:

$$\alpha_k = \alpha_{opt} = \frac{2}{\lambda_{min}(A) + \lambda_{max}(A)}. \tag{6}$$

- Gradient if :

$$\alpha_k = \frac{(\mathbf{r}^{(k)})^T \mathbf{r}^{(k)}}{(\mathbf{r}^{(k)})^T A \mathbf{r}^{(k)}}, \qquad k \geq 0. \tag{7}$$

Convergence of Richardson for SPD matrices

When A and P are SPD and with the two optimal choices for α, we can show that the preconditioned Richardson method converges to $\mathbf{x}$ when $k \to \infty$ for all the choices of $\mathbf{x}^{(0)} \in \mathbb{R}^{n \times n}$, and that

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_A \leq \left(\frac{K(P^{-1}A) - 1}{K(P^{-1}A) + 1} \right)^k \|\mathbf{x}^{(0)} - \mathbf{x}\|_A, \quad k \geq 0, \tag{8}$$

where $\|\mathbf{v}\|_A = \sqrt{\mathbf{v}^T A \mathbf{v}}$ and $K(P^{-1}A)$ is the condition number of $P^{-1}A$.

Remark If A and P are SPD, we have that

$$K(P^{-1}A) = \frac{\lambda_{max}}{\lambda_{min}}.$$

Convergence of Richardson for SPD matrices

Proof for stationary Richardson The iteration matrix of the method is given by $B_\alpha = I - \alpha P^{-1}A$, where the eigenvalues of B_α are of the form $1 - \alpha\lambda_i$. The method is convergent if and only if $|1 - \alpha\lambda_i| < 1$ for $i = 1, \ldots, n$, therefore $-1 < 1 - \alpha\lambda_i < 1$ for $i = 1, \ldots, n$. As $\alpha > 0$, this is the equivalent to $-1 < 1 - \alpha\lambda_{max}$, from where the necessary and sufficient for convergence remains $\alpha < 2/\lambda_{max}$. Consequently, $\rho(B_\alpha)$ is minimal if $1 - \alpha\lambda_{max} = \alpha\lambda_{min} - 1$, i.e., for $\alpha_{opt} = 2/(\lambda_{min} + \lambda_{max})$. By substitution, we obtain

$$\rho_{opt} = \rho(B_{opt}) = 1 - \alpha_{opt}\lambda_{min} = 1 - \frac{2\lambda_{min}}{\lambda_{min} + \lambda_{max}} = \frac{\lambda_{max} - \lambda_{min}}{\lambda_{min} + \lambda_{max}}$$

what allows us to complete the proof. □

Gradient methods

For A SPD, solve $Ax = b$ by minimizing the quadratic function

$$\begin{aligned} \phi(x) &= \frac{1}{2}\mathbf{x}^T A\mathbf{x} - \mathbf{b}^T x \\ \bigtriangledown\phi(x) &= A\mathbf{x} - \mathbf{b} = 0 \end{aligned}$$

The new iterate is computed in the direction given by

$$r_k = - \bigtriangledown \phi(x^{(k)})$$

and α_k chosen such that it minimizes the error in this direction.

Theorem (Gradient method)

If A and preconditioner P are SPD, the optimal choice for α_k is given by

$$\alpha_k = \frac{(\mathbf{r}^{(k)}, \mathbf{z}^{(k)})}{(A\mathbf{z}^{(k)}, \mathbf{z}^{(k)})}, \qquad k \geq 0 \tag{9}$$

where

$$\mathbf{z}^{(k)} = P^{-1}\mathbf{r}^{(k)}. \tag{10}$$

Proof We have

$$\mathbf{r}^{(k)} = \mathbf{b} - A\mathbf{x}^{(k)} = A(\mathbf{x} - \mathbf{x}^{(k)}) = -A\mathbf{e}^{(k)}, \tag{11}$$

and thus, using (10),

$$P^{-1}A\mathbf{e}^{(k)} = -\mathbf{z}^{(k)}, \tag{12}$$

where $\mathbf{e}^{(k)} = \mathbf{x} - \mathbf{x}^{(k)}$ represents the error at step k. We also have:

$$\mathbf{e}^{(k+1)} = \mathbf{e}^{(k+1)}(\alpha) = \underbrace{(I - \alpha P^{-1}A)}_{B_\alpha}\mathbf{e}^{(k)}.$$

