An Exponential Integrator for ODEs with polynomial parameterization

Antti Koskela
KTH Royal Institute of Technology
Dept. of Mathematics - Numerical Analysis group

joint work with
Elias Jarlebring, KTH
Michiel Hochstenbach, TU Eindhoven

SIAM Conference on Applied Linear Algebra,
Atlanta, Ocotber 26, 2015

Problem

Let $A_0, A_1, \ldots, A_N \in \mathbb{C}^{n\times n}$ and consider the parameterized linear ODE

$$\frac{\partial u}{\partial t}(t,\varepsilon) = A(\varepsilon)\, u(t,\varepsilon), \quad u(0,\varepsilon) = u_0,$$

where A is the matrix polynomial

$$A(\varepsilon) := A_0 + \varepsilon A_1 + \cdots + \varepsilon^N A_N.$$

Specifically considered: problems arising from spatial semidiscretizations of partial differential equations (i.e., the matrices A_ℓ large and sparse).

Series representation

Let the coefficients of the Taylor expansion of the solution with respect to the parameter ε be denoted by $c_0(t)$, $c_1(t)$, $\ldots$, i.e.,

$$u(t,\varepsilon) = \exp(tA(\varepsilon))\, u_0 = \sum_{\ell=0}^{\infty} \varepsilon^{\ell} c_{\ell}(t). \qquad (*)$$

As $\exp(tA(\varepsilon))$ is an entire function of a matrix polynomial, the expansion (*) exists for all $\varepsilon \in \mathbb{C}$.

Approximation

Consider the approximation stemming from
the truncation of the Taylor series and
from an approximation of the Taylor coefficients:

$$\begin{aligned} u_k(t,\varepsilon) &:= \sum_{\ell=0}^{k-1} \varepsilon^\ell c_\ell(t) \\ &\approx \sum_{\ell=0}^{k-1} \varepsilon^\ell \widetilde{c}_\ell(t) =: \widetilde{u}_k(t,\varepsilon). \end{aligned} \qquad (*)$$

Our approach gives an explicit parameterization w.r.t. t of the approximate coefficients $\widetilde{c}_0(t),\ldots,\widetilde{c}_{k-1}(t)$.

On the other hand, (*) gives an explicit parametrization w.r.t. ε.

As a result, we can efficiently approximate the solution $u(t,\varepsilon)$ for different values of t and ε.

Main theorem

The Taylor coefficients $c_0(t), \ldots, c_{m-1}(t)$ are explicitly given by

$$\operatorname{vec}(c_0(t), \ldots, c_{m-1}(t)) = \exp(tL_m)\, \widetilde{u}_0,$$

where

$$L_m := \begin{bmatrix} A_0 & & & & & \\ A_1 & \ddots & & & & \\ \vdots & \ddots & \ddots & & & \\ A_{\widehat{N}} & \ddots & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & A_{\widehat{N}} & \ldots & A_1 & A_0 \end{bmatrix} \in \mathbb{C}^{mn \times mn}, \quad \widetilde{u}_0 = \begin{bmatrix} u_0 \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

and $\widehat{N} = \min(m-1, N)$.

Related work

Case $N = 1$ considered in

I.Najfeld and T.F. Havel. *Derivatives of the matrix exponential and their computation.* Advances in Applied Mathematics 16.3 (1995).

The main theorem can also be obtained from a theorem in

R. Mathias. *A chain rule for matrix functions and applications.* SIAM Journal on Matrix Analysis and Applications 17.3 (1996).

Recent related work:

D.A. Bini, S. Dendievel, G. Latouche and B. Meini. *Computing the exponential of large block-triangular block-Toeplitz matrices encountered in fluid queues.* Linear Algebra and its Applications (2015).

N.J. Higham and S.D. Relton. *Estimating the condition number of the Fréchet derivative of a matrix function.* SIAM Journal on Scientific Computing 36.6 (2014).

Krylov approximation of matrix functions

The Arnoldi iteration gives an orthogonal basis $Q_k \in \mathbb{R}^{n\times k}$ for the Krylov subspace

$$\mathcal{K}_k(A, b) = \mathrm{span}\{b, Ab, A^2b, ..., A^{k-1}b\},$$

and the Hessenberg matrix $H_k = Q_k^{\mathsf{T}} A Q_k \in \mathbb{R}^{k\times k}$.

