Challenges in coupling iterative algebraic computations with modeling and discretisation PART I - Basic (mostly algebraic) settings

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ERC-CZ MORE, 2012, Praha

Cornelius Lanczos, March 9, 1947

"The reason why I am strongly drawn to such
approximation mathematics problems is ... the fact that
a very "economical" solution is possible only when it is very "adequate".

To obtain a solution in very few steps
means nearly always that one has found a way
that does justice to the inner nature of the problem."

Albert Einstein, March 18, 1947

“Your remark on the importance of adapted approximation methods makes very good sense to me, and I am convinced that this is a fruitful mathematical aspect, and not just a utilitarian one.”

Algebraic iterative computations

- Computational cost of finding sufficiently accurate approximation to the exact solution heavily depends on the particular data, i.e.,
  - on the underlying real world problem,
  - on the mathematical model,
  - on its discretisation.
- Evaluation of cost must take into account rounding errors.
- Evaluation of accuracy of the computed approximation can not be done within the algebra.

Krylov subspace methods for linear problems

A relatively small number of nonlinear iterations which

- in principle (assuming exact arithmetic) form, when continued, a finite process
- can not be treated as a sequence of linearisations,
- are possibly significantly affected by rounding errors.

Always preconditioning!

If the preconditioned matrix approximates identity, then any reasonable iterative method performs well, and the iterative life is greatly simplified.

The story goes a way back ...

- Euclid (300BC), Hippassus from Metapontum (before 400BC), ... ,
- Bhascara II (1150), Brouncker and Wallis (1655-56): Three term recurences (for numbers)
- Euler (1737, 1748), ... , Brezinski (1991), Khrushchev (2008)
- Gauss (1814), Jacobi (1826), Christoffel (1858, 1857), ... , Chebyshev (1855, 1859), Markov (1884), Stieltjes (1884, 1893-94): Orthogonal polynomials, quadrature, analytic theory of continued fractions, problem of moments, minimal partial realization, Riemann-Stieltjes integral
  Gautschi (1981, 2004), Brezinski (1991), Van Assche (1993), Kjeldsen (1993),
- Hilbert (1906, 1912), ... , Von Neumann (1927, 1932), Wintner (1929) resolution of unity, integral representation of operator functions in quantum mechanics

In the language of matrix computations

- Krylov (1931), Gantmakher (1934), Lanczos (1950–52, 1952c), Hestenes and Stiefel (1952), Rutishauser (1953), Henrici (1958), Stiefel (1958), Rutishauser (1959), Vorobyev (1958, 1965), ...
- Gordon (1968), Schlesinger and Schwartz (1966), Reinhard (1979), ... , Horáček (1983), Laptev, Nabokov and Safronov (2003), Simon (2007)
- Paige (1971), Reid (1971), Greenbaum (1978, 1989), ...
- Paige and Saunders (1975, 1982), van der Vorst (1982), Elman (1982), Saad and Schultz (1986), ...
- Magnus (1962a,b), Gragg (1974), Kalman (1979), Gragg, Lindquist (1983), Gallivan, Grimme, Van Dooren (1994), ...

Are there still any challenges left ?

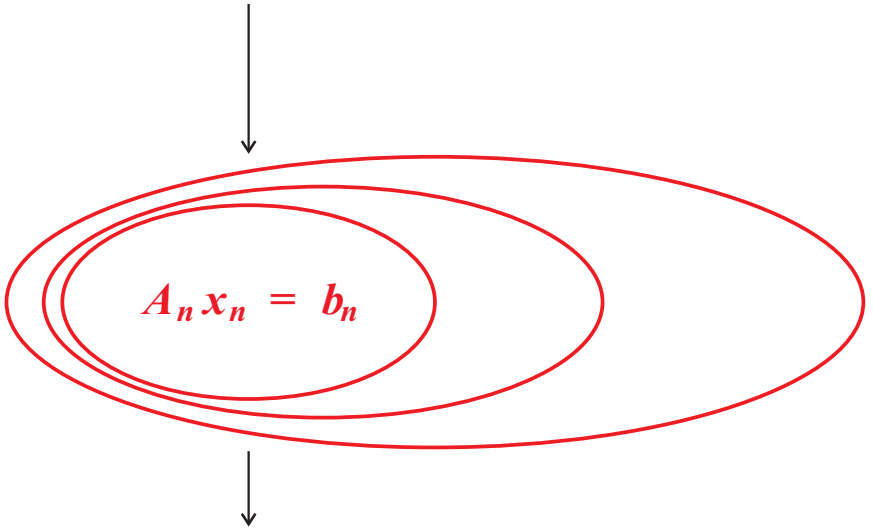
Outline

1. Nonlinearity of Krylov subspace methods
2. CG and the convergence bound for CSI
3. Clusters = fast convergence ?
4. Algebraic error in numerical PDEs
5. Conclusions

Point 1: Nonlinearity of Krylov subspace methods

1 Krylov subspace methods

$$A\,x \;=\; b$$



x_n approximates the solution x
using the subspace of small dimension.

$$\mathcal{S}_n \;\equiv\; \mathcal{K}_n(A, r_0) \;\equiv\; span\,\{r_0, Ar_0, \cdots, A^{n-1}r_0\} \;\longrightarrow\; \text{moments !}$$

1 Conjugate gradients (CG): A HPD

$$\|x - x_n\|_A \;=\; \min_{u \,\in\, x_0 + \mathcal{K}_n(A,r_0)} \|x - u\|_A$$

with the formulation via the Lanczos process, $w_1 = r_0/\|r_0\|$,

$$A\,W_n \;=\; W_n\,T_n \;+\; \delta_{n+1} w_{n+1} e_n^T\,, \quad T_n \;=\; W_n^*(A, r_0)\,A\,W_n(A, r_0)\,,$$

and the CG approximation given by

$$T_n\,y_n \;=\; \|r_0\| e_1\,, \quad x_n \;=\; x_0 \;+\; W_n\,y_n\,.$$

$$A_n \;=\; Q_n\,A\,Q_n \;=\; W_n W_n^*\,A\,W_n W_n^* \;=\; W_n\,T_n\,W_n^*\,,$$

1 Computational algorithm

Given x_0 (in approximating $b^* A^{-1} b$ we set $x_0 = 0$), $r_0 = b - Ax_0$, $p_0 = r_0$

For $n = 1, 2, \ldots$

$$
\begin{aligned}
 & \gamma_{n-1} = (r_{n-1}, r_{n-1})/(p_{n-1}, Ap_{n-1}) \\
x_n &= x_{n-1} + \gamma_{n-1}\, p_{n-1} \\
r_n &= r_{n-1} - \gamma_{n-1}\, Ap_{n-1} \\
 & \delta_n = (r_n, r_n)/(r_{n-1}, r_{n-1}) \\
p_n &= r_n + \delta_n\, p_{n-1}.
\end{aligned}
$$

Search directions are given by the modified residuals, γ_{n-1} gives the line search minimum, δ_n ensures the local A-orthogonality of the direction vectors. No moments are visible. If we wish to get an insight, we need them.

