

Optimality and resonances in a class of compact finite difference schemes of high order

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Motivation : Understand construction and qualitative properties of compact *finite difference* schemes of high order for *elliptic problems* .

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Motivation : Understand construction and qualitative properties of compact *finite difference* schemes of high order for *elliptic problems* .

Problem : It is too general ! So we focus on an elementary problem: *homogeneous Dirichlet problem in dimension 1*.

For a given $f : \mathbb{R} \rightarrow \mathbb{C}$, find $u : [0, 1] \rightarrow \mathbb{C}$ such that

$$\begin{cases} -u''(x) = f(x), \quad \forall x \in]0, 1[, \\ u(0) = u(1) = 0. \end{cases}$$

Compact finite difference scheme ?

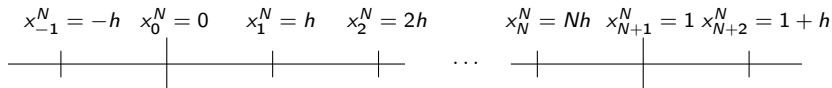


Figure: Regular grid with N points into $]0, 1[$.

A compact finite difference scheme is a linear system

$$\mathbf{D}_N \mathbf{u}^N = h^2 \mathbf{S}_N \mathbf{f}^{N,ex}$$

where

- $\mathbf{f}^{N,ex} = (f(x_j^N))_{j \in \mathbb{Z}}$,
- $\mathbf{u}^N \simeq (u(x_j^N))_{j=1 \dots N}$ is an approximation of the solution of the Dirichlet problem,
- \mathbf{D}_N and \mathbf{S}_N are matrices.

Examples:

$$\mathbf{D}_N = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \in \mathcal{L}(\mathbb{C}^N).$$

and (small abuse of notations)

$$\mathbf{S}_N = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & & 1 & \\ & & & & 1 \end{pmatrix} \in \mathcal{L}(\mathbb{C}^N).$$

Expectations: convergence of u^N

$$\lim_{N \rightarrow \infty} \sup_{j=1, \dots, N} |u_j^N - u(x_j^N)| = 0.$$

In general, we expect there exists $n \in \mathbb{N}^*$, the *order of the scheme*, and $C > 0$ such that

$$|u_j^N - u(x_j^N)| \leq Ch^n, \quad \forall N, \forall j.$$

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Questions:

- In general, are these schemes convergent ?
- Are some of them more efficient than others ?

1 Consistency + Stability \Rightarrow Convergence

2 Construction of the schemes

3 Optimality

4 Resonances

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Consistency: (order n) $\forall f \in C^\infty(\mathbb{R}), \exists c > 0, \forall N \in \mathbb{N}^*$,

$$\|\mathbf{D}_N \mathbf{u}^{N,\text{ex}} - h^2 \mathbf{S}_N \mathbf{f}^{N,\text{ex}}\|_\infty \leq ch^{n+2}.$$

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Weak Consistency: (order n) $\exists l \in \mathbb{N}, \forall f \in C^\infty(\mathbb{R}), \exists c > 0, \forall N \in \mathbb{N}^*$,

$$\left| \left(\mathbf{D}_N \mathbf{u}^{N,ex} \right)_j - h^2 \left(\mathbf{S}_N \mathbf{f}^{N,ex} \right)_j \right| \leq \begin{cases} ch^{n+2} & \text{if } l < j < N + 1 - l, \\ ch^n & \text{else.} \end{cases}$$

A scheme $(\mathbf{D}_N, \mathbf{S}_N)_N$ (or a sequence of matrix $(\mathbf{D}_N)_N$) is

- stable, if there exists a positive constant $c > 0$ such that for all $N \in \mathbb{N}^*$, we have

$$\forall \mathbf{v} \in \mathbb{C}^N, c \|\mathbf{v}\|_\infty \leq h^{-2} \|\mathbf{D}_N \mathbf{v}\|_\infty.$$

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- strongly stable, if for all $l \in \mathbb{N}$, there exists a positive constant $c > 0$ such that for all $N \in \mathbb{N}^*$,

$$\forall \mathbf{v} \in \mathbb{C}^N, c \|\mathbf{v}\|_\infty \leq \sup_{j=1, \dots, N} \begin{cases} h^{-2} (\mathbf{D}_N \mathbf{v})_j & \text{if } l < j < N + 1 - l, \\ (\mathbf{D}_N \mathbf{v})_j & \text{else.} \end{cases} .$$