For any polynomial p_n of degree $n \leq k-1$ it holds

$$p_n(A)b = Q_k p_n(H_k) Q_k^* b = Q_k p_n(H_k) e_1.$$

We use the approximation

$$\exp(A)b \approx Q_k \exp(H_k) Q_k^{\mathsf{T}} b.$$

Bounds for the norm and logarithmic norm of L_m

Recall the field of values of a matrix $A \in \mathbb{C}^{n\times n}$:

$$\mathcal{F}(A) = \{x^* A x \,:\, x \in \mathbb{C}^n,\ \|x\| = 1\}.$$

Let $L_m \in \mathbb{C}^{mn\times mn}$ be the block Toeplitz matrix defined by $A_0, A_1, \ldots, A_N \in \mathbb{C}^{n\times n}$. Then,

$$\|L_m\| \leq \sum_{\ell=0}^{N} \|A_\ell\|$$

and

$$\mathcal{F}(L_m) \subset \{z \in \mathbb{C} \,:\, d(\mathcal{F}(A_0), z) \leq \sum_{\ell=1}^{N} \|A_\ell\|\}.$$

Thus

$$\mu(L_m) \leq \mu(A_0) + \sum_{\ell=1}^{N} \|A_\ell\|,$$

where $\mu(A_0)$ denotes the logarithmic 2-norm of A_0.

Matvecs for the Arnoldi iteration

When running the Arnoldi iteration on $\mathcal{K}_k(L_m, \widetilde{u}_0)$, we use the following:

Suppose $x = \mathrm{vec}(x_1, \ldots, x_j, 0, \ldots, 0) = \mathrm{vec}(X) \in \mathbb{C}^{nm}$, where $x_1, \ldots, x_j \in \mathbb{C}^n$ and $m > j + N$. Then,

$$L_m x = \mathrm{vec}(y_1, \ldots, y_{j+N}, 0, \ldots, 0),$$

where

$$y_\ell = \sum_{i=\max(0,\ell-k)}^{\min(N,\ell-1)} A_i x_{\ell-i}, \quad \ell = 1, \ldots, j+N.$$

Infinite Arnoldi algorithm

The Arnoldi approximation of $\exp(tL_m)\widetilde{u}_0$ can be formulated as an *infinite Arnoldi algorithm*, see

E. Jarlebring, W. Michiels, and K. Meerbergen. *A linear eigenvalue algorithm for the nonlinear eigenvalue problem.* Numerische Mathematik 122.1 (2012): 169-195.

The following procedures generate identical results.

(i) p iterations of the Arnoldi iteration started with u_0 and $A_0, \ldots, A_N$;

(ii) p iterations of Arnoldi's method applied to L_m with starting vector $e_1 \otimes u_0 \in \mathbb{C}^{nm}$ for any $m \geq Np$;

(iii) p iterations of Arnoldi's method applied to the infinite matrix L_∞ with the infinite starting vector $e_1 \otimes u_0 \in \mathbb{C}^\infty$.

Integral representation of the coefficients

In order to derive error bounds, we need integral formulas for the coefficients $c_\ell(t)$. The case $N = 1$ is given in

I.Najfeld and T.F. Havel. *Derivatives of the matrix exponential and their computation.* Advances in Applied Mathematics 16.3 (1995): 321-375.

From the main theorem we see that

$$c_j'(t) = \sum_{i=0}^{\min(N,j)} A_i c_{j-i}(t).$$

Using the variation-of-constants formula

$$u(t) = \mathrm{e}^{tA_0} u_0 + \int_0^t \mathrm{e}^{(t-\tau)A} g(u(\tau))\,\mathrm{d}\tau,$$

which gives the the exact solution at time t for the semilinear ODE

$$u'(t) = A_0 u(t) + g(u(t)), \quad u(0) = u_0,$$

we get an integral formula for the coefficients $c_\ell(t)$.