1 Numerical PDE connection of CG

Find $u \equiv u(\xi_1, \xi_2)$, where ξ_1, ξ_2 denote the space variables, such that

$$-\nabla^2 u \;=\; f \quad \text{in a bounded domain } \; \Omega \subset \mathbb{R}^2 \,,$$

$$u \;=\; g_{\mathcal{D}} \;\text{ on }\; \partial\Omega_{\mathcal{D}}, \quad \text{and} \quad \frac{\partial u}{\partial n} \;=\; g_{\mathcal{N}} \;\text{ on }\; \partial\Omega_{\mathcal{N}} \,,$$

where $\partial\Omega_{\mathcal{D}} \cup \partial\Omega_{\mathcal{N}} \;=\; \partial\Omega$, and $\partial\Omega_{\mathcal{D}} \cap \partial\Omega_{\mathcal{N}} \;=\; \emptyset$.

For the Galerkin FEM approximation

$$\|\nabla(u - u_h^{(n)})\|^2 \;=\; \|\nabla(u - u_h)\|^2 \;+\; \|x - x_n\|_A^2 \,.$$

1 CG $\equiv$ matrix formulation of the Gauss q.

$$
\begin{array}{ccc}
A, w_1 = r_0/\|r_0\| & \longleftrightarrow & \omega(\lambda), \quad \int f(\lambda)\, d\omega(\lambda) \\
\uparrow & & \uparrow \\
T_n, e_1 & \longleftrightarrow & \omega^{(n)}(\lambda), \quad \sum_{i=1}^{n} \omega_i^{(n)}\, f\left(\theta_i^{(n)}\right)
\end{array}
$$

$$
\omega^{(n)}(\lambda) \longrightarrow \omega(\lambda)
$$

Point 2: CG and the convergence bound for CSI

2 CG as a model reduction matching $2n$ moments

$$\int \lambda^{-1}\, d\omega(\lambda) \;=\; \sum_{i=1}^{n} \omega_i^{(n)} \left(\theta_i^{(n)}\right)^{-1} \;+\; R_n(f)$$

$$\frac{\|x - x_0\|_A^2}{\|r_0\|^2} \;=\; n\text{-th Gauss quadrature} \;+\; \frac{\|x - x_n\|_A^2}{\|r_0\|^2}$$

With $x_0 = 0,$ $\qquad b^* A^{-1} b \;=\; \sum_{j=0}^{n-1} \gamma_j \|r_j\|^2 \;+\; r_n^* A^{-1} r_n\,.$

Hesteness and Stiefel, Vorobyev, Golub, Meurant, Brezinski, Reichel, Boley, Gutknecht, Saylor, Smolarski, ... , Meurant and S (2006), Golub and Meurant (2010), S and Tichý (2011),

Liesen, S, Krylov subspace methods, OUP (2012)

2 A linear bound for the nonlinear method

$$\|x - x_n\|_A \;=\; \{\, \|x - x_0\|_A \;-\; \|r_0\|^2 \; n\text{-th Gauss quadrature} \,\}^{\frac{1}{2}} \,.$$

Using the shifted Chebyshev polynomials on the interval $[\lambda_1, \lambda_N]$,

$$\|x - x_n\|_A \;\leq\; \|x - x_n^{CSI}\|_A \;\leq\; 2 \left(\frac{\sqrt{\kappa(A)} - 1}{\sqrt{\kappa(A)} + 1} \right)^n \|x - x_0\|_A \,.$$

This widely used bound does NOT describe, apart from very special cases, the convergence behaviour of CG.

2 Minimization property and the bound

- Markov (1890)
- Flanders and Shortley (1950)
- Lanczos (1953), Kincaid (1947), Young (1954, ...)
- Stiefel (1958), Rutishauser (1959)
- Meinardus (1963), Kaniel (1966)
- Daniel (1967a, 1967b)
- Luenberger (1969)

The bound is relevant to the Chebyshev method.

2 Composite bounds with s large outliers

The following statement reappears in literature (1977, ... , 2009, 2011, ...)

