

# Numerical Analysis - Part II

Anders C. Hansen

Lecture 21

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*Iterative methods for linear algebraic systems*

# The conjugate gradient method

Here it is.

(A) For any initial vector  $\mathbf{x}^{(0)}$ , set  $\mathbf{d}^{(0)} = \mathbf{r}^{(0)} = \mathbf{b} - A\mathbf{x}^{(0)}$ ;

(B) For  $k \geq 0$ , calculate  $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}$  and the residual

$$\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha_k A\mathbf{d}^{(k)}, \quad \text{with}$$
$$\alpha_k := \{ \mathbf{r}^{(k+1)} \perp \mathbf{d}^{(k)} \} = \frac{(\mathbf{r}^{(k)}, \mathbf{d}^{(k)})}{(A\mathbf{d}^{(k)}, \mathbf{d}^{(k)})}, \quad k \geq 0. \quad (1)$$

(C) For the same  $k$ , the next conjugate direction is the vector

$$\mathbf{d}^{(k+1)} = \mathbf{r}^{(k+1)} + \beta_k \mathbf{d}^{(k)}, \quad \text{with}$$
$$\beta_k := \{ \mathbf{d}^{(k+1)} \perp A\mathbf{d}^{(k)} \} = -\frac{(\mathbf{r}^{(k+1)}, A\mathbf{d}^{(k)})}{(\mathbf{d}^{(k)}, A\mathbf{d}^{(k)})}, \quad k \geq 0. \quad (2)$$

## Theorem 1 (Properties of CGM)

For every  $m \geq 0$ , the conjugate gradient method has the following properties.

- (1) The linear space spanned by the residuals  $\{\mathbf{r}^{(i)}\}$  is the same as the linear space spanned by the conjugate directions  $\{\mathbf{d}^{(i)}\}$  and it coincides with the space spanned by  $\{A^i \mathbf{r}^{(0)}\}$ :

$$\text{span}\{\mathbf{r}^{(i)}\}_{i=0}^m = \text{span}\{\mathbf{d}^{(i)}\}_{i=0}^m = \text{span}\{A^i \mathbf{r}^{(0)}\}_{i=0}^m.$$

- (2) The residuals satisfy the orthogonality conditions:  $(\mathbf{r}^{(m)}, \mathbf{r}^{(i)}) = (\mathbf{r}^{(m)}, \mathbf{d}^{(i)}) = 0$  for  $i < m$ .
- (3) The directions are conjugate ( $A$ -orthogonal):  $(\mathbf{d}^{(m)}, \mathbf{d}^{(i)})_A = (\mathbf{d}^{(m)}, A\mathbf{d}^{(i)}) = 0$  for  $i < m$ .

# The CGM – Theoretical aspects

**Proof.** We use induction on  $m \geq 0$ , the assertions being trivial for  $m = 0$ , since  $\mathbf{d}^{(0)} = \mathbf{r}^{(0)}$  and (2)-(3) are void. Therefore, assuming that the assertions are true for some  $m = k$ , we ask if they remain true when  $m = k + 1$ .

(1) Formula (2)

$$\mathbf{d}^{(k+1)} = \mathbf{r}^{(k+1)} + \beta_k \mathbf{d}^{(k)}$$

readily implies that equivalence of the spaces spanned by  $(\mathbf{r}^{(i)})_0^k$  and  $(\mathbf{d}^{(i)})_0^k$ , is preserved when  $k$  is increased to  $k + 1$ . Similarly, from  $\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha_k A \mathbf{d}^{(k)}$  in (1), and from the inductive assumption  $\mathbf{r}^{(k)}, \mathbf{d}^{(k)} \in \text{span}\{A^i \mathbf{r}^{(0)}\}_{i=0}^k$ , it follows that  $\mathbf{r}^{(k+1)} \in \text{span}\{A^i \mathbf{r}^{(0)}\}_{i=0}^{k+1}$ . To see that  $A^{k+1} \mathbf{r}^{(0)} \in \text{span}\{\mathbf{r}^{(i)}\}_{i=0}^{k+1}$ , since  $\alpha_k \neq 0$ , the claim follows by (5) if  $\mathbf{d}^{(k)}$  has a non-zero component from  $A^k \mathbf{r}^{(0)}$ , and if not the claim follows from the induction hypothesis.