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- stable relatively to a sequence $(\eta_N)_{N \in \mathbb{N}^*}$ of positive numbers, if there exists a positive constant $c > 0$ such that for all $N \in \mathbb{N}^*$, we have

$$\forall \mathbf{v} \in \mathbb{C}^N, c \|\mathbf{v}\|_\infty \leq \eta_N \|\mathbf{D}_N \mathbf{v}\|_\infty.$$

Theorem: Lax

- A scheme that is strongly stable and weakly consistent of order n is convergent of order n .
- If $\eta_N h^{n+2} \rightarrow_{N \rightarrow \infty} 0$ then a scheme that is stable relative to the sequence $(\eta_N)_{N \in \mathbb{N}^*}$ and consistent of order n is convergent at the rate $\epsilon_N = \eta_N h^{n+2}$.

Proof.

$$\mathbf{D}_N \mathbf{v} = \mathbf{D}_N \left(\mathbf{u}^{N,ex} - \mathbf{u}^N \right) = \mathbf{D}_N \mathbf{u}^{N,ex} - h^2 \mathbf{S}_N \mathbf{f}^{N,ex}.$$



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A couple of *finite difference formulas* $(d, s) \in (\mathbb{C}^{\mathbb{Z}})^2$ is consistent of order n , if

$$\forall u \in C^\infty(\mathbb{R}), \sum_{j \in \mathbb{Z}} d_j u(x_j^N) + h^2 s_j u''(x_j^N) = \mathcal{O}(h^{n+2}).$$

Example: $d = 2\mathbb{1}_{\{0\}} - \mathbb{1}_{\{-1,1\}} = "(-1, 2, -1)"$ and $s = \mathbb{1}_{\{0\}} = "(1)"$.

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Remark : We only consider *symmetric* finite difference formulas

$$\forall j \in \mathbb{Z}, d_j = d_{-j} \text{ and } s_j = s_{-j}.$$

Choosing $u \equiv 1$ we get

$$\sum_{j \in \mathbb{Z}} d_j = 0.$$

It is easy to get such couples. For example, choose any $d \in \mathbb{C}(\mathbb{Z})$ symmetric and satisfying

$$\sum_{j \in \mathbb{Z}} d_j = 0$$

then we can get $s \in \mathbb{C}(\mathbb{Z})$ such that (d, s) is consistent of order n solving the linear system

$$\left(\frac{s_0}{2}, s_1, \dots, s_{\frac{n}{2}-1}\right) \left((i-1)^{2j-2} \right)_{1 \leq i, j \leq \frac{n}{2}} = - \sum_{j>0} d_j \left(\frac{j^2}{2}, \dots, \frac{j^n}{n(n-1)} \right).$$

To design matrices \mathbf{D}_N and \mathbf{S}_N from the formulas d and s , a natural choice would be the following:

$$(\mathbf{D}_N \mathbf{u})_i = \sum_{j \in \mathbb{Z}} d_{i-j} \mathbf{u}_j \text{ and } (\mathbf{S}_N \mathbf{f})_i = \sum_{j \in \mathbb{Z}} s_{i-j} \mathbf{f}_j.$$

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Problem: it does not make sense on the boundary !

If we define *the size of the stencil* of d as

$$\tau(d) = \max\{j \in \mathbb{Z} \mid d_j \neq 0\},$$

then the previous formula involves terms like $\mathbf{u}_{1-\tau(d)}$.

Solution: To introduce formulas (d^i, s^i) consistent of order n (or $n - 2$) at a distance i of the boundary.

$$(\mathbf{D}_N \mathbf{u})_i := \begin{cases} \sum_{j>0} d_{j-i}^i \mathbf{u}_j & \text{if } 1 \leq i \leq \tau(d), \\ \sum_{j \in \mathbb{Z}} d_{j-i} \mathbf{u}_j & \text{if } \tau(d) < i < N + 1 - \tau(d), \\ \sum_{j < N+1} d_{-j+i}^{N+1-i} \mathbf{u}_j & \text{if } N + 1 - \tau(d) \leq i \leq N + 1. \end{cases}$$

$$(\mathbf{S}_N \mathbf{f})_i := \begin{cases} \sum_{j \in \mathbb{Z}} s_{j-i}^i \mathbf{f}_j & \text{if } 1 \leq i \leq \tau(d), \\ \sum_{j \in \mathbb{Z}} s_{j-i} \mathbf{f}_j & \text{if } \tau(d) < i < N + 1 - \tau(d), \\ \sum_{j \in \mathbb{Z}} s_{-j+i}^{N+1-i} \mathbf{f}_j & \text{if } N + 1 - \tau(d) \leq i \leq N + 1. \end{cases}$$