Theorem

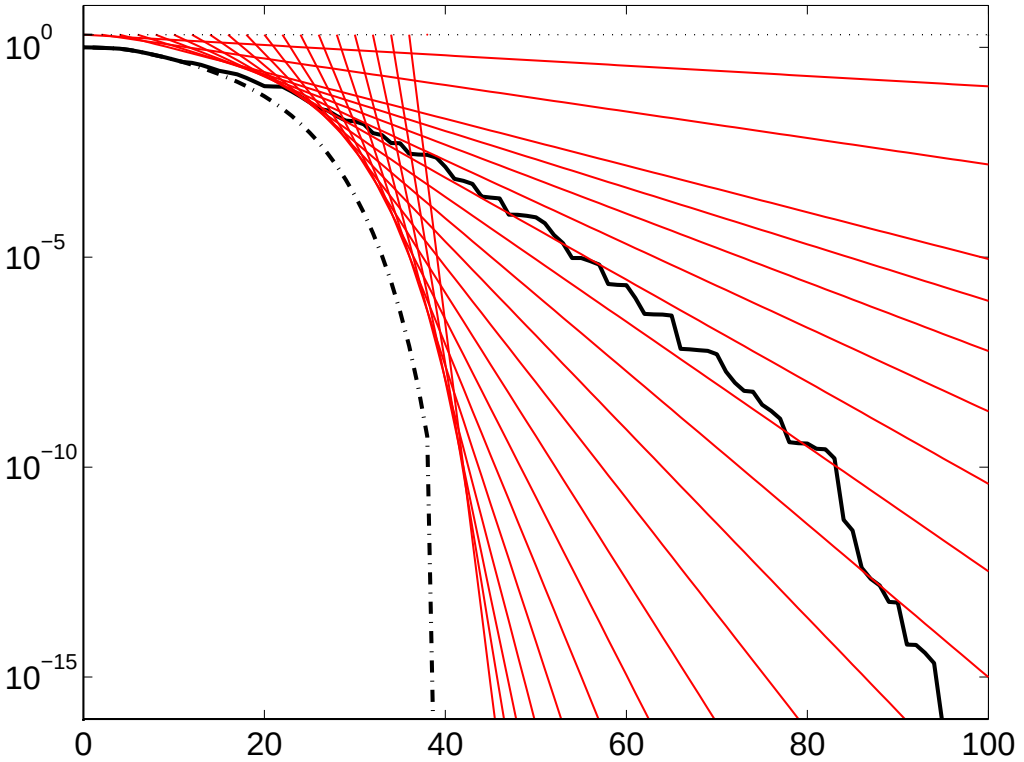
Consider the desired accuracy ϵ . Then

$$\mathbf{k} \;=\; \mathbf{s} \;+\; \left\lceil \frac{\ln(2/\epsilon)}{2}\sqrt{\kappa_s(A)} \right\rceil \;, \quad \kappa_s(A) \equiv \frac{\lambda_{N-s}}{\lambda_1}$$

CG steps will produce the approximate solution x_n satisfying

$$\|x - x_n\|_A \;\leq\; \epsilon\, \|x - x_0\|_A \,.$$

2 Liesen, S (2012); Gergelits, S (2012)



Finite precision arithmetic computations, inexact Krylov spce methods?

Point 3: Clusters = fast convergence ?

Point 3: HPD problem and CG

- in exact arithmetic, CG applied to a matrix with the spectrum consisting of t tight clusters of eigenvalues does not find, in general, a reasonably close approximation to the solution within t steps.

- Finite precision arithmetic CG computation can be viewed as exact CG applied to a larger matrix with the individual original eigenvalues replaced by tight clusters.

- Finite precision arithmetic CG computation with a matrix having t isolated well separated eigenvalues may require for reaching a reasonable approximate solution a significantly larger number of steps than t .

3 Any GMRES convergence with any spectrum

Theorem

1° The spectrum of A is $\{\lambda_1, \ldots, \lambda_N\}$ and GMRES(A, b) yields residuals with the prescribed nonincreasing sequence

$$\|r_0\| \geq \|r_1\| \geq \cdots \geq \|r_{N-1}\| > \|r_N\| = 0\,.$$

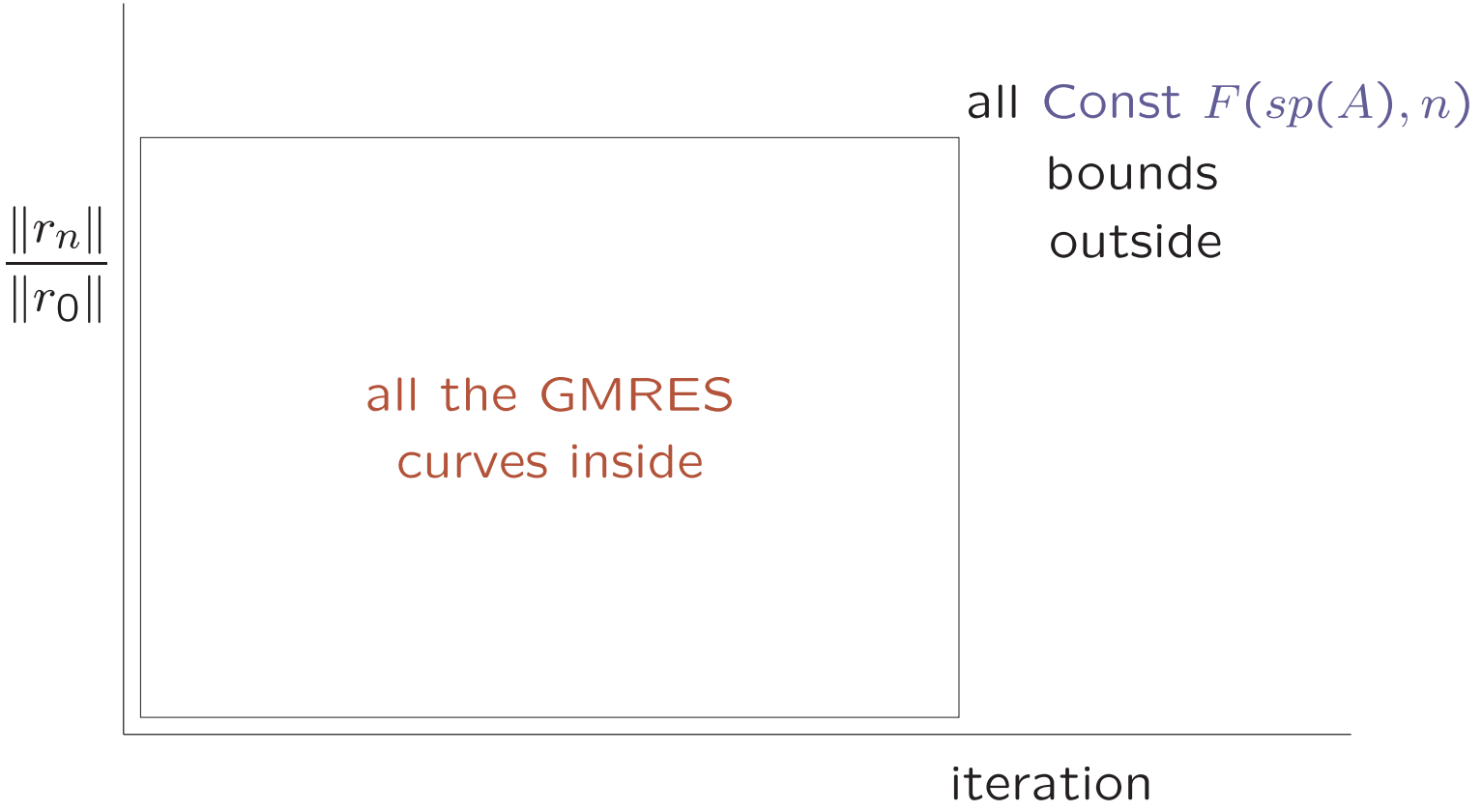
2° Matrix A is of the form $A = WRCR^{-1}W^*$ and $b = Wh$ where C is the spectral companion matrix, W is unitary and R a nonsingular upper triangular matrix such that $Rs = h$.