We notice that, in order to update the residual, we have the relation

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha A\mathbf{z}^{(k)} = \mathbf{r}^{(k)} - \alpha AP^{-1}\mathbf{r}^{(k)}.$$

Thus, expressing as $\|\cdot\|_A$ the vector norm associated to the scalar product $(\mathbf{x},\mathbf{y})_A = (A\mathbf{x},\mathbf{y})$, what means, $\|\mathbf{x}\|_A = (A\mathbf{x},\mathbf{x})^{1/2}$ we can write

$$\begin{aligned}
\|\mathbf{e}^{(k+1)}\|_A^2 &= (A\mathbf{e}^{(k+1)},\mathbf{e}^{(k+1)}) = -(\mathbf{r}^{(k+1)},\mathbf{e}^{(k+1)}) \\
&= -(\mathbf{r}^{(k)} - \alpha AP^{-1}\mathbf{r}^{(k)}, \mathbf{e}^{(k)} - \alpha P^{-1}A\mathbf{e}^{(k)}) \\
&= -(\mathbf{r}^{(k)},\mathbf{e}^{(k)}) + \alpha[(\mathbf{r}^{(k)}, P^{-1}A\mathbf{e}^{(k)}) + (A\mathbf{z}^{(k)},\mathbf{e}^{(k)})] \\
&\quad -\alpha^2(A\mathbf{z}^{(k)}, P^{-1}A\mathbf{e}^{(k)})
\end{aligned}$$

Now we choose α as the α_k that minimises $\|\mathbf{e}^{(k+1)}(\alpha)\|_A$:

$$\frac{d}{d\alpha}\|\mathbf{e}^{(k+1)}(\alpha)\|_A\Big|_{\alpha=\alpha_k} = 0$$

We then obtain

$$\alpha_k = \frac{1}{2}\frac{(\mathbf{r}^{(k)}, P^{-1}A\mathbf{e}^{(k)}) + (A\mathbf{z}^{(k)}, \mathbf{e}^{(k)})}{(A\mathbf{z}^{(k)}, P^{-1}A\mathbf{e}^{(k)})} = \frac{1}{2}\frac{-(\mathbf{r}^{(k)}, \mathbf{z}^{(k)}) + (A\mathbf{z}^{(k)}, \mathbf{e}^{(k)})}{-(A\mathbf{z}^{(k)}, \mathbf{z}^{(k)})}$$

and using the equality $(A\mathbf{z}^{(k)}, \mathbf{e}^{(k)}) = (\mathbf{z}^{(k)}, A\mathbf{e}^{(k)})$ knowing that A is symmetric definite positive, and noting that $A\mathbf{e}^{(k)} = -\mathbf{r}^{(k)}$, we find

$$\alpha_k = \frac{(\mathbf{r}^{(k)}, \mathbf{z}^{(k)})}{(A\mathbf{z}^{(k)}, \mathbf{z}^{(k)})}$$

□

Preconditioned gradient method

The preconditioned gradient method can be written as:
Let $\mathbf{x}^{(0)}$ be given, set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, then for $k \geq 0$,

$$
\begin{aligned}
P\mathbf{z}^{(k)} &= \mathbf{r}^{(k)} \\
\alpha_k &= \frac{(\mathbf{z}^{(k)})^T \mathbf{r}^{(k)}}{(\mathbf{z}^{(k)})^T A\mathbf{z}^{(k)}} \\
\mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \alpha_k \mathbf{z}^{(k)} \\
\mathbf{r}^{(k+1)} &= \mathbf{r}^{(k)} - \alpha_k A\mathbf{z}^{(k)}.
\end{aligned}
$$

We have to apply once A and inverse P at each iteration. P should then be such that the resolution of the associated system results easy (i.e. it requires a reasonable amount of cumputing cost). For example, we can choose a diagonal P (like in the gradient or stationary Richardson cases) or triangular.