# The CGM – Theoretical aspects

**Proof. Cont.** (2) Turning to assertion (2), we need  $\mathbf{r}^{(k+1)} \perp \mathbf{r}^{(i)}$  for  $i \leq k$ , which by (1) is equivalent to

$$\mathbf{r}^{(k+1)} \perp \mathbf{d}^{(i)} \quad \text{for } i \leq k.$$

We have  $\mathbf{r}^{(k+1)} \perp \mathbf{d}^{(k)}$  by the definition of  $\alpha_k$  in (1), so we need

$$\mathbf{r}^{(k+1)} \stackrel{(1)}{=} \mathbf{r}^{(k)} - \alpha_k \mathbf{Ad}^{(k)} \perp \mathbf{d}^{(i)} \quad \text{for } i < k,$$

and this follows from the inductive assumptions  $\mathbf{r}^{(k)} \perp \mathbf{d}^{(i)}$  and  $\mathbf{Ad}^{(k)} \perp \mathbf{d}^{(i)}$ .

**Proof. Cont.** (3) It remains to justify (3), namely that  $\mathbf{d}^{(k+1)}$  defined in (2) satisfies

$$\mathbf{d}^{(k+1)} \perp \mathbf{Ad}^{(i)} \quad \text{for } i \leq k.$$

The value of  $\beta_k$  in (2) is defined to give  $\mathbf{d}^{(k+1)} \perp \mathbf{Ad}^{(k)}$ , so we need

$$\mathbf{d}^{(k+1)} \stackrel{(2)}{=} \mathbf{r}^{(k+1)} + \beta_k \mathbf{d}^{(k)} \perp \mathbf{Ad}^{(i)} \quad \text{for } i < k.$$

By the inductive hypothesis  $\mathbf{d}^{(k)} \perp \mathbf{Ad}^{(i)}$ , hence it remains to establish that  $\mathbf{r}^{(k+1)} \perp \mathbf{Ad}^{(i)}$  for  $i < k$ . Now, the formula (1) yields  $\mathbf{Ad}^{(i)} = (\mathbf{r}^{(i)} - \mathbf{r}^{(i+1)})/\alpha_i$ , therefore we require the conditions  $\mathbf{r}^{(k+1)} \perp (\mathbf{r}^{(i)} - \mathbf{r}^{(i+1)})$  for  $i < k$ , and they are a consequence of the assertion (2) for  $m = k + 1$  obtained previously.  $\square$

## Corollary 2 (A termination property)

*If the conjugate gradient method is applied in exact arithmetic, then, for any  $\mathbf{x}^{(0)} \in \mathbb{R}^n$ , termination occurs after at most  $n$  iterations.*

*More precisely, termination occurs after at most  $s$  iterations, where  $s = \dim \text{span}\{A^i \mathbf{r}_0\}_{i=0}^{n-1}$  (which can be smaller than  $n$ ).*



# Termination property

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**Proof.** Assertion (2) of Theorem 1 states that residuals  $(\mathbf{r}^{(k)})_{k \geq 0}$  form a sequence of mutually orthogonal vectors in  $\mathbb{R}^n$ , therefore at most  $n$  of them can be nonzero. Since they also belong to the space  $\text{span}\{A^i \mathbf{r}_0\}_{i=0}^{n-1}$ , their number is bounded by the dimension of that space.  $\square$

# The Krylov subspaces

## Definition 3 (The Krylov subspaces)

Let  $A$  be an  $n \times n$  matrix,  $\mathbf{v} \in \mathbb{R}^n$  nonzero, and  $m \in \mathbb{N}$ . The linear space  $K_m(A, \mathbf{v}) := \text{span}\{A^i \mathbf{v}\}_{i=0}^{m-1}$  is called the  $m$ -th Krylov subspace of  $\mathbb{R}^n$ .

## Theorem 4 (Number of iterations in CGM)

Let  $A > 0$ , and let  $s$  be the number of its distinct eigenvalues. Then, for any  $\mathbf{v}$ ,

$$\dim K_m(A, \mathbf{v}) \leq s \quad \forall m. \quad (3)$$

Hence, for any  $A > 0$ , the number of iterations of the CGM for solving  $A\mathbf{x} = \mathbf{b}$  is bounded by the number of distinct eigenvalues of  $A$ .