Complete parametrization. Set of measure zero?

Greenbaum, Ptak, Arioli and S (1994 - 98); Eirmann and Ernst (2001); Meurant (2012); Meurant and Duintjer Tebbens (2012); Meurant, Duintjer Tebbens and S (2012); .....

3 Claims based only on the spectrum

The bounds Const $F_n(sp(A), N)$ do not intersect the rectangle $(1,0) - (1,N) - (0,N) - (0,0)$.



3 Functional analytic point of view

- "... useful insight is gained as to the relationship between Hilbert space and matrix condition numbers and translating Hilbert space fixed point iterations into matrix computations provides new ways of motivating and explaining some classic iteration schemes." Kirby, SIREV, 2010

- "... in the early sweeps the convergence is very rapid but slows down, this is the sublinear behavior. The convergence then settles down to a roughly constant linear rate ... Towards the end new speed may be picked up again, corresponding to the superlinear behavior. ...
  In practice all phases need not be identifiable, nor need they appear only once and in this order." Nevanlinna, 1993, Section 1.8

- "However, if the operator has a few eigenvalues far away from the rest of the spectrum, then the estimate is not sharp. In fact, a few 'bad eigenvalues' will have almost no effect on the asymptotic convergence of the method ..." Mardal and Winther, NLAA, 2011

3 An example

Consider a fixed point iteration in the Banach space with the bounded operator $\mathcal{B}$,

$$u = \mathcal{B}\,u + f\,, \quad u^{(\ell+1)} = \mathcal{B}\,u^{(\ell)} + f\,.$$

Using polynomial acceleration we can do better,

$$u - u^{(\ell)} = p_\ell(\mathcal{B})\,(u - u^{(0)})\,.$$

Separating the operator polynomial from the initial error, *it seems natural* to minimize the appropriate norm of the operator polynomial

$$\|p_\ell(\mathcal{B})\| \qquad \text{subject to } \; p_\ell(0) = 0\,.$$

3 An example continues

Consider now a numerical (finite dimensional) approximation $\mathcal{B}_h$ of the bounded operator $\mathcal{B}$. Then

$$p(\mathcal{B}) - p(\mathcal{B}_h) = \frac{1}{2\pi\imath} \int_\Gamma p(\lambda) \left[(\lambda\mathcal{I} - \mathcal{B})^{-1} - (\lambda\mathcal{I} - \mathcal{B}_h)^{-1} \right] d\lambda \,.$$

This is considered a sufficient argument why to study algebraic iterations directly in abstract (infinite dimensional) Banach spaces.

At this level of abstraction, many challenges which one must deal with in studying finite computational processes at finite dimensional spaces are simply not visible. Abstract Banach space settings make things certainly easier (it does not see the trouble). It, however, does not answer the question about the cost of the algebraic computations (and therefore also about the cost of the whole solution process).

3 A way to get together

- Assumptions used in derivations of the statements should be strictly respected when the statements are further used.
- Statements should be interpreted more rigorously.
- Questions challenging common views may inspire further progress. One should be open to consider them.

Computation is performed within the finite dimensional algebraic setting. Analysis of the finite dimensional algebraic problem can not be done on the model problem level using functional analysis in infinite dimensional Banach or Hilbert spaces. Such approaches do not see discretisation and computation in an adequate way. On the other hand, analysis of the finite dimensional algebraic problem must “do justice” to the original (non-algebraic) problem as much as possible.

Point 4: Algebraic error in numerical PDEs

4 Verification and validation

Knupp and Salari, 2003:

"There may be incomplete iterative convergence (IICE) or round-off-error that is polluting the results. If the code uses an iterative solver, then one must be sure that the iterative stopping criteria is sufficiently tight so that the numerical and discrete solutions are close to one another. Usually in order-verification tests, one sets the iterative stopping criterion to just above the level of machine precision to circumvent this possibility."

In solving tough problems this can not be afforded.

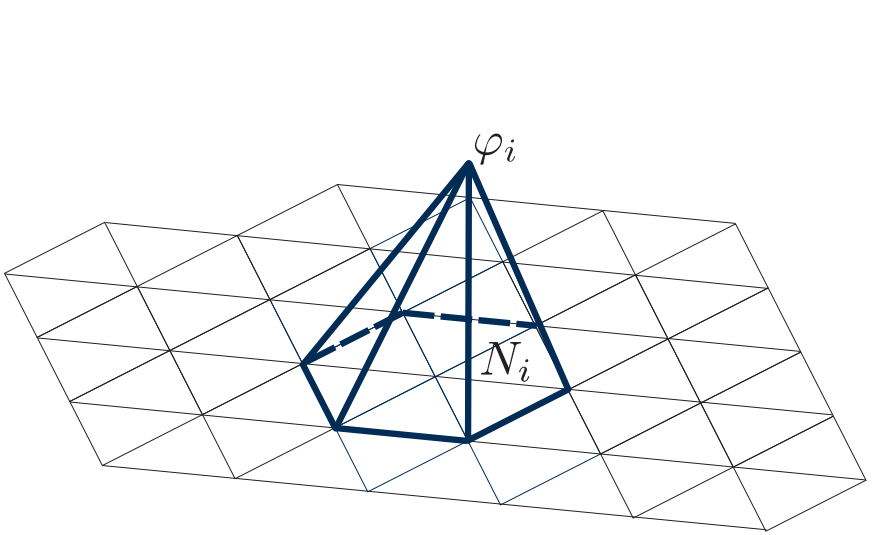
How to measure the algebraic error ?