For the stationary and the dynamic case, we can prove that, if A and P are SPD, the series $\{\mathbf{x}^{(k)}\}$ given by the Richardson method (stationary and dynamic) converges towards $\mathbf{x}$ when $k \to \infty$, and

$$\|\mathbf{e}^{(k)}\|_A := \|\mathbf{x}^{(k)} - \mathbf{x}\|_A \leq \left(\frac{K(P^{-1}A) - 1}{K(P^{-1}A) + 1}\right)^k \|\mathbf{x}^{(0)} - \mathbf{x}\|_A, \quad k \geq 0, \tag{13}$$

where $\|\mathbf{v}\|_A = \sqrt{\mathbf{v}^T A \mathbf{v}}$ and $K(P^{-1}A)$ is the conditioning of the matrix $P^{-1}A$.

Remark. In the case of the gradient method or the Richardson stationary method the error estimation becomes

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_A \leq \left(\frac{K(A)-1}{K(A)+1}\right)^k \|\mathbf{x}^{(0)} - \mathbf{x}\|_A, \quad k \geq 0. \tag{14}$$

Remark. If A and P are symmetric definite positive, we have

$$K(P^{-1}A) = \frac{\lambda_{max}(P^{-1}A)}{\lambda_{min}(P^{-1}A)}.$$

Conjugate gradient (Hestenes, Stieffel, 52)

(Sec. 6.3.6)

When A is SPD, there exists a very efficient and effective method to iteratively solve the system: the conjugate gradient method

- Solve $A\mathbf{x} = \mathbf{b}$ by minimizing the quadratic function

$$\begin{aligned} \phi(x) &= \frac{1}{2}\mathbf{x}^T A\mathbf{x} - \mathbf{b}^T\mathbf{x} \\ \bigtriangledown\phi(x) &= A\mathbf{x} - \mathbf{b} = 0 \end{aligned}$$

Start from $\mathbf{x}^{(0)}$, $\mathbf{p}^{(0)} = \mathbf{r}^{(0)}$ and compute the new iterate as:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{p}^{(k)}$$

where $\mathbf{p}_k$ is A-conjugate (A-orthogonal) to all previous search directions,

$$\mathbf{p}^{(k)\,T} A\mathbf{p}^{(i)} = 0, \text{for all } i < k$$

and α_k chosen to minimize $\phi(\mathbf{x}^{(k+1)}) = \phi(\mathbf{x}^{(k)} + \alpha_k \mathbf{p}^{(k)})$ with respect to α_k.

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and α_k chosen to minimize $\phi(\mathbf{x}^{(k+1)}) = \phi(\mathbf{x}^{(k)} + \alpha_k \mathbf{p}^{(k)})$ with respect to α_k.

Conjugate gradient method

Compute the new search direction A-conjugate to previous ones by using Gram-Schmidt:

$$\mathbf{p}^{(k+1)} = \mathbf{r}^{(k+1)} - \sum_{i \leq k} \frac{{\mathbf{p}^{(i)}}^{\mathsf{T}} A \mathbf{r}^{(k+1)}}{{\mathbf{p}^{(i)}}^{\mathsf{T}} A \mathbf{p}^{(i)}} \mathbf{p}^{(i)}$$

It can be shown that $\mathbf{p}^{(k+1)}$ is already A-conjugate to all previous search directions, except last one. We obtain:

$$\mathbf{p}^{(k+1)} = \mathbf{r}^{(k+1)} - \beta_k \mathbf{p}^{(k)}, \beta_k = \frac{{\mathbf{p}^{(k)}}^{T} A \mathbf{r}^{(k+1)}}{{\mathbf{p}^{(k)}}^{T} A \mathbf{p}^{(k)}}$$

Conjugate gradient method

Let $\mathbf{x}^{(0)}$ be given; we compute $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, $\mathbf{p}^{(0)} = \mathbf{r}^{(0)}$,then for $k \geq 0$,

$$
\begin{aligned}
\alpha_k &= \frac{{\mathbf{p}^{(k)}}^T \mathbf{r}^{(k)}}{{\mathbf{p}^{(k)}}^T A\mathbf{p}^{(k)}} \\
\mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \alpha_k \mathbf{p}^{(k)} \\
\mathbf{r}^{(k+1)} &= \mathbf{r}^{(k)} - \alpha_k A\mathbf{p}^{(k)} \\
\beta_k &= \frac{{\mathbf{p}^{(k)}}^T A\mathbf{r}^{(k+1)}}{{\mathbf{p}^{(k)}}^T A\mathbf{p}^{(k)}} \\
\mathbf{p}^{(k+1)} &= \mathbf{r}^{(k+1)} - \beta_k \mathbf{p}^{(k)} .
\end{aligned}
$$