# The Krylov subspaces

**Proof.** Inequality (3) is true not just for positive definite  $A > 0$ , but for any  $A$  with  $n$  linearly independent eigenvectors ( $\mathbf{u}_i$ ). Indeed, in that case one can expand  $\mathbf{v} = \sum_{i=1}^n a_i \mathbf{u}_i$ , and then group together eigenvectors with the same eigenvalues: for each  $\lambda_\nu$  we set  $\mathbf{w}_\nu = \sum_{k=1}^{m_\nu} a_{i_k} \mathbf{u}_{i_k}$  if  $A \mathbf{u}_{i_k} = \lambda_\nu \mathbf{u}_{i_k}$ . Then

$$\mathbf{v} = \sum_{\nu=1}^s c_\nu \mathbf{w}_\nu, \quad c_\nu \in \{0, 1\},$$

hence  $A^i \mathbf{v} = \sum_{\nu=1}^s c_\nu \lambda_\nu^i \mathbf{w}_\nu$ , thus for any  $m$  we get  $K_m(A, \mathbf{v}) \subseteq \text{span}\{\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_s\}$ , and that proves (3). By Corollary 2, the number of iteration in CGM is bounded by  $\dim K_m(A, \mathbf{r}^{(0)})$ , hence the final conclusion. □

## Remark 5

Theorem 4 shows that, unlike other iterative schemes, the conjugate gradient method is both iterative and direct: each iteration produces a reasonable approximation to the exact solution, and the exact solution itself will be recovered after  $n$  iterations at most.

# Simplifying the CGM-algorithm

We now simplify and reformulate the CGM-algorithm.

Firstly, we rewrite expressions for the parameters  $\alpha_k$  and  $\beta_k$  in (1)-(2) as follows:

$$\alpha_k = \frac{(\mathbf{r}^{(k)}, \mathbf{d}^{(k)})}{(\mathbf{d}^{(k)}, \mathbf{Ad}^{(k)})} \stackrel{(c)}{=} \frac{\|\mathbf{r}^{(k)}\|^2}{(\mathbf{d}^{(k)}, \mathbf{Ad}^{(k)})} > 0,$$

$$\beta_k = -\frac{(\mathbf{r}^{(k+1)}, \mathbf{Ad}^{(k)})}{(\mathbf{d}^{(k)}, \mathbf{Ad}^{(k)})} \stackrel{(a)}{=} -\frac{(\mathbf{r}^{(k+1)}, \mathbf{r}^{(k+1)} - \mathbf{r}^{(k)})}{(\mathbf{d}^{(k)}, \mathbf{r}^{(k+1)} - \mathbf{r}^{(k)})} \stackrel{(b)}{=} \frac{\|\mathbf{r}^{(k+1)}\|^2}{(\mathbf{d}^{(k)}, \mathbf{r}^{(k)})} \stackrel{(c)}{=} \frac{\|\mathbf{r}^{(k+1)}\|^2}{\|\mathbf{r}^{(k)}\|^2} > 0.$$

Here, for  $\beta$ , we used in (a) the fact that  $\mathbf{Ad}^{(k)}$  is a multiple of  $\mathbf{r}^{(k+1)} - \mathbf{r}^{(k)}$  by (1), and in (b) orthogonality of  $\mathbf{r}^{(k+1)}$  to both  $\mathbf{r}^{(k)}, \mathbf{d}^{(k)}$  proved in Theorem 1(2). Then, for both  $\beta$  and  $\alpha$ , we used in (c) the property  $(\mathbf{d}^{(k)}, \mathbf{r}^{(k)}) = \|\mathbf{r}^{(k)}\|^2$  which follows from (2) with index  $k + 1$ , taking in account orthogonality  $\mathbf{r}^{(k+1)} \perp \mathbf{d}^{(k)}$ .

Secondly, we let  $\mathbf{x}^{(0)}$  be the zero vector.

# Standard form of the conjugate gradient method

Here it is.

- (1) Set  $k = 0$ ,  $\mathbf{x}^{(0)} = \mathbf{0}$ ,  $\mathbf{r}^{(0)} = \mathbf{b}$ , and  $\mathbf{d}^{(0)} = \mathbf{r}^{(0)}$ ;
- (2) Calculate the matrix-vector product  $\mathbf{v}^{(k)} = \mathbf{A}\mathbf{d}^{(k)}$  and  $\alpha_k = \|\mathbf{r}^{(k)}\|^2 / (\mathbf{d}^{(k)}, \mathbf{v}^{(k)}) > 0$ ;
- (3) Apply the formulae  $\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha_k \mathbf{d}^{(k)}$  and  $\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \alpha_k \mathbf{v}^{(k)}$ ;
- (4) Stop if  $\|\mathbf{r}^{(k+1)}\|$  is acceptably small;
- (5) Set  $\mathbf{d}^{(k+1)} = \mathbf{r}^{(k+1)} + \beta_k \mathbf{d}^{(k)}$ , where  $\beta_k = \|\mathbf{r}^{(k+1)}\|^2 / \|\mathbf{r}^{(k)}\|^2 > 0$ ;
- (6) Increase  $k \rightarrow k + 1$  and go back to (2).