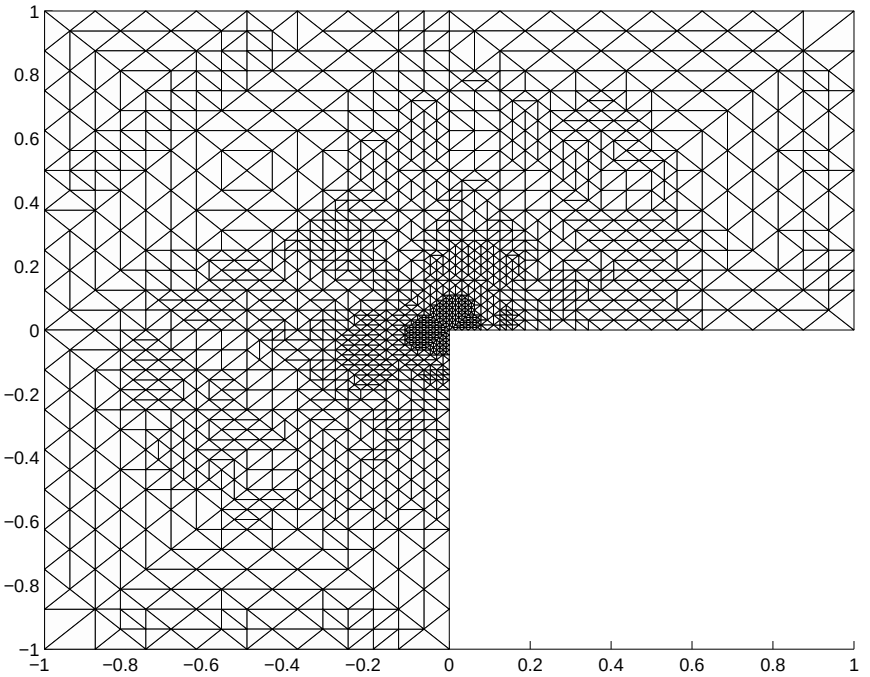
4 Local discretisation and global computation

Discrete (piecewise polynomial) solution $u_h = \sum_{j=1}^{N} \zeta_j \varphi_j$.

- If ζ_j is known exactly, then the global information is approximated as the (exact) linear combination of the local basis functions.
- Apart from trivial cases, $\zeta_j,\ j = 1, 2, \ldots,$ that supply the global information, are not known exactly. Then

$$\underbrace{u - u_h^{(n)}}_{\text{total error}} = \underbrace{u - u_h}_{\text{discretisation error}} + \underbrace{u_h - u_h^{(n)}}_{\text{algebraic error}} .$$


φ_i
N_i


1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.8
−0.6
−0.4
−0.2
0
0.2
0.4
0.6
0.8
1

4 Global energy norm of the error

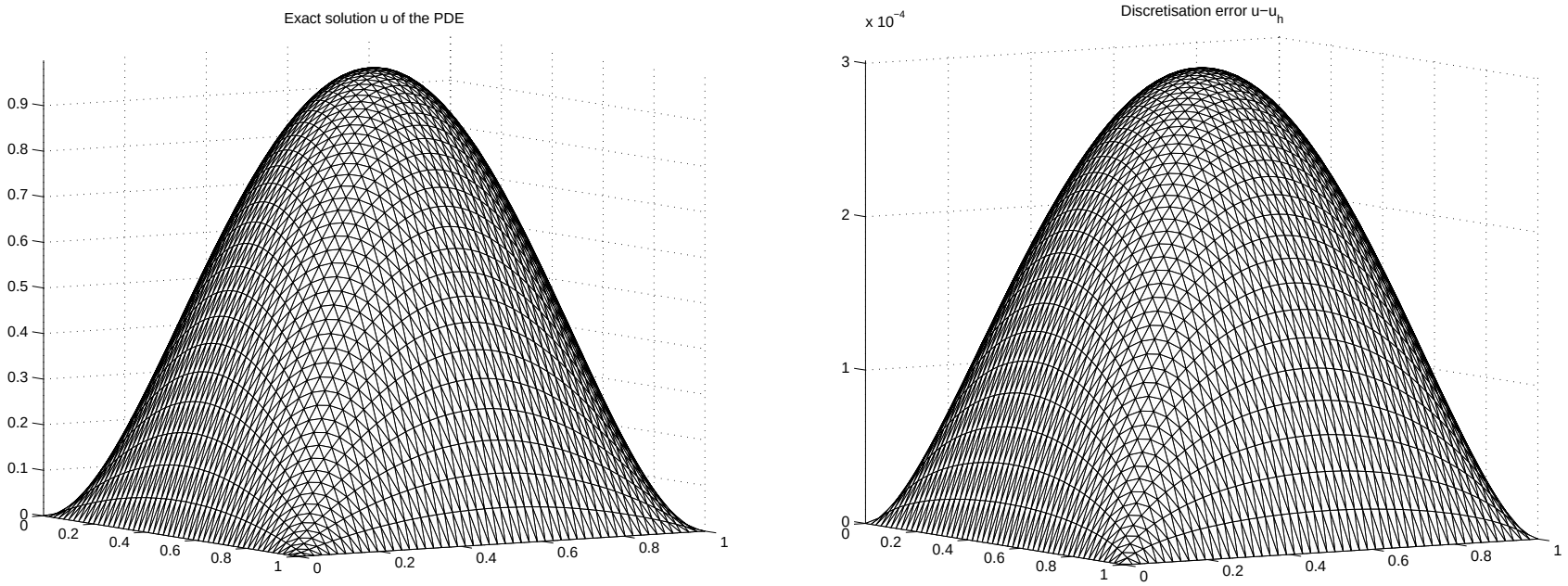
Theorem

Up to a small inaccuracy proportional to machine precision,

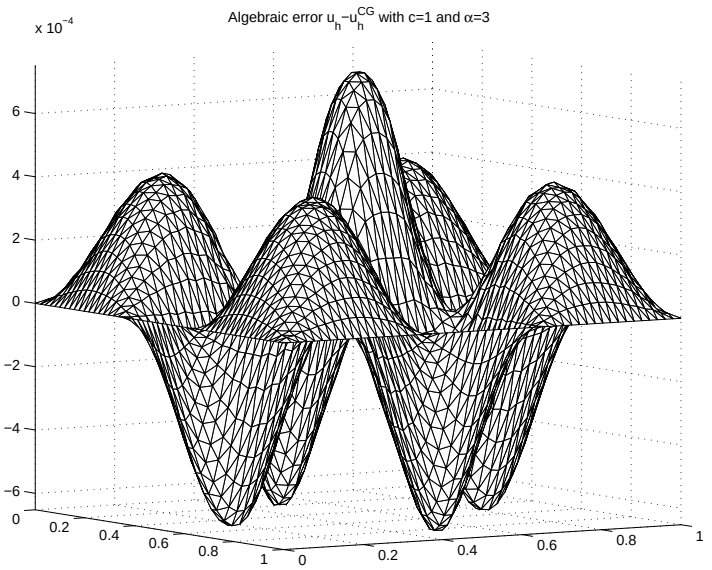
$$\begin{aligned} \|\nabla(u - u_h^{(n)})\|^2 &= \|\nabla(u - u_h)\|^2 + \|\nabla(u_h - u_h^{(n)})\|^2 \\ &= \|\nabla(u - u_h)\|^2 + \|x - x_n\|_A^2 \,. \end{aligned}$$