Integral representation of the coefficients

Let ℓ and N be positive integers such that $N \leq \ell$. Denote by C_ℓ the set of compositions of ℓ, i.e.,

$$C_\ell = \{(i_1, \ldots, i_r) \in \mathbb{N}_+^r \,:\, i_1 + \cdots + i_r = \ell\},$$

and further denote

$$C_{\ell,N} := \{(i_1, \ldots, i_r) \in C_\ell \,:\, i_s \leq N \ \text{ for all } \ 1 \leq s \leq r\}.$$

Then,

$$c_0(t) = \mathrm{e}^{tA_0} u_0,$$

$$c_\ell(t) = \sum_{(i_1,\ldots,i_r)\in C_{\ell,N}} \int_0^t \mathrm{e}^{(t-t_{i_1})A_0} A_{i_1} \int_0^{t_{i_1}} \mathrm{e}^{(t_{i_1}-t_{i_2})A_0} A_{i_2}$$

$$\ldots \int_0^{t_{i_{r-1}}} \mathrm{e}^{(t_{i_{r-1}}-t_{i_r})A_0} A_{i_r} c_0(t_{i_r})\, \mathrm{d}t_{i_1} \ldots \mathrm{d}t_{i_r} \quad \text{for} \quad \ell > 0.$$

Bound for the coefficients

Using the above integral formulas
we obtain bounds for the norms of $c_\ell(t)$.

For example when $N = 1$, we have

$$\|c_\ell(t)\| = \| \int_0^t \mathrm{e}^{(t-t_{i_1})A_0} A_1 \dots \int_0^{t_{i_{\ell-1}}} \mathrm{e}^{(t_{i_{\ell-1}}-t_{i_\ell})A_0} A_1 \mathrm{e}^{t_{i_\ell}\mu(A_0)} u_0 \,\mathrm{d}t_{i_1} \dots \mathrm{d}t_{i_\ell} \| \leq \mathrm{e}^{t\mu(A_0)} \frac{(t\|A_1\|)^\ell}{\ell!} \|u_0\|,$$

where $\mu(A_0)$ denotes the logarithmic 2-norm of A_0.

Notice: $\|\mathrm{e}^{tA_0}\| \leq \mathrm{e}^{t\mu(A_0)}$ for every $t > 0$.

A priori error bound

After p steps, the error

$$\begin{aligned}\mathrm{err}_p(t,\varepsilon) :=& \|u(t,\varepsilon)-\widetilde{u}_p(t,\varepsilon)\| \\ \leq& \|u(t,\varepsilon)-u_p(t,\varepsilon)\| + \|u_p(t,\varepsilon)-\widetilde{u}_p(t,\varepsilon)\|\end{aligned}$$

is bounded as (assuming $\|A_\ell\| \leq a$ for all ℓ)

$$\mathrm{err}_p(t,\varepsilon) \leq \mathrm{e}^{t\mu(A_0)}\|u_0\|\Bigg(C_1(t,\varepsilon)\sum_{\ell=0}^{N-1}\frac{C_2(t,\varepsilon)^{p+\ell-1}\mathrm{e}^{C_2(t,\varepsilon)}}{(p+\ell-2)!} + 2\sqrt{\frac{1-|\varepsilon|^{2N(p-1)}}{1-|\varepsilon|^2}}\frac{(t\alpha)^p}{p!}\Bigg),$$

where

$$C_1(t,\varepsilon) = |\varepsilon|^{\mathrm{sign}(|\varepsilon|-1)}\,\mathrm{e}^{t\mathrm{e}Na+C_2(t,\varepsilon)-1},$$

$$C_2(t,\varepsilon) = |\varepsilon|^N\,\mathrm{e}\,Nta,$$

and

$$\alpha = \sum_{\ell=0}^{N}\|A_\ell\| \qquad \text{and} \qquad \gamma = \sum_{\ell=1}^{N}\|A_\ell\|,$$

and $\mu(A_0)$ denotes the logarithmic 2-norm of A_0.

A posteriori error estimate

A posteriori error estimates obtained using techniques given in

- Y.Saad. *Analysis of some Krylov subspace approximations to the matrix exponential operator.* SIAM J. Numer. Anal., 29 (1992), pp. 209–228.

For the Arnoldi approximation of $\mathrm{e}^{A}b$ it holds that

$$\mathrm{e}^{A}b - Q_p \exp(H_p)e_1 = h_{p+1,p}\sum_{\ell=1}^{\infty} e_p^T \varphi_\ell(H_p)e_1\, A^{\ell-1}q_{p+1}, \qquad (*)$$

where $h_{p+1,p}$ is the subdiagonal element of the Hessenberg matrix, and $\varphi_\ell(z) = \sum_{j=0}^{\infty} \frac{z^j}{(j+\ell)!}$.