# Standard form of the conjugate gradient method

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The total work is dominated by the number of iterations, multiplied by the time it takes to compute  $\mathbf{v}^{(k)} = A\mathbf{d}^{(k)}$ . Thus the conjugate gradient algorithm is highly suitable when most of the elements of  $A$  are zero, i.e. when  $A$  is *sparse*.

# Preconditioning

In  $A\mathbf{x} = \mathbf{b}$ , we change variables,  $\mathbf{x} = P^T\hat{\mathbf{x}}$ , where  $P$  is a nonsingular  $n \times n$  matrix, and multiply both sides with  $P$ . Thus, instead of  $A\mathbf{x} = \mathbf{b}$ , we are solving the linear system

$$PAP^T\hat{\mathbf{x}} = P\mathbf{b} \quad \Leftrightarrow \quad \hat{A}\hat{\mathbf{x}} = \hat{\mathbf{b}}. \quad (4)$$

Note that symmetry and positive definiteness of  $A$  imply that  $\hat{A} = PAP^T$  is also symmetric and positive definite since  $(\hat{A}\mathbf{y}, \mathbf{y}) = (PAP^T\mathbf{y}, \mathbf{y}) = (AP^T\mathbf{y}, P^T\mathbf{y}) > 0$ . Therefore, we can apply conjugate gradients to the new system. This results in the solution  $\hat{\mathbf{x}}$ , hence  $\mathbf{x} = P^T\hat{\mathbf{x}}$ . This procedure is called the *preconditioned conjugate gradient method* and the matrix  $P$  is called the *preconditioner*.



# Condition number and convergence rate of CGM

The *condition number* of a matrix  $A$  is the value

$\kappa(A) := \|A\| \cdot \|A^{-1}\|$ , so for a symmetric positive definite matrix  $A$  it is the ratio between its largest and smallest eigenvalues,

$$\kappa(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} \geq 1.$$

The closer this number is to 1, the faster the convergence is of CGM. More precisely, for the rate of convergence of CGM, we have the upper estimate

$$\|\mathbf{e}^{(k)}\|_A \leq 2\rho^k \|\mathbf{e}^{(0)}\|_A, \quad \rho = \rho_A = \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} < 1. \quad (5)$$

The main idea of preconditioning is to pick  $P$  in (4) so that  $\kappa(\hat{A})$  is much smaller than  $\kappa(A)$ , thus accelerating convergence.

## Preconditioning – Choosing $P$

To this end, we note that the similarity transform  $B \rightarrow C^{-1}BC$  preserves spectrum, hence

$$\kappa(\hat{A}) = \kappa(PAP^T) = \kappa(P^{-1}[PAP^T]P) = \kappa(AP^T P),$$

and if we set

$$S^{-1} := P^T P =: (QQ^T)^{-1},$$

then it is suggestive to choose  $S$  as an approximation to  $A$  which is easy to Cholesky-factorize, i.e.,  $S = QQ^T$  (or already in this form), and then take  $P = Q^{-1}$ . Then  $AP^T P = AS^{-1}$  is close to identity, hence

$$\kappa(\hat{A}) = \kappa(AP^T P) \approx \kappa(I) = 1 \quad \Rightarrow \quad \kappa(\hat{A}) \ll \kappa(A),$$

and the preconditioned system (4) will be solved much faster because of (5).

## Preconditioning – Extra cost

Each step in the CGM for solving  $A\mathbf{x} = \mathbf{b}$  requires one matrix-vector product  $A\mathbf{y}$ , so with  $P = Q^{-1}$ , additional expense in each step of the CGM for the preconditioned system (4) while computing  $\hat{A}\mathbf{y} = PAP^T\mathbf{y}$  is two additional computations

$$\mathbf{u} = P^T\mathbf{y} = Q^{-T}\mathbf{y}, \quad \mathbf{v} = P\mathbf{z} = Q^{-1}\mathbf{z},$$

for some  $\mathbf{y}, \mathbf{z} \in \mathbb{R}^n$ , but note that computing  $Q^{-1}\mathbf{z}$  is the same as solving the linear system  $Q\mathbf{v} = \mathbf{z}$ , which is cheap (via forward substitution) as  $Q$  is a lower triangular matrix.