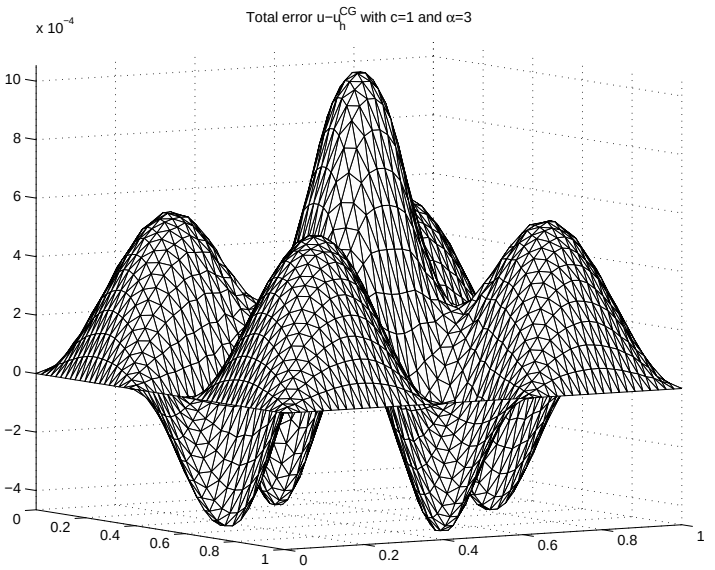
Question: What is the distribution of the algebraic error in the functional space ?

4 A simple model boundary value problem



Exact solution u of the Poisson model problem (left)
and the MATLAB `trisurf` plot of the discretisation error $u - u_h$ (right).

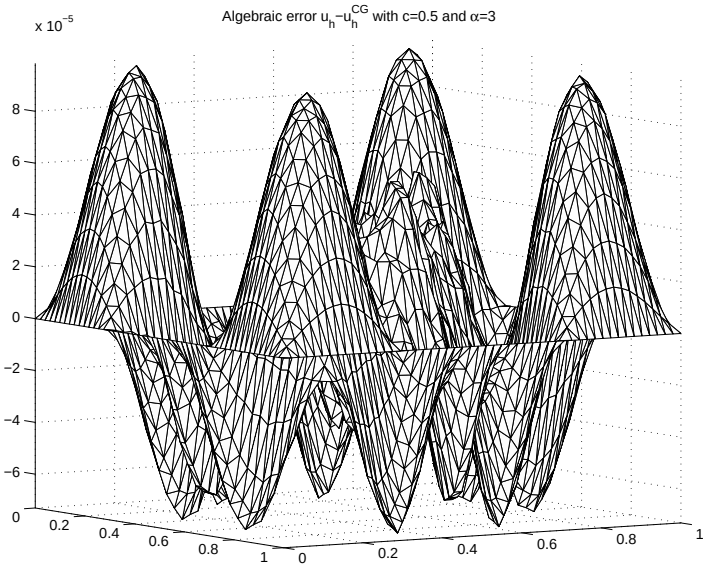


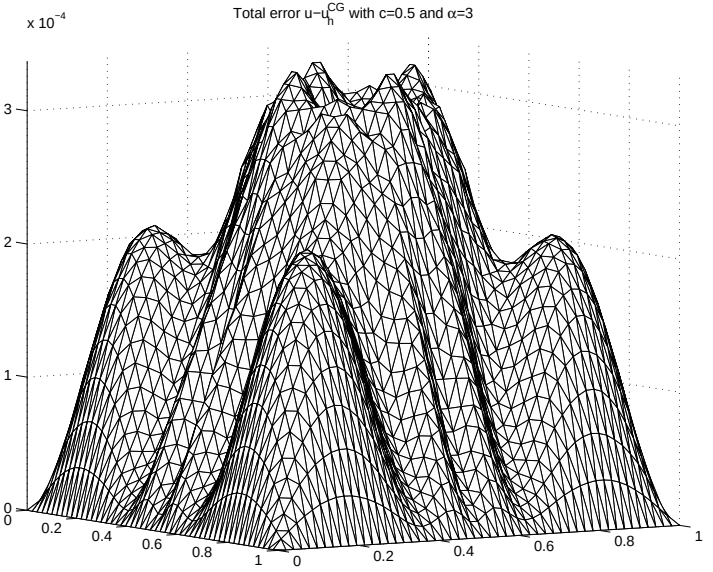


Algebraic error $u_h - u_h^{(n)}$ (left) and the MATLAB `trisurf` plot of the total error $u - u_h^{(n)}$ (right),

$$\begin{aligned} \|\nabla(u - u_h^{(n)})\|^2 &= \|\nabla(u - u_h)\|^2 + \|x - x_n\|_A^2 \\ &= 5.8444e-03 + 1.4503e-05\,. \end{aligned}$$