To construct an a posteriori estimate

we take into account the first 2 terms in (*), and use the fact that

$$\begin{bmatrix} I_p & 0 \end{bmatrix} \exp\left(\begin{bmatrix} H_p & e_1 & e_1 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \right)$$
$$= \begin{bmatrix} \exp(H_p) & \varphi_1(H_p)e_1 + \varphi_2(H_p)e_1 & \varphi_1(H_p)e_1 \end{bmatrix}.$$

Scaling

Let $\gamma > 0$ and define $\Sigma_m := \mathrm{diag}(1, \gamma, \ldots, \gamma^{m-1}) \otimes I_n$. Then it holds

$$\widehat{c}(t) = \exp(tL_m)\,\widetilde{u}_0 = \Sigma_m \exp(t\Sigma_m^{-1} L_m \Sigma_m)\,\widetilde{u}_0$$
$$= \Sigma_m \exp(t\widehat{L}_m)\,\widetilde{u}_0,$$

Related scaling can be found in:
A.H. Al-Mohy and N.J. Higham, *Computing the action of the matrix exponential, with an application to exponential integrators*, SIAM J. Sci. Comput. 33 (2011).

Thus, we see that using this scaling strategy corresponds to the changes

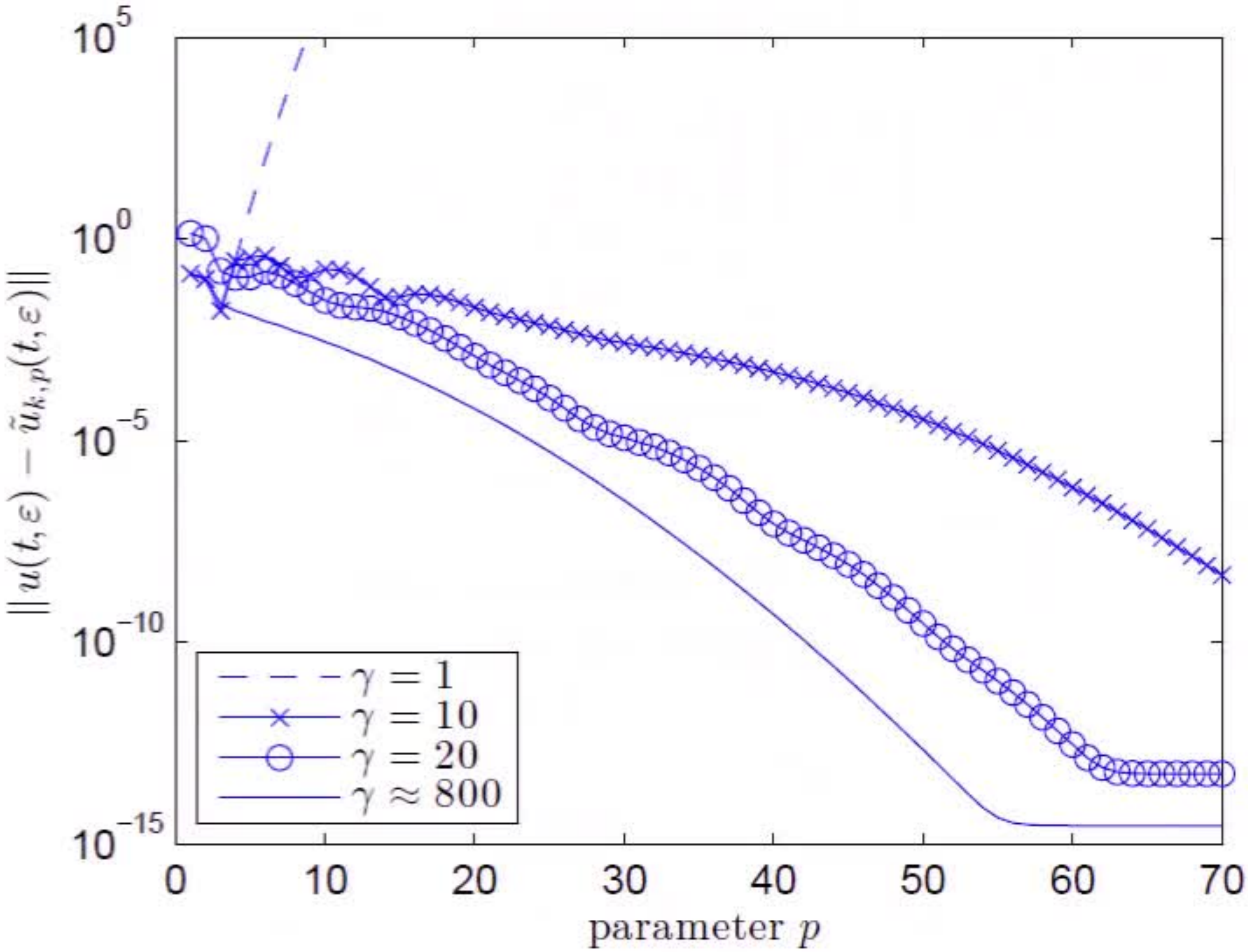
$$\epsilon \to \gamma\epsilon \quad \text{and} \quad A_\ell \to \gamma^{-\ell} A_\ell$$