Precondtioned Conjugate gradient method

(Sec. 6.3.6)

When A and P are SPD, we use the preconditioned conjugate gradient method

Let $\mathbf{x}^{(0)}$ be given; we compute $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, $\mathbf{z}^{(0)} = P^{-1}\mathbf{r}^{(0)}$, $\mathbf{p}^{(0)} = \mathbf{z}^{(0)}$,then for $k \geq 0$,

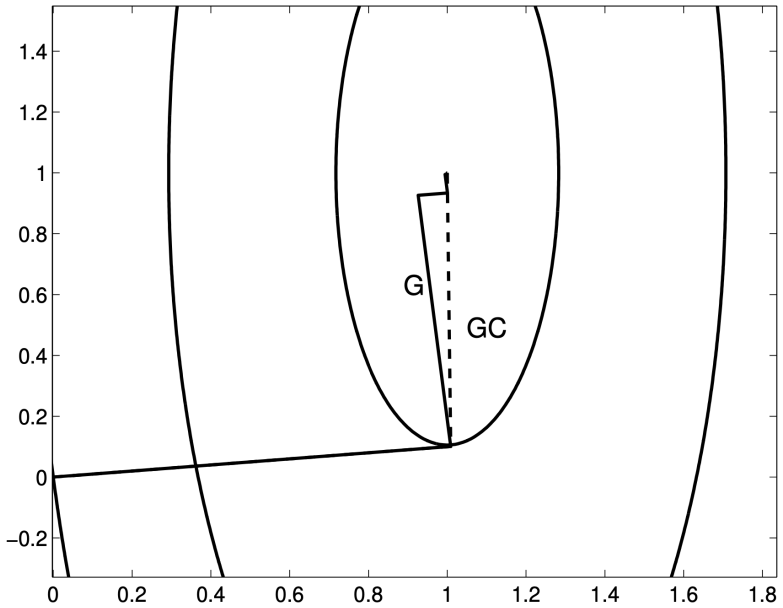
$$
\begin{aligned}
\alpha_k &= \frac{{\mathbf{p}^{(k)}}^T \mathbf{r}^{(k)}}{{\mathbf{p}^{(k)}}^T A\mathbf{p}^{(k)}} \\
\mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \alpha_k \mathbf{p}^{(k)} \\
\mathbf{r}^{(k+1)} &= \mathbf{r}^{(k)} - \alpha_k A\mathbf{p}^{(k)} \\
P\mathbf{z}^{(k+1)} &= \mathbf{r}^{(k+1)} \\
\beta_k &= \frac{{\mathbf{p}^{(k)}}^T A\mathbf{z}^{(k+1)}}{{\mathbf{p}^{(k)}}^T A\mathbf{p}^{(k)}} \\
\mathbf{p}^{(k+1)} &= \mathbf{z}^{(k+1)} - \beta_k \mathbf{p}^{(k)} .
\end{aligned}
$$

Convergence of conjugate gradient

Proposition (6.16)

If A and $P \in \mathbb{R}^{n\times n}$ are SPD, the conjugate gradient converges to $x \in \mathbb{R}^{n\times n}$ for all $x^{(0)} \in \mathbb{R}^n$ in at most n iterations (in exact arithmetic). The error estimate is given by

$$\|\mathbf{x}^{(k)} - \mathbf{x}\|_A \leq \frac{2c^k}{1+c^{2k}} \|\mathbf{x}^{(0)} - \mathbf{x}\|_A, \quad k \geq 0 \quad \text{with } c = \frac{\sqrt{K_2(P^{-1}A)} - 1}{\sqrt{K_2(P^{-1}A)} + 1}. \tag{15}$$



Convergence Criteria for iterative methods
(Sec. 6.3.7)