### Example 6

- 1) The simplest choice of  $S$  is  $D = \text{diag } A$ , then  $P = D^{-1/2}$  in (4).
- 2) Another possibility is to choose  $S$  as a band matrix with small bandwidth. For example, solving the Poisson equation with the five-point formula, we may take  $S$  to be the tridiagonal part of  $A$ .
- 3) One can also take  $P = L^{-1}$ , where  $L$  is the lower triangular part of  $A$  (maybe imposing some changes). For example, for the Poisson equation, with  $m = 20$  hence dealing with  $400 \times 400$  system, we take  $P^{-1}$  as the lower triangular part of  $A$ , but change the diagonal elements from 4 to  $\frac{5}{2}$ . Then we get a computer precision after just 30 iterations.

## Preconditioning – Examples

For the tridiagonal system  $A\mathbf{x} = \mathbf{b}$  below, we choose the preconditioner as follows.

$$A = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & -1 & 2 \end{bmatrix}, \quad Q = \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & \ddots & \ddots & & \\ & & & -1 & 1 \end{bmatrix},$$
$$S = QQ^T = \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & & -1 & 2 \end{bmatrix}.$$

## Preconditioning – Examples

The matrix  $S$  coincides with  $A$  except at the  $(1, 1)$ -entry. The matrix

$$\hat{A} = Q^{-1}AQ^{-T}$$

for the preconditioned CGM has just two distinct eigenvalues, and we recover the exact solution just in two steps. To see the latter, note that  $\hat{A}$  is similar to

$$Q^{-T}Q^{-1}A = S^{-1}A,$$

hence it has the same spectrum. Since  $A = S + \mathbf{e}_1\mathbf{e}_1^T$ , we have

$$S^{-1}A = I + \mathbf{u}\mathbf{e}_1^T,$$

a rank-1 perturbation of the identity matrix, with all eigenvalues but one equal 1 (the remaining one equal  $1 + u_1$ ).

# Rate of convergence of CGM

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## Theorem 7

*Consider the CGM. We then have the upper estimate*

$$\|\mathbf{e}^{(k)}\|_A \leq 2\rho^k \|\mathbf{e}^{(0)}\|_A, \quad \rho = \rho_A = \frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} < 1,$$

where  $\mathbf{e}^{(k)} = \mathbf{x}^* - \mathbf{x}^{(k)}$  and  $\mathbf{x}^{(k)}$  is the  $k$ -th output of the CGM.

# Conjugate gradient - Global approach

## Theorem 8 (Non-examinable)

Given  $A \in \mathbb{R}^{n \times n}$ ,  $A > 0$ , let  $\{\mathbf{d}^{(k)}\}_{k=0}^{m-1}$  be a set of the conjugate directions, i.e.,  $(A\mathbf{d}^{(k)}, \mathbf{d}^{(i)}) = 0$  for  $i < k$ , and consider

$$F(\mathbf{x}^{(k)}) := \|\mathbf{x}^* - \mathbf{x}^{(k)}\|_A^2 = \|\mathbf{e}^{(k)}\|_A^2.$$

Then the value of  $F(\mathbf{x}^{(m+1)})$  obtained through the CGM coincides with the minimum of  $F(\mathbf{y})$  taken over all  $\mathbf{y} = \mathbf{x}^{(0)} + \sum_{k=0}^m c_k \mathbf{d}^{(k)}$  simultaneously, namely

$$\arg \min_{c_0, \dots, c_m} F(\mathbf{y}) = \mathbf{x}^{(m+1)} = \mathbf{x}^{(0)} + \sum_{k=0}^m \alpha_k \mathbf{d}^{(k)}.$$



# Rate of convergence of CGM

**Proof of Theorem 7.** As we have seen, every direction  $\mathbf{d}^{(i)}$  in CGM is a linear combination of the vectors  $(A^s \mathbf{r}^{(0)})_{s=0}^i$ , therefore, any vector of the form  $\hat{\mathbf{x}}^{(k)} = \mathbf{x}^{(0)} + \sum_{i=0}^{k-1} a_i \mathbf{d}^{(i)}$  can be represented as

$$\hat{\mathbf{x}}^{(k)} = \mathbf{x}^{(0)} + \sum_{i=0}^{k-1} c_i A^i \mathbf{r}^{(0)}. \quad (6)$$