when performing the Arnoldi approximation of the product $\exp(t\widehat{L}_m)\,\widetilde{u}_0$.

We scale the norms of coefficients A_ℓ, $1 \leq \ell \leq N$, such that they are of the order 1 or less. We use the heuristic choice

$$\gamma = \max_{1 \leq \ell \leq N} \|A_\ell\|^{1/\ell}.$$

Scaling



2-norm errors of approximations $\tilde{u}_p(t,\varepsilon)$ using different scalings. The last option corresponds to the heuristic choice.

Numerical example

Consider the damped wave equation inside the 3D unit box:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} u(t) \\ u'(t) \end{bmatrix} = \begin{bmatrix} 0 & I \\ -M^{-1}K & -M^{-1}C(\gamma) \end{bmatrix}\begin{bmatrix} u(t) \\ u'(t) \end{bmatrix}, \quad \begin{bmatrix} u(0) \\ u'(0) \end{bmatrix} = \begin{bmatrix} u_0 \\ u_0' \end{bmatrix} \in \mathbb{R}^{2n}$$

where $C(\gamma_1, \gamma_2) = \gamma_1 C_1 + \gamma_2 C_2$.

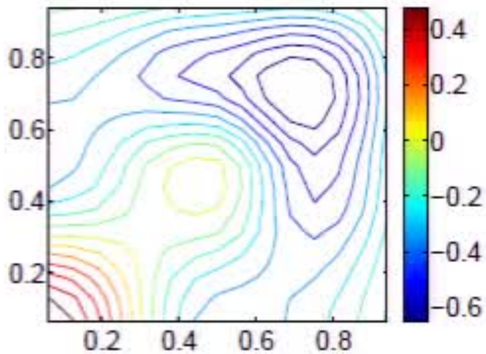
ODE obtained by finite differences with 15 discretization points in each dimension, i.e., $n = 15^3$.

K denotes the discretized Laplacian,
$C(\gamma_1, \gamma_2)$ the damping matrix stemming from boundary conditions, and M the mass matrix.

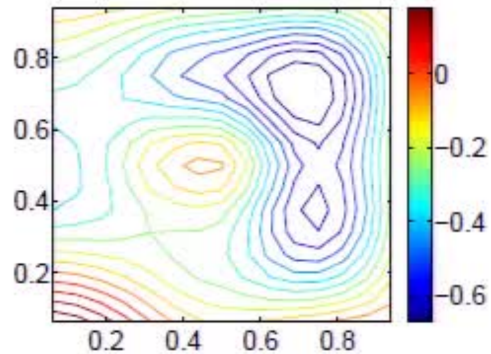
Reformulate the ODE by setting

$$A_0 = \begin{bmatrix} 0 & I \\ -M^{-1}K & -M^{-1}\gamma_1 C_1 \end{bmatrix}, \quad A_1 = \begin{bmatrix} 0 & 0 \\ 0 & -M^{-1}C_2 \end{bmatrix}.$$