(d^i, s^i) is consistent of order $\mu \in \{n, n-2\}$ at a distance i of the boundary if

$$\forall u \in C^\infty(\mathbb{R}), u(0) = 0 \Rightarrow \sum_{j>-i} d_j^i u(x_{j+i}^N) + h^2 \sum_{j \in \mathbb{Z}} s_j^i u''(x_{j+i}^N) = \mathcal{O}(h^{\mu+2}), \quad (1)$$

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$$\forall u \in C^\infty(\mathbb{R}), u(0) = 0 \Rightarrow \sum_{j > -i} d_j^i u(x_{j+i}^N) + h^2 \sum_{j \in \mathbb{Z}} s_j^i u''(x_{j+i}^N) = \mathcal{O}(h^{\mu+2}), \quad (1)$$

Lemma

This scheme is consistent of order n (weakly if (d^i, s^i) consistent of order $n-2$).

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Question : How to choose (d^i, s^i) ?

This choice is *crucial* to hope stability. For example, we could choose $d^i = s^i = 0$ but the scheme would not be stable !

There are methods based on *monotonicity* (i.e. $(\mathbf{D}_N^{-1})_{i,j} \geq 0$) but these methods are not very general and it is not clear if arbitrarily high order schemes may be designed.

Our choice: We keep the relation

$$(\mathbf{D}_N \mathbf{u})_i = \sum_{j \in \mathbb{Z}} d_{i-j} \mathbf{u}_j, \quad \forall j = 1, \dots, N,$$

extending \mathbf{u} as an odd sequence in 0 and $N + 1$.

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$$d_j^i = d_j - d_{2i+j}, \quad i = 1, \dots, \tau(d), \quad j \in \mathbb{Z}$$

Lemma

There exists \mathbf{s}^i such that (d^i, \mathbf{s}^i) is consistent of order $\mu \in \{n, n - 2\}$ at a distance i of the boundary.

Sketch of proof: Let $u \in C^\infty(\mathbb{R})$ such that $u(0) = 0$

$$\begin{aligned} \sum_{j>-i} d_j^i u(x_{i+j}^N) &= \sum_{j \in \mathbb{Z}} d_j u(x_{j+i}^N) - \sum_{j<-i} d_j u(x_{j+i}^N) - \sum_{j>-i} d_{j+2i} u(x_{j+i}^N) \\ &= -h^2 \sum_{j \in \mathbb{Z}} s_j u''(x_{j+i}^N) - \sum_{j>0} d_{i+j} \left(u(x_j^N) + u(x_{-j}^N) \right) + \mathcal{O}(h^{n+2}). \end{aligned}$$

However, we have

$$u(x_j^N) + u(x_{-j}^N) = u(x_j^N) + u(x_{-j}^N) - 2u(0) = -h^2 \sum_{l \in \mathbb{Z}} b_l^j u''(x_l^N) + \mathcal{O}(h^{\mu+2}),$$

where b^j is obtained solving the linear system

$$\left(\frac{b_0^j}{2}, s_1, \dots, b_{\frac{\mu}{2}-1}^j \right) \left((i-1)^{2j-2} \right)_{1 \leq i, j \leq \frac{\mu}{2}} = - \left(\frac{j^2}{2}, \dots, \frac{j^\mu}{\mu(\mu-1)} \right).$$

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However, if $\mathbf{a} = 2\mathbb{1}_{\{0\}} - \mathbb{1}_{\{-1,1\}} = "(-1, 2, -1)"$ then

$$\begin{array}{l} \mathbb{C}[X] \rightarrow \mathcal{S}_{\mathbb{C}} \\ P \mapsto P(\mathbf{a}) \end{array} \text{ is an isomorphism of algebra.}$$

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However, if $a = 2\mathbb{1}_{\{0\}} - \mathbb{1}_{\{-1,1\}} = "(-1, 2, -1)"$ then

$$\begin{aligned}\mathbb{C}[X] &\rightarrow \mathcal{S}_{\mathbb{C}} \\ P &\mapsto P(a)\end{aligned} \text{ is an isomorphism of algebra.}$$