Subtracting both parts of (6) from the exact solution  $\mathbf{x}^*$  we obtain  $\hat{\mathbf{e}}^{(k)} = \mathbf{e}^{(0)} - \sum_{i=0}^{k-1} c_i A^i \mathbf{r}^{(0)}$ , and since  $\mathbf{r}^{(0)} = A \mathbf{e}^{(0)}$ , we can express the error  $\hat{\mathbf{e}}^{(k)} = \mathbf{x}^* - \hat{\mathbf{x}}^{(k)}$  as

$$\hat{\mathbf{e}}^{(k)} = (I - \sum_{i=1}^k c_i A^i) \mathbf{e}^{(0)} = P_k(A) \mathbf{e}^{(0)}, \quad (7)$$

where  $P_k$  is a polynomial of degree  $\leq k$ , which satisfies  $P_k(0) = 1$ .

# Rate of convergence of CGM

**Proof. Cont.** Now recall from Theorem 8 that, at the  $k$ -th stage, the CGM produces the vector  $\mathbf{x}^{(k)}$  that minimizes the functional

$$F(\widehat{\mathbf{x}}^{(k)}) = \|\widehat{\mathbf{e}}^{(k)}\|_A^2 = (A\widehat{\mathbf{e}}^{(k)}, \widehat{\mathbf{e}}^{(k)})$$

over all vectors  $\widehat{\mathbf{x}}^{(k)}$  of the form  $\widehat{\mathbf{x}}^{(k)} = \mathbf{x}^{(0)} + \sum_{i=0}^{k-1} a_i \mathbf{d}^{(i)}$ , hence over all  $\widehat{\mathbf{e}}^{(k)}$  of the form (7). Expressing  $\mathbf{e}^{(0)}$  as  $\mathbf{e}^{(0)} = \sum \gamma_i \mathbf{w}_i$ , where  $(\mathbf{w}_i)$  are orthonormal eigenvectors of  $A$ , we find from (7) that  $\widehat{\mathbf{e}}^{(k)} = \sum_i \gamma_i P_k(\lambda_i) \mathbf{w}_i$ , and  $A\widehat{\mathbf{e}}^{(k)} = \sum_i \gamma_i P_k(\lambda_i) \lambda_i \mathbf{w}_i$ , and respectively

$$\|\widehat{\mathbf{e}}^{(k)}\|_A^2 = \sum_i [P_k(\lambda_i)]^2 \lambda_i \gamma_i^2 \leq \max_{\lambda \in \sigma(A)} [P_k(\lambda)]^2 \|\mathbf{e}^{(0)}\|_A^2.$$

Hence, because of the minimization property of CGM,

$$\|\mathbf{e}^{(k)}\|_A = \min_{P_k} \|\widehat{\mathbf{e}}^{(k)}\|_A \leq \min_{P_k} \max_{\lambda \in \sigma(A)} |P_k(\lambda)| \|\mathbf{e}^{(0)}\|_A.$$

# Rate of convergence of CGM

**Proof. Cont.** Now, assume that, for the spectrum  $\sigma(A)$ , we know the largest and the smallest eigenvalues, or some lower and upper bounds, say,  $0 < m \leq \lambda \leq M$ . Then the following minimization problem, on the class of polynomials of degree  $k$ , arises:

$$P_k(0) = 1, \quad \max_{x \in [m, M]} |P_k(x)| \rightarrow \min .$$

This problem has a classical solution  $P_k^* = T_k^*$ , where  $T_k^*$  is the Chebyshev polynomial on the interval  $[m, M]$ , which is obtained by dilation and translation of the standard Chebyshev polynomial  $T_k$  given on the interval  $[-1, 1]$ :

$$T_k(x) = \cos k\theta, \quad x = \cos \theta, \quad \theta \in [0, \pi].$$

One can show that  $|T_k^*(x)| \leq 2\rho^k$  on the interval  $[m, M]$ , hence the rate of convergence of CGM admits the following estimate:

$$\|\mathbf{e}^{(k)}\|_A \leq 2\rho^k \|\mathbf{e}^{(0)}\|_A, \quad \rho = \frac{\sqrt{M} - \sqrt{m}}{\sqrt{M} + \sqrt{m}} < 1, \quad \sigma(A) \in [m, M].$$