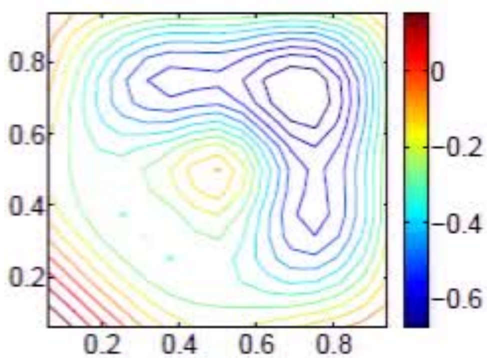
Linear example 2



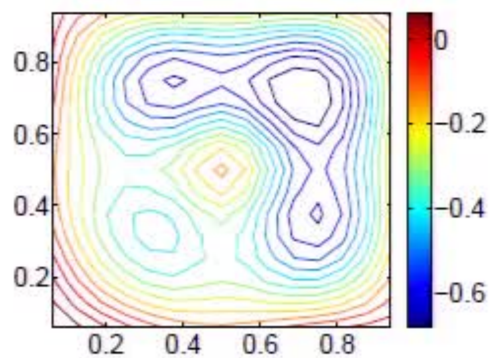
(a) $\gamma_1 = \gamma_2 = 0$



(b) $\gamma_1 = 2,\ \gamma_2 = 0$



(c) $\gamma_1 = 1,\ \gamma_2 = 1$



(d) $\gamma_1 = 2,\ \gamma_2 = 2$

Figure : The solution in the plane $z = 0.5$, for different values of (γ_1, γ_2) at $t = 1$.

Numerical example

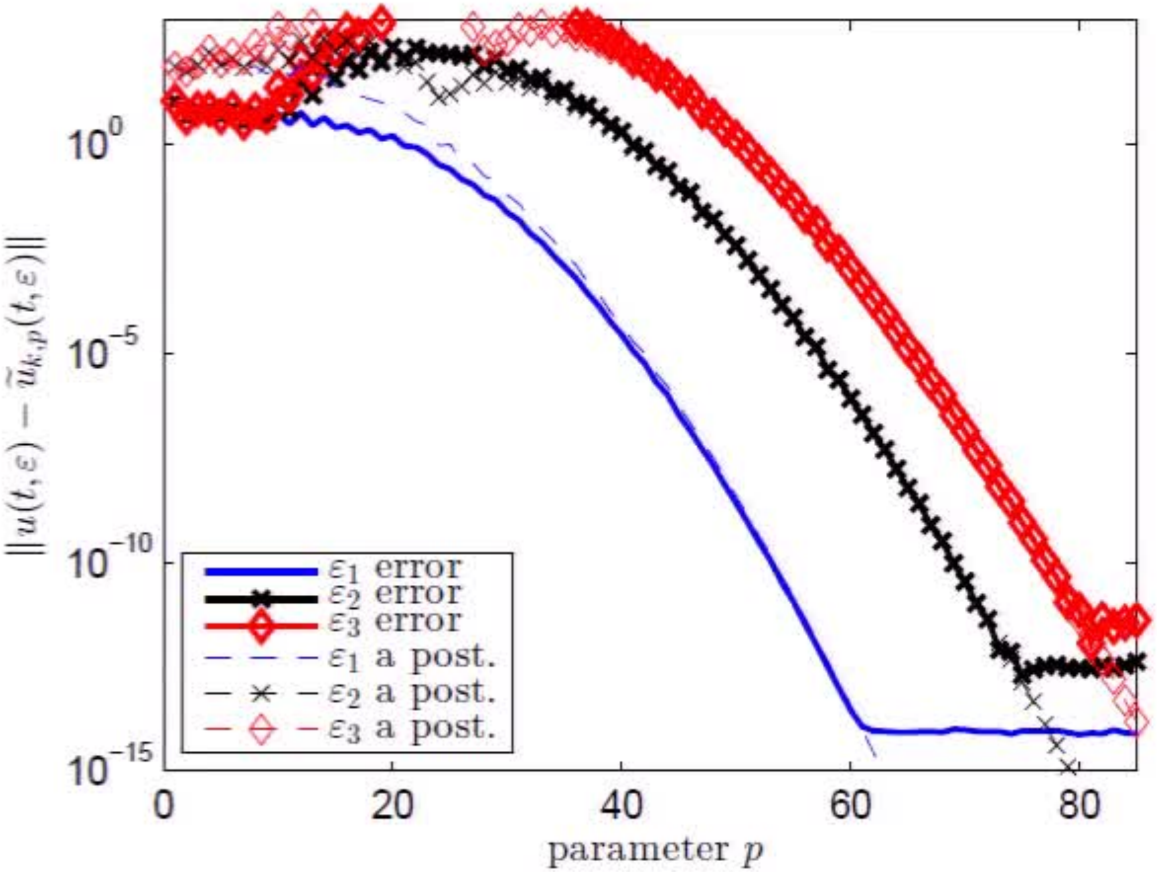


Figure : 2-norm errors of approximations $\widetilde{u}_p(t,\varepsilon)$ and the error estimates, when $\gamma_1 = 2$ and γ_2 has the values $\varepsilon_1 = 1$, $\varepsilon_2 = 1.5$ and $\varepsilon_3 = 2$.