Conclusion: if $d = P(a)$ then

$$\mathbf{D}_N(d) = \mathbf{D}_N(P(a)) = P(\mathbf{D}_N(a)) =: P(\mathbf{A}_N).$$

\mathbf{A}_N is the square matrix defined by

$$\mathbf{A}_N = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \in \mathcal{L}(\mathbb{C}^N).$$

It is a well known matrix whose spectral decomposition is given by

$$\mathbf{A}_N \mathbf{e}_k^N = 4 \sin^2 \left(\frac{\pi}{2} kh \right) \mathbf{e}_k^N, \quad \text{with } \mathbf{e}_k^N := (\sin(\pi khj))_{j=1, \dots, N}.$$

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Conclusion: To get convergence, we just have to study stability of matrices of the type $P(\mathbf{A}_N)$!

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We can look for symmetric formulas d, s as polynomial of a

$$d = P(a) \text{ and } s = Q(a).$$

Considering formulas of consistency order larger than or equal 2, necessarily we have $P(0) = 0$. Consequently, it can be factorized

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Lemma

(d, s) is consistent of order $n = 2k$ if and only if

$$R(X) = C(X)Q(X) \pmod{X^k}.$$

where

$$C(X) := 4 \left(\frac{\arcsin\left(\frac{\sqrt{X}}{2}\right)}{\sqrt{X}} \right)^2 = 2 \sum_{n \in \mathbb{N}} \frac{X^n}{(n+1)^2 C_{2n+2}^{n+1}}.$$

Looking for a solution of $R(X) = C(X)Q(X) \pmod{X^k}$ with $\deg R \leq l$ and $\deg Q \leq m$ we get a linear system with

- k equations,
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So, if $l + m + 1 \geq k$ there is at least one non trivial solution.

Lemma

For any fixed, l, m, k such that $l + m + 1 = k$, this solution is unique up to multiplication by a constant.

We denote it $R_{l,m}$ and $Q_{l,m}$ (choosing $R_{l,m}(0) = 1$).

Sketch of proof: It is a classical problem of *Padé approximant*.

Indeed, we are looking for a rational approximation $\frac{R}{Q}$ of C in $X = 0$.

Following classical theory, this result is a corollary of the fact that $C(-4X)$ is a Stieltjes transform of a positive function $\rho : (0, 1) \rightarrow \mathbb{R}$,

$$C(-4X) = \int_0^1 \frac{\rho(s)}{1 + sX} ds.$$

Theorem: D. Karp and E. Prilepkina (2012)

$$\text{If } \begin{cases} 1 \leq \alpha_1 \leq \dots \leq \alpha_q, \\ 0 < \beta_1 \leq \dots \leq \beta_q, \\ \forall k \in \llbracket 1, q \rrbracket, \sum_{j=1}^k \alpha_j \leq \sum_{j=1}^k \beta_j \end{cases}$$

then ${}_{q+1}F_q \left[\begin{matrix} 1, \alpha_1, \dots, \alpha_q \\ \beta_1, \dots, \beta_q \end{matrix}; -X \right]$ is a Stieltjes transform of a positive function $\rho : (0, 1) \rightarrow \mathbb{R}$.

$${}_pF_q \left[\begin{matrix} \alpha_1, \dots, \alpha_p \\ \beta_1, \dots, \beta_q \end{matrix}; X \right] := \sum_{k \in \mathbb{N}} \frac{(\alpha_1)_k \dots (\alpha_p)_k}{(\beta_1)_k \dots (\beta_q)_k} \frac{X^k}{k!} \text{ with } (\gamma)_k = \prod_{j=0}^{k-1} \gamma + j.$$

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$$C(X) = {}_3F_2 \left[\begin{matrix} 1, 1, 1 \\ \frac{3}{2}, 2 \end{matrix}; \frac{X}{4} \right].$$

Corollary: Zero points of $R_{l,m}$ are localised in $(4, \infty)$.

Theorem

Let $P \in \mathbb{C}[X]$ be a polynomial such that

$$P(0) = 0, \quad P'(0) \neq 0 \quad \text{and} \quad \forall x \in]0, 4], \quad P(x) \neq 0.$$

Then the sequence of matrices $(P(\mathbf{A}_N))_{N \in \mathbb{N}^*}$ is strongly stable.

Application: $P = XR_{l,m}$.

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Conclusion: If we want a scheme of order $n = 2k$ with $l = \tau(d) + 1$ and $m = \tau(m)$ as small as possible, we have to choose $l + m + 1 = k$. In this case there exists an unique normalized scheme given by $d = (XR_{l,m})(a)$ and $s = Q_{l,m}(a)$. Furthermore, this scheme is strongly stable and so convergent of order n .

