CG-method for $Ax^* = b$

Notation:

1. initial vector x_0, initial residual, $r_0 := b - Ax_0$, init. error $e_0 := x^* - x_0$
2. residual in l-th step: $r_l := b - Ax_l$
3. Krylov subspace: $\mathcal{K}_l := \text{span}\{r_0, Ar_0, \cdots, A^{l-1}r_0\}$

abstract definition of x_l:

l-th approximation x_l is defined by:

$$\text{find } x_l \in x_0 + \mathcal{K}_l \text{ s.t. } \quad \|x^* - x_l\|_A \le \|x^* - x\|_A \qquad \forall x \in x_0 + \mathcal{K}_l$$

residual in l-th step: $r_l := b - Ax_l$

- $\mathcal{K}_{l+1} \supset \mathcal{K}_l$
- $\exists l^* \le N$ s.t. $r_{l^*} = 0$
- $\forall l \le l^* : \dim\mathcal{K}_l = l$

CG-method for $Ax^* = b$, cont'd

Theorem 1. The following are equivalent:

(i) x_l solves the minimization problem: $\|x^* - x_l\|_A \leq \|x^* - x\|_A \; \forall x \in x_0 + \mathcal{K}_l$

(ii) the error is orthogonal to $\mathcal{K}_l$ in the A-inner product:
$(x^* - x_l, v)_A = 0 \; \forall v \in \mathcal{K}_l$

(iii) residual is orthog. to $\mathcal{K}_l$ in euclid. inner product: $(r_l, v) = 0 \; \forall v \in \mathcal{K}_l$

Theorem 2. For $l \leq l^*$ the set $\{r_0, \ldots, r_{l-1}\}$ is an orthogonal basis of $\mathcal{K}_l$

A-orthogonal bases of $\mathcal{K}_l$:

- the sequence of residuals $r_0, \ldots,$ spans the spaces $\mathcal{K}_l$:
  $\{r_0, \ldots, r_{l-1}\}$ is an orthogonal basis w.r.t. $(\cdot, \cdot)$ of $\mathcal{K}_l$
- Gram-Schmidt $\rightarrow$ yields sequence d_0, $d_1, \ldots,$ with
  $\{d_0, \ldots, d_{l-1}\}$ is an orthogonal basis w.r.t. $(\cdot, \cdot)_A$ of $\mathcal{K}_l$

orthogonalities imply short recurrence relations

$\{r_0, \dots, r_{l-1}\}$ is orthogonal basis w.r.t. $(\cdot,\cdot)$ of $\mathcal{K}_l$

$\{d_0, \dots, d_{l-1}\}$ is orthogonal basis w.r.t. $(\cdot,\cdot)_A$ of $\mathcal{K}_l$

For suitable $\beta_{l-1},\ \alpha_l \in \mathbb{R}$:

$$d_l = r_l + \beta_{l-1} d_{l-1} \qquad \text{by GS and orthogonality } (r_l, \mathcal{K}_{l-1}) = 0 \tag{1}$$

$$x_l = x_{l-1} + \alpha_l d_{l-1} \qquad \text{by } \mathcal{K}_l = \mathcal{K}_{l-1} \oplus_A \operatorname{span}\{d_{l-1}\} \text{ and min. property} \tag{2}$$

$$r_l = r_{l-1} - \alpha_l A d_{l-1} \qquad \text{from (2)} \tag{3}$$

α_l and β_{l-1} result from orthogonalities:

$$(3) \text{ und } (r_l, r_{l-1}) = 0 \Longrightarrow \alpha_l = -\frac{\|r_{l-1}\|^2}{(Ad_{l-1}, r_{l-1})} = \cdots = \frac{\|r_{l-1}\|^2}{\|d_{l-1}\|_A^2}$$

$$(1) \text{ und } (d_l, d_{l-1})_A = 0 \Longrightarrow \beta_{l-1} = -\frac{(r_l, d_{l-1})_A}{\|d_{l-1}\|_A^2} = \cdots = \frac{\|r_l\|^2}{\|r_{l-1}\|^2}$$

Hence recursive evaluation: $r_{l-1},\ d_{l-1}$ yield $\alpha_l \to x_l \to r_l \to \beta_{l-1} \to d_l$.