- Stop the iterative method when error estimator $\tilde{e}^{(k)} < tol$.
- Possible error estimators and associated stopping criteria:
  - **The (absolute) residual**, for which

$$\tilde{e}^{(k)} = \|\mathbf{r}^{(k)}\|,$$

    where $\mathbf{r}^{(k)}$ denotes the residual at iteration k.
  - **The relative residual**, for which

$$\tilde{e}^{(k)}_{\text{rel}} = \mathbf{r}^{(k)}_{\text{rel}} := \frac{\|\mathbf{r}^{(k)}\|}{\|\mathbf{b}\|}$$

    is used to estimate the relative error

$$e^{(k)}_{\text{rel}} := \frac{\|\mathbf{x} - \mathbf{x}^{(k)}\|}{\|\mathbf{x}\|}, \quad \text{for } \mathbf{x} \neq 0.$$

  - **The difference of successive iterates**, for which

$$\tilde{e}^{(k)} = \|\delta^{(k)}\|, \text{ where } \delta^{(k)} := \mathbf{x}^{(k+1)} - \mathbf{x}^{(k)}, \quad \text{for } k \geq 0.$$

Convergence Criteria for iterative methods

We have the following error bound:
If A is SPD, then

$$e_{rel}^{(k)} := \frac{\|\mathbf{x}^{(k)} - \mathbf{x}\|}{\|\mathbf{x}\|} \leq K_2(A) \frac{\|\mathbf{r}^{(k)}\|}{\|\mathbf{b}\|}. \tag{16}$$

In case of a preconditioned system:

$$e_{rel}^{(k)} := \frac{\|\mathbf{x}^{(k)} - \mathbf{x}\|}{\|\mathbf{x}\|} \leq K_2(P^{-1}A) \frac{\|P^{-1}\mathbf{r}^{(k)}\|}{\|P^{-1}\mathbf{b}\|}.$$

Example

Let's consider the following linear system:

$$\begin{cases} 2x_1 + x_2 &= 1 \\ x_1 + 3x_2 &= 0 \end{cases} \tag{17}$$

whose matrix is $A = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$ is SPD. The solution to this system is $x_1 = 3/5 = 0.6$ et $x_2 = -1/5 = -0.2$.

Example

Some convergence studies

- A is strictly diagonal dominant by row. Hence Jacobi and Gauss-Seidel methods converge.
- A is nonsingular, tridiagonal with non-zero diagonal elements. Then $\rho(B_{GS}) = \rho(B_J)^2$. Therefore we expect a quicker convergence of Gauss-Seidel w.r.t. Jacobi.
- A is SPD, hence the gradient and the conjugate gradient methods converge. Moreover (see error estimates), the CG shall converge faster.

Example

We want to approximate the solution with an iterative methode starting with

$$\mathbf{x}^{(0)} = \begin{pmatrix} x_1^{(0)} \\ x_2^{(0)} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix}.$$

We can see that

$$\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)} = \begin{pmatrix} -\frac{3}{2} \\ -\frac{5}{2} \end{pmatrix}$$

and

$$\|\mathbf{r}^{(0)}\|_2 = \sqrt{(\mathbf{r}^{(0)})^T \mathbf{r}^{(0)}} = \frac{\sqrt{34}}{2} \approx 2.9155.$$

Example

Jacobi method

$$\mathbf{x}^{(k+1)} = B_J \mathbf{x}^{(k)} + \mathbf{g}_J, \quad k \geq 0, \qquad \text{where } B_J = I - D^{-1}A \text{ and } \mathbf{g}_J = D^{-1}\mathbf{b}.$$

We have

$$B_J = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} = \begin{pmatrix} 0 & -\frac{1}{2} \\ -\frac{1}{3} & 0 \end{pmatrix}$$

$$\mathbf{g}_J = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix}$$

and $\rho(B_J) = max|\lambda_i(B_J)| = \texttt{max(abs(eig(}B_J\texttt{)))} = 0.4082.$

Example

For $k = 0$ (first iteration) we find:

$$\mathbf{x}^{(1)} = B_J \mathbf{x}^{(0)} + \mathbf{g}_J = \begin{pmatrix} 0 & -\frac{1}{2} \\ -\frac{1}{3} & 0 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} \\ -\frac{1}{3} \end{pmatrix} \approx \begin{pmatrix} 0.25 \\ -0.3333 \end{pmatrix}.$$