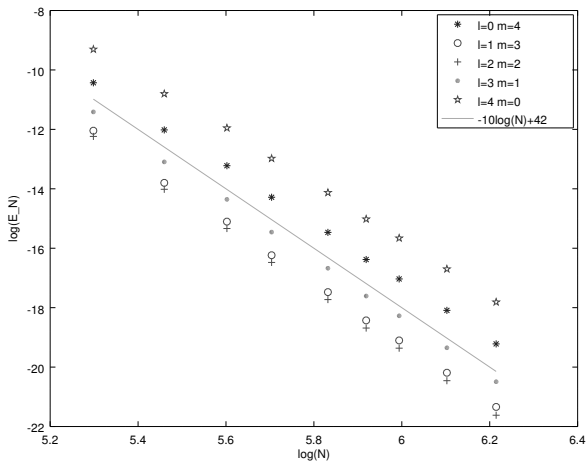


Figure: Convergence curves, with $u(x) = x(1-x)e^{4\cos(41x)}$ and $E_N := \|\mathbf{u}^N - \mathbf{u}^{N,ex}\|_\infty$, $N \in \{200, 235, 271, 300, 341, 372, 401, 447, 500\}$, for the optimal schemes, with $n = 10$, $\mu = 8$, $d = d^{l,m}$ and $s = s^{l,m}$.

Sketch of proof: This property is well known for \mathbf{A}_N , so we just have to prove that if R does not vanish on $[0, 4]$ then

$$\sup_{N \in \mathbb{N}^*} \|R(\mathbf{A}_N)^{-1}\|_{\infty} < \infty.$$

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Consequently, we have

$$R(\mathbf{A}_N)^{-1} = \sum_{n \in \mathbb{N}} a_n \mathbf{D}_N\left(\frac{\mathbb{1}_{\{-n, n\}}}{2}\right).$$

However, we have obviously $\|\mathbf{D}_N(\frac{\mathbb{1}_{\{-n, n\}}}{2})\|_\infty = 1$, so we get

$$\|R(\mathbf{A}_N)^{-1}\|_\infty \leq \|(a_n)\|_{\ell^1}.$$

1 Consistency + Stability \Rightarrow Convergence

2 Construction of the schemes

3 Optimality

4 Resonances

Consider a scheme where $\mathbf{D}_N(d) = P(\mathbf{A}_N)$. If we don't take care in the construction of d , P could vanish into $(0, 4)$.

However, we have

$$\text{Sp}_{\mathbb{C}} \mathbf{D}_N(d) = \left\{ P \left(4 \sin^2 \left(\frac{\pi kh}{2} \right) \right) \mid k = 1, \dots, N \right\}.$$

So $\mathbf{D}_N(d)$ could have very small eigenvalues. (stability \simeq control of $h^2 \|\mathbf{D}_N^{-1}\|$)

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Questions:

- In general, does P really have zero points into $(0, 4)$?
- Are small eigenvalues of $\mathbf{D}_N(d)$ large enough to allow stability ?

Theorem

For almost all symmetric \mathbb{C} valued formula d such that

$$\sum_{j \in \mathbb{Z}} d_j = 0,$$

P does not vanish in $]0, 4]$, $P(0) = 0$ and $P'(0) \neq 0$.

Corollary: Almost all complex valued scheme (consistent of order larger than or equal to 2) is strongly stable !

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Problem: In practice, we consider real valued formulas. And for any $l > 0$,

$$\text{Int}\{R \in \mathbb{R}_l[X] \mid \exists x_0 \in (0, 4), R(x_0) = 0\} \neq \emptyset.$$

It can not be a null set.

A numerical experiment:

- Fix $l \geq 1$ and $n \in 2\mathbb{N}^*$,
- Choose randomly a formula d of sum 0 such that $\tau(d) \leq l + 1$,
- Determine s to get a couple (d, s) consistent of order n ,
- Assemble the matrices $\mathbf{D}_N(d)$ and \mathbf{S}_N ,
- Choose a test function $u \in C^\infty(\mathbb{R})$ such that $u(0) = u(1) = 0$ and define $f = -u''$,
- Plot the convergence curves.