4 Algebraic and total errors

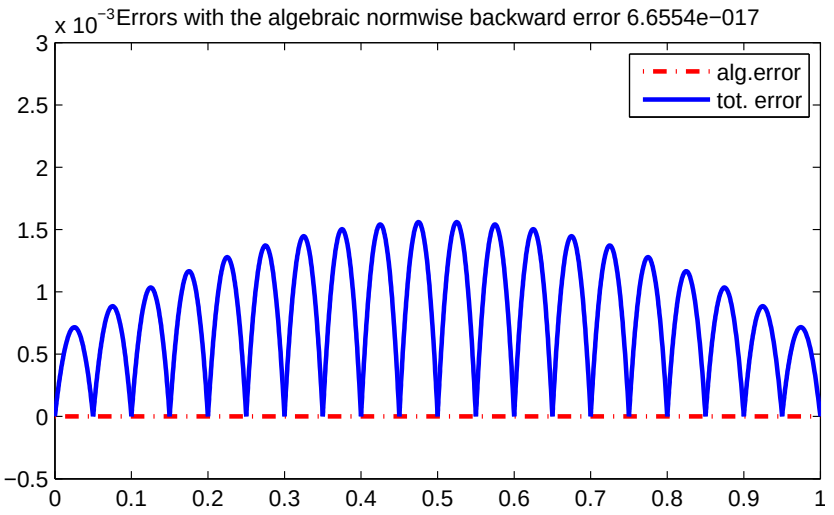


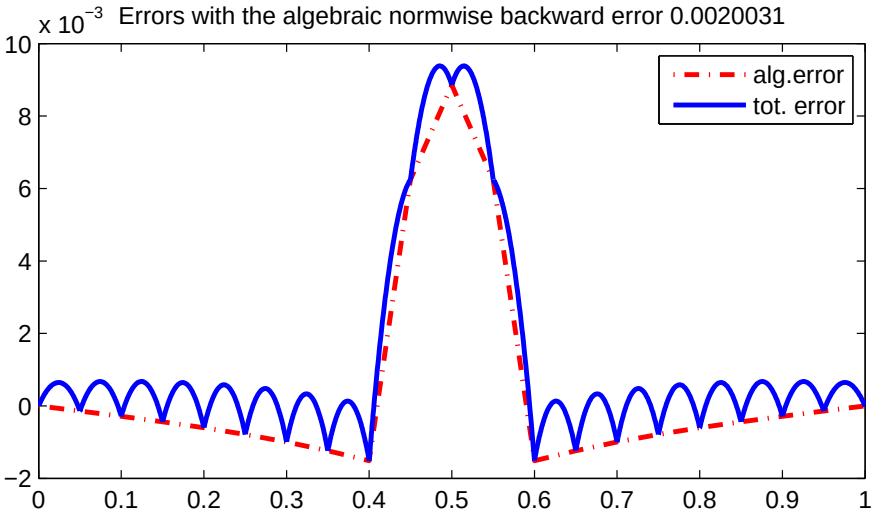


Algebraic error $u_h - u_h^{(n)}$ (left) and the MATLAB `trisurf` plot of the total error $u - u_h^{(n)}$ (right),

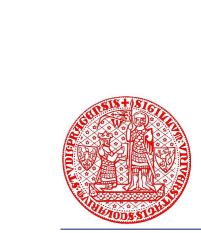
$$\begin{aligned} \|\nabla(u - u_h^{(n)})\|^2 &= \|\nabla(u - u_h)\|^2 + \|x - x_n\|_A^2 \\ &= 5.8444e-03 + 5.6043e-07\,. \end{aligned}$$

4 1D analogy, Papež and S (2012)

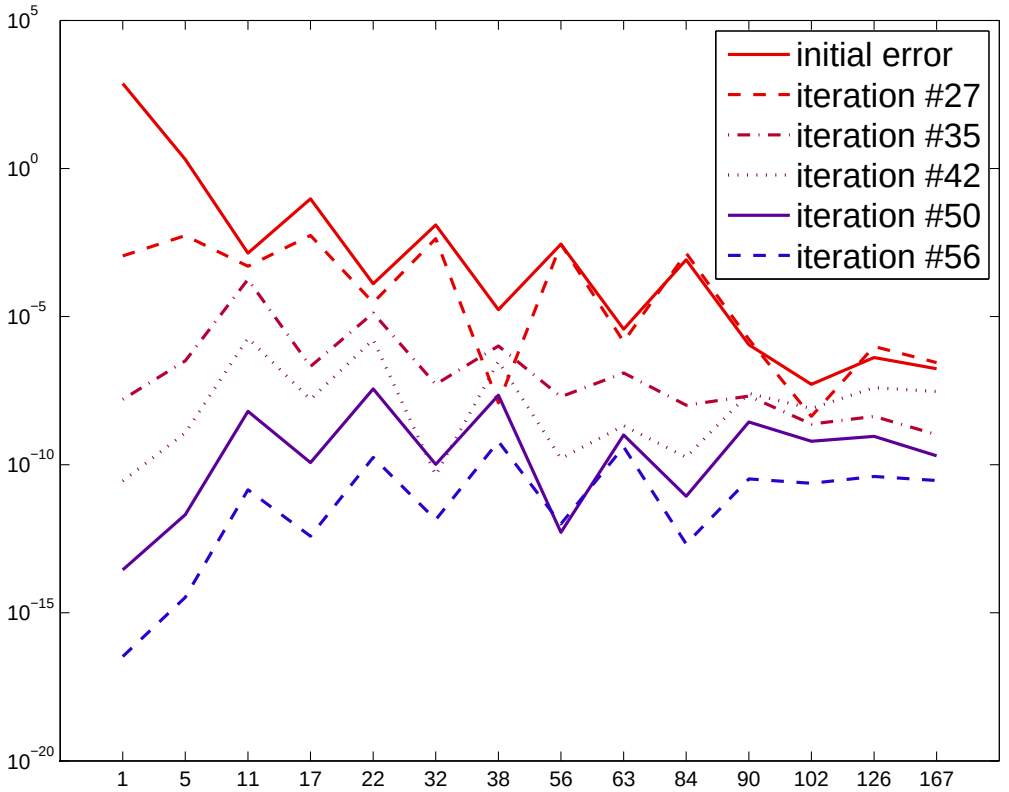




The discretisation error (left),
the algebraic and the total error (right),



4 Why? Moment matching.



Krylov subspace methods represent matching moments model reduction!

4 Backward error challenge

We need fully computable *a-posteriori* error bounds (no hidden constants) which are:

- Locally efficient,
- and allow to compare the local contribution of the discretisation error and the algebraic error to the total error.

Challenges for the algebraic backward error theory:

- We need componentwise relative forward error.
- Functional backward error (perturbation of the bilinear form) modifies the problem to be solved.
- Projecting the backward error into the FEM basis makes the basis functions non-local.

4 Loss of locality

Consider the transformation of the FEM basis functions $\Phi = [\varphi_1, \ldots, \varphi_n]$ (in the model problem the continuous piecewise linear hat functions) to the basis $\widehat{\Phi} = [\widehat{\varphi}_1, \ldots, \widehat{\varphi}_n]$ represented by a square matrix $\mathbf{D} \in \mathbb{R}^{n \times n}$, $\mathbf{D} = [D_{\ell j}]$,

$$\widehat{\varphi}_j = \varphi_j + \sum_{\ell=1}^{n} D_{\ell j}\, \varphi_\ell\,, \quad j = 1, \ldots, n\,.$$

or, in the compact form

$$\widehat{\Phi} = \Phi\,(\mathbf{I} + \mathbf{D})\,,$$

where $\mathbf{D}$ accounts for the numerical errors in solving the discretised finite dimensional algebraic problem.