Notice that

$$\mathbf{r}^{(1)} = \mathbf{b} - A\mathbf{x}^{(1)} = \begin{pmatrix} 0.8333 \\ 0.75 \end{pmatrix} \qquad \text{and } \|\mathbf{r}^{(1)}\|_2 = 1.1211.$$

Example

Gauss-Seidel method

$$\mathbf{x}^{(k+1)} = B_{GS}\mathbf{x}^{(k)} + \mathbf{g}_{GS}, \quad k \geq 0, \quad \text{where } B_{GS} = (D-E)^{-1}(D-E-A)$$

$$\text{and } \mathbf{g}_{GS} = (D-E)^{-1}\mathbf{b}.$$

We have

$$B_{GS} = \begin{pmatrix} 2 & 0 \\ 1 & 3 \end{pmatrix}^{-1} \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ -\frac{1}{6} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\frac{1}{2} \\ 0 & \frac{1}{6} \end{pmatrix}$$

$$\mathbf{g}_{GS} = \begin{pmatrix} \frac{1}{2} & 0 \\ -\frac{1}{6} & \frac{1}{3} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{6} \end{pmatrix}$$

In this case $\rho(B_{GS}) = max|\lambda_i(B_{GS})| = \texttt{max(abs(eig(}B_{GS}\texttt{)))} = 0.1667$.
We can verify that $\rho(B_{GS}) = \rho(B_J)^2$.

Example

For $k = 0$ (first iteration) we find:

$$\mathbf{x}^{(1)} = B_{GS}\mathbf{x}^{(0)} + \mathbf{g}_{GS} = \begin{pmatrix} 0 & -\frac{1}{2} \\ 0 & \frac{1}{6} \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{6} \end{pmatrix} = \begin{pmatrix} \frac{1}{4} \\ -\frac{1}{12} \end{pmatrix} \approx \begin{pmatrix} 0.25 \\ -0.0833 \end{pmatrix}.$$

We have

$$\mathbf{r}^{(1)} = \mathbf{b} - A\mathbf{x}^{(1)} = \begin{pmatrix} 0.5833 \\ 0 \end{pmatrix} \qquad \text{and } \|\mathbf{r}^{(1)}\|_2 = 0.5833.$$

Example

Preconditioned gradient method with $P = D$

We set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} -\frac{3}{2} \\ -\frac{5}{2} \end{pmatrix}$.

For $k = 0$, we have:

$$P\mathbf{z}^{(0)} = \mathbf{r}^{(0)} \quad \Leftrightarrow \quad \mathbf{z}^{(0)} = P^{-1}\mathbf{r}^{(0)} = \begin{pmatrix} -\frac{3}{4} \\ -\frac{5}{6} \end{pmatrix}$$

$$\alpha_0 = \frac{(\mathbf{z}^{(0)})^T \mathbf{r}^{(0)}}{(\mathbf{z}^{(0)})^T A\mathbf{z}^{(0)}} = \frac{77}{107}$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha_0 \mathbf{z}^{(0)} = \begin{pmatrix} 0.4603 \\ -0.0997 \end{pmatrix}$$

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} - \alpha_0 A\mathbf{z}^{(0)} = \begin{pmatrix} 0.1791 \\ -0.1612 \end{pmatrix} \quad \text{and } \|\mathbf{r}^{(1)}\|_2 = 0.2410.$$

Example

Conjugated preconditioned gradient method with $P = D$

We set $\mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$, $\mathbf{z}^{(0)} = P^{-1}\mathbf{r}^{(0)}$ and $\mathbf{p}^{(0)} = \mathbf{z}^{(0)}$. For $k = 0$, we have:

$$\alpha_0 = \frac{(\mathbf{p}^{(0)})^T \mathbf{r}^{(0)}}{(\mathbf{p}^{(0)})^T A\mathbf{p}^{(0)}} = \frac{(\mathbf{z}^{(0)})^T \mathbf{r}^{(0)}}{(\mathbf{z}^{(0)})^T A\mathbf{z}^{(0)}}$$

$$\mathbf{x}^{(1)} = \mathbf{x}^{(0)} + \alpha_0 \mathbf{p}^{(0)} = \mathbf{x}^{(0)} + \alpha_0 \mathbf{z}^{(0)}$$

$$\mathbf{r}^{(1)} = \mathbf{r}^{(0)} - \alpha_0 A\mathbf{p}^{(0)} = \mathbf{r}^{(0)} - \alpha_0 A\mathbf{z}^{(0)}.$$