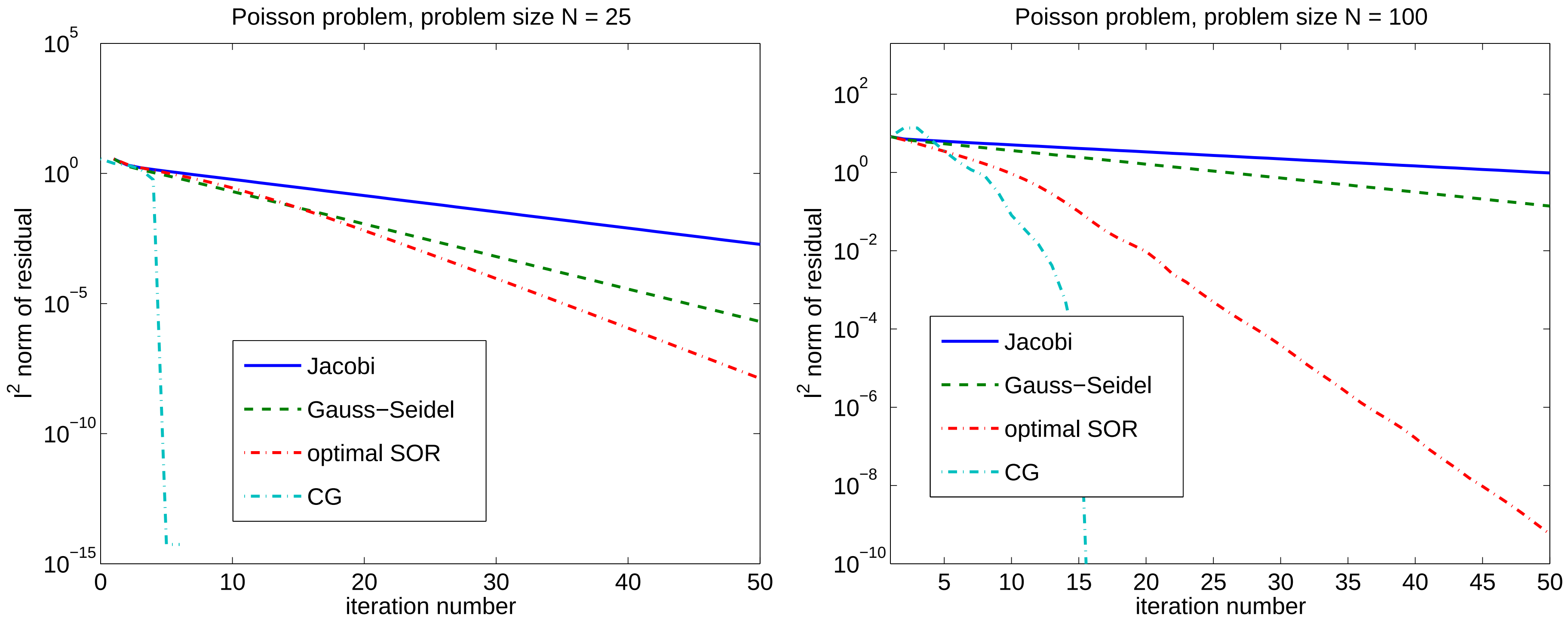
CG algorithm

%input: SPD matrix A, rhs b, initial vector x_0

Compute $r_0 = b - Ax_0$, $d_0 = r_0$
for $j = 1, 2, \ldots,$ until convergence do
    $\alpha_l = (r_l, r_l)/(Ad_l, d_l)$
    $x_{j+1} = x_{l-1} + \alpha_l d_{l-1}$
    $r_l = r_{l-1} - \alpha_l A d_{l-1}$
    $\beta_{l-1} = (r_l, r_l)/(r_{l-1}, r_{l-1})$
    $d_l = r_l + \beta_{l-1} d_{l-1}$
end for

memory requirement: store merely 4 vectors of length N (x_l, r_l, d_l, memory for Ad_{l-1})

different iterative methods for Poisson problem (problem size $N = 25$ and $N = 100$)



N	λ_{min}	λ_{max}
25	0.54	7.46
100	0.16	7.8
2500	0.04	7.9