Gratton, Jiránek and Vasseur (2012); Papež, S (2012)

4 Loss of locality - meaning of $\mathbf{D}$

We look for $\mathbf{D}$ such that the Galerkin solution

$$u_h = \Phi\mathbf{x}, \quad \mathbf{A}\mathbf{x} = \mathbf{b}$$

of the discretised problem

$$a(u_h, \varphi_i) = \ell(\varphi_i), \quad i = 1, \ldots, n$$

can be expressed as the exact solution

$$u_h = \Phi(\mathbf{I} + \mathbf{D})\widehat{\mathbf{x}}, \quad \widehat{\mathbf{A}}\widehat{\mathbf{x}} = \mathbf{b}$$

of the same infinite dimensional problem discretised via the transformed basis functions $\Phi(\mathbf{I} + \mathbf{D})$ and the original test functions $\varphi_i,\ i = 1, \ldots, n$. Here the algebraic vector $\widehat{\mathbf{x}}$ which approximates $\mathbf{x}$ solves exactly the algebraic system determined by the Petrov-Galerkin discretisation of the infinite dimensional problem.

4 Loss of locality - determining $\mathbf{D}$

Using the algebraic backward error we immediately get that the given approximate solution $\widehat{\mathbf{x}}$ of $\mathbf{A}\mathbf{x} = \mathbf{b}$ solves exactly the perturbed algebraic system

$$(\mathbf{A} + \mathbf{E})\,\widehat{\mathbf{x}} = \mathbf{b}$$

where

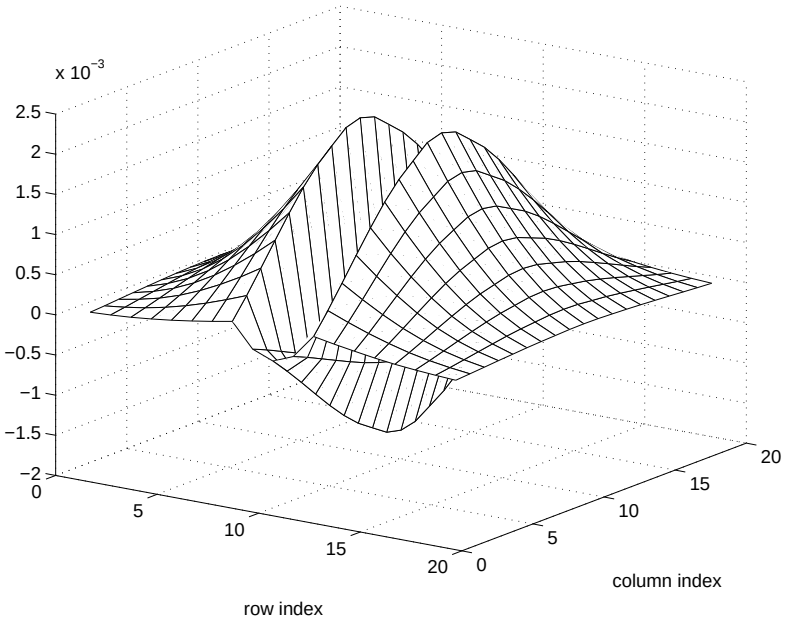
$$\mathbf{E} = \frac{(\mathbf{b} - \mathbf{A}\widehat{\mathbf{x}})\widehat{\mathbf{x}}^T}{\|\widehat{\mathbf{x}}\|^2}\,.$$

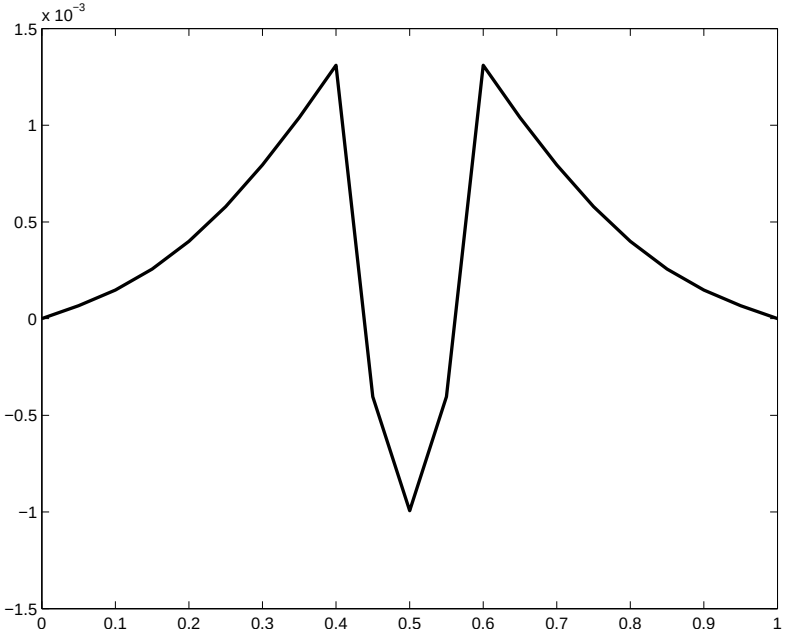
Finally, setting

$$\mathbf{E} = \mathbf{A}\mathbf{D} \quad \text{i.e.} \quad \mathbf{D} = \mathbf{A}^{-1}\mathbf{E}$$

finishes the result.

4 Loss of locality





The MATLAB `surf` plot of the transformation matrix $\mathbf{D}$ (left) and the difference $\widehat{\varphi}_j - \varphi_j$ (right).

Conclusions

Patrick J. Roache's book *Validation and Verification in Computational Science*, 1998, p. 387:

"With the often noted tremendous increases in computer speed and memory, and with the less often acknowledged but equally powerful increases in algorithmic accuracy and efficiency, a natural question suggest itself. What are we doing with the new computer power? with the new GUI and other set-up advances? with the new algorithms? What *should* we do? ... *Get the right answer."*

This can not be done without considering modelling, discretisation, analysis and computation tightly coupled parts of
a single solution process.

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Principles and Analysis

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Numerical Mathematics and Scientific Computation
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Price: GBP 75.00 (60.00)

Papež, Liesen and S (2012); Gergelits and S (2012); Rannacher (2012); Ern and Vohralik (2012); Jiranek, S, Vohralik (2010); Arioli, Loghin and Wathen (2005); ... ...

Thank you for your kind patience