We see that the first iteration $\mathbf{x}^{(1)}$ matches with the one obtained by the preconditioned gradient method.

Example

We then complete the first iteration of the preconditioned conjugate gradient method:

$$P\mathbf{z}^{(1)} = \mathbf{r}^{(1)} \quad \Leftrightarrow \quad \mathbf{z}^{(1)} = P^{-1}\mathbf{r}^{(1)} = \begin{pmatrix} 0.0896 \\ -0.0537 \end{pmatrix}$$

$$\beta_0 = \frac{(A\mathbf{p}^{(0)})^T\mathbf{z}^{(1)}}{(A\mathbf{p}^{(0)})^T A\mathbf{p}^{(0)}} = \frac{(A\mathbf{z}^{(0)})^T\mathbf{z}^{(1)}}{(A\mathbf{z}^{(0)})^T\mathbf{z}^{(0)}} = -0.0077$$

$$\mathbf{p}^{(1)} = \mathbf{z}^{(1)} - \beta_0\mathbf{p}^{(0)} = \mathbf{z}^{(1)} - \beta_0\mathbf{z}^{(0)} = \begin{pmatrix} 0.0838 \\ -0.0602 \end{pmatrix}.$$

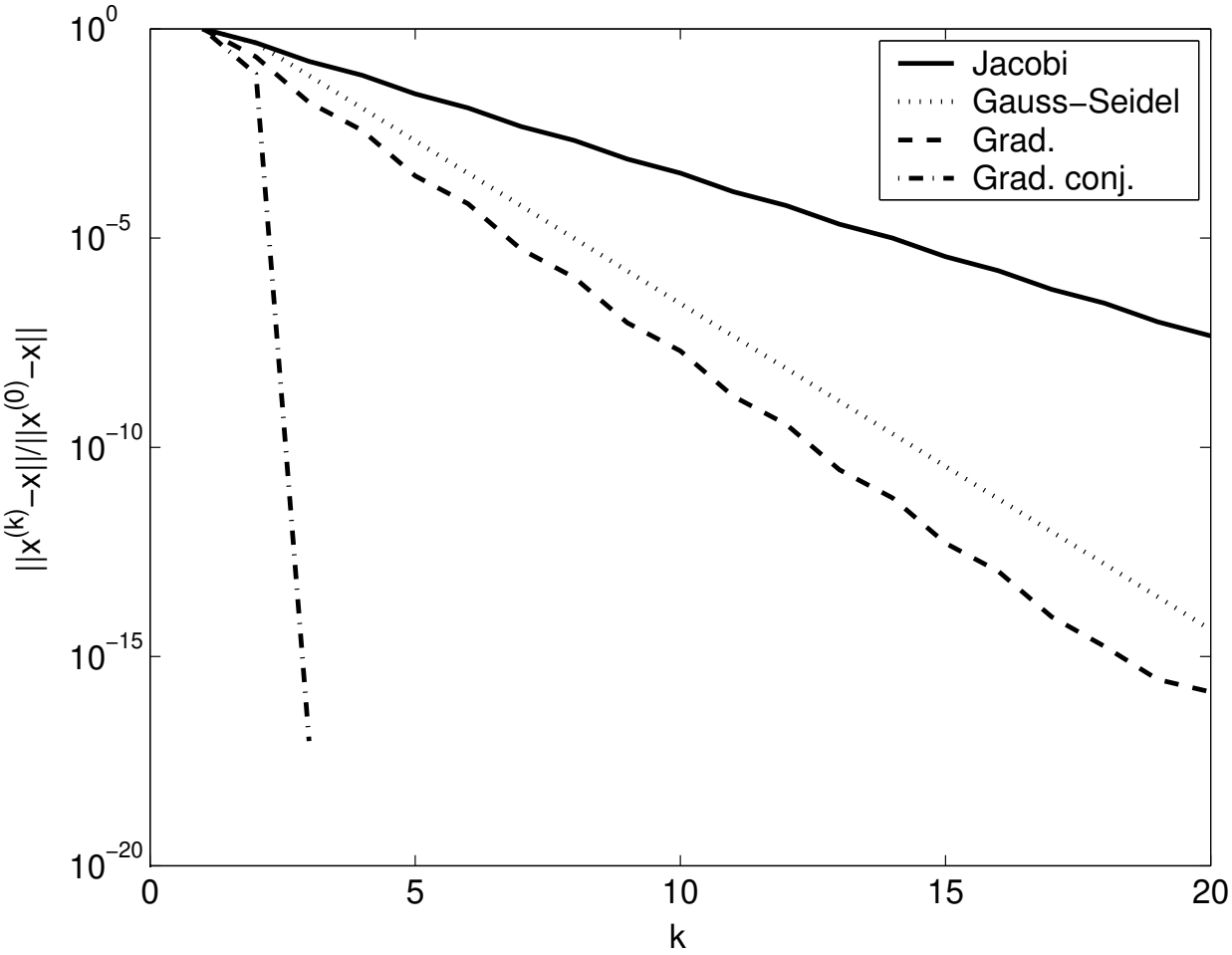
Example

At the second iteration, with the four different methods, we have:

Method	$\mathbf{x}^{(2)}$	$\mathbf{r}^{(2)}$	$\|\mathbf{r}^{(2)}\|_2$
Jacobi	$\begin{pmatrix} 0.6667 \\ -0.0833 \end{pmatrix}$	$\begin{pmatrix} -0.2500 \\ -0.4167 \end{pmatrix}$	0.4859
Gauss-Seidel	$\begin{pmatrix} 0.5417 \\ -0.1806 \end{pmatrix}$	$\begin{pmatrix} 0.0972 \\ 0 \end{pmatrix}$	0.0972
PG	$\begin{pmatrix} 0.6070 \\ -0.1877 \end{pmatrix}$	$\begin{pmatrix} -0.0263 \\ -0.0438 \end{pmatrix}$	0.0511
PCG	$\begin{pmatrix} 0.60000 \\ -0.2000 \end{pmatrix}$	$\begin{pmatrix} -0.2220 \\ -0.3886 \end{pmatrix} \cdot 10^{-15}$	$4.4755 \cdot 10^{-16}$

Example

