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The error structure of the Douglas–Rachford splitting method for stiff linear problems

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Abstract

The Lie splitting algorithm is frequently used when splitting stiff ODEs or, more generally, dissipative evolution equations. It is unconditionally stable and is considered to be a robust choice of method in most settings. However, it possesses a rather unfavorable local error structure. This gives rise to order reductions if the evolution equation does not satisfy extra compatibility assumptions. To remedy the situation one can add correction-terms to the splitting scheme which, e.g., yields the first-order Douglas–Rachford (DR) scheme. In this paper we derive a rigorous error analysis in the setting of linear dissipative operators and inhomogeneous evolution equations. We also illustrate the order reduction of the Lie splitting, as well as the far superior performance of the DR splitting.

Keywords: Douglas–Rachford splitting, error analysis, order reduction, stiff linear problems, inhomogeneous evolution equations, dissipative operators.

1. Introduction

Consider the inhomogeneous evolution equation

$$u'(t) = (A + B)u(t) + g(t), \quad u(0) = u_0, \quad (1)$$

where A and B are linear dissipative operators, e.g., arising in reaction-diffusion models. Splitting schemes often constitute a competitive choice of temporal discretization if the actions of the flows governed by A and B , respectively, can

be more efficiently approximated than the flow of the full vector field $A + B$. One of the most commonly used splitting schemes is the Lie splitting

$$u_{n+1} = (I - hB)^{-1}(I - hA)^{-1}(u_n + hg(t_n)), \quad (2)$$

where u_n is an approximation of the solution u at time $t_n = nh$. This first-order scheme is often considered to be a robust choice of method in most settings.

It is well known that exponential splitting schemes may suffer from severe order reductions if the sequence of the operators A and B is chosen carelessly, as exemplified in the context of ODEs with vector fields consisting of a stiff and a non-stiff component [3, 8]. Order reductions also arise when utilizing high-order splitting schemes for discretizing linear parabolic equations with non-periodic boundary conditions [2]. However, even the Lie splitting requires a rather artificial structure of the evolution equation (1) in order to obtain first-order convergence. This can easily be seen via a