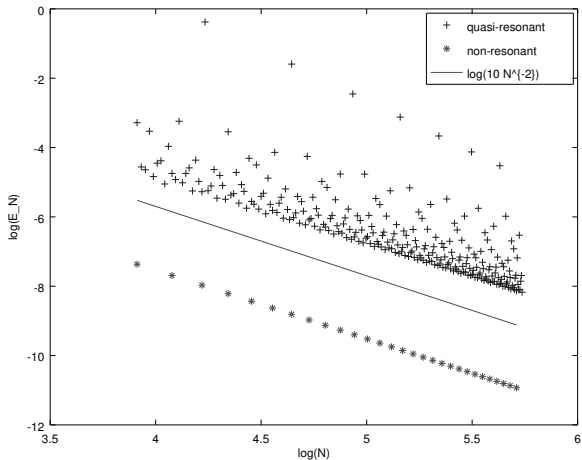


Figure: Convergence curves with $u(x) = x(1-x)e^{2x}$, $n = 2$ and $E_N := \|\mathbf{u}^N - \mathbf{u}^{N,ex}\|_\infty$. For the non-resonant scheme $d = 2\mathbb{1}_{\{0\}} - \mathbb{1}_{\{-1,1\}}$ and for the quasi-resonant scheme $d = (2 - 6z)\mathbb{1}_{\{0\}} + (4z - 1)\mathbb{1}_{\{-1,1\}} - z\mathbb{1}_{\{-2,2\}}$ with $z = 0.358946420670826$.

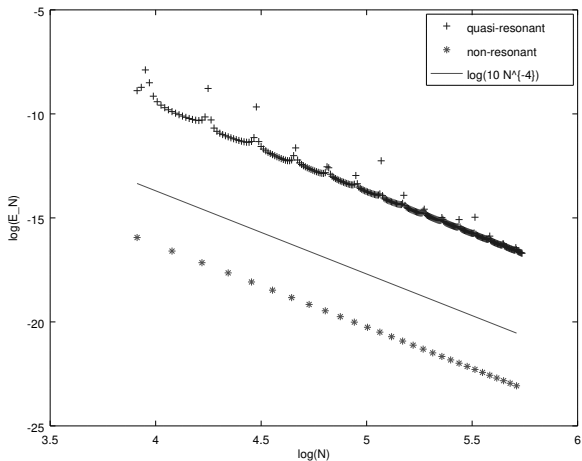


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Observations:

- Two kinds of behaviours.
- Resonant case $\iff P$ vanishes into $]0, 4]$
- In the resonant case the scheme seems convergent with the good rate.

Theorem

Let $P \in \mathbb{C}[X]$ be a polynomial and let Λ be the set of the roots of P in $[0, 4]$ and assume that P satisfies the following assumptions:

- i) $0 \in \Lambda$,
- ii) $4 \notin \Lambda$,
- iii) the roots of P in $[0, 4]$ are simple,
- iv) $\exists \delta : \mathbb{N}^* \rightarrow \mathbb{R}_+^*$,

$$\forall \lambda \in \Lambda, \forall q \in \mathbb{N}^*, \forall 1 \leq p \leq q-1, \quad 0 < \delta_q \leq \left| \lambda - 4 \sin^2 \left(\frac{\pi p}{2q} \right) \right|.$$

Then the sequence of finite difference matrices $(P(\mathbf{A}_N))_{N \in \mathbb{N}^*}$ is stable relatively to the sequence $\eta_N = \frac{1}{\delta_{N+1}}$

Remark: If $\delta_{N+1} = h^2$ then $P(\mathbf{A}_N)$ is stable.

Theorem Khinchin's

Let $(\nu_q)_q$ be a sequence of positive real numbers such that the series $\sum \nu_q$ converges. Then, for almost all $\alpha \in \mathbb{R}$, there exists a constant $c > 0$ such that for all $p, q \in \mathbb{Z} \times \mathbb{N}^*$, one has

$$\left| \alpha - \frac{p}{q} \right| \geq c \frac{\nu_q}{q}.$$

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"Corollary"

If $\delta_q = \frac{\nu_q}{q}$ and $q\nu_q$ is bounded then for all $l \geq 1$ and almost all $P \in X\mathbb{R}_l[X]$, if Λ is the set of the roots of P into $[0, 4]$ then there exists $C > 0$ s.t.

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In practice we can choose $\nu_q = \frac{1}{q \log^2 q}$.

Conclusion: Almost all real valued consistent scheme of order $n \geq 2$ is convergent at the rate $h^n \log^2(h)$.

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Thank you for your attention