Behavior of the relative error applied to the system (17) :



Example

Let's now consider another example:

$$\begin{cases} 2x_1 + x_2 & = 1 \\ -x_1 + 3x_2 & = 0 \end{cases} \tag{18}$$

whose solution is $x_1 = 3/7$, $x_2 = 1/7$.

Example

Preliminary convergence studies

The associatd matrix is $A = \begin{pmatrix} 2 & 1 \\ -1 & 3 \end{pmatrix}$.

- A is strictly diagonal dominant by row. Hence Jacobi and Gauss-Seidel methods converge.
- A is nonsingular, tridiagonal with non-zero diagonal elements. Then $\rho(B_{GS}) = \rho(B_J)^2$. Therefore we expect a quicker convergence of Gauss-Seidel w.r.t. Jacobi.
- A **is not SPD**, therefore we have no idea if the gradient or the conjugate gradient converge.

Example

We approximate the solution with an iterative method starting from

$$\mathbf{x}^{(0)} = \begin{pmatrix} x_1^{(0)} \\ x_2^{(0)} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{1}{2} \end{pmatrix}.$$

The following figure shows the value of $\frac{\|\mathbf{x}^{(k)} - \mathbf{x}\|}{\|\mathbf{x}^{(0)} - \mathbf{x}\|}$ for the Jacobi, Gauss-Seidel, Richardson stationary (preconditioned with $\alpha = 0.5$ and $P = D = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$), and the preconditioned (with $P = D$) conjugate gradient methods.

Remark that this time the preconditioned conjugate gradient method doesn't converge.

Example

Behavior of the relative error applied to the system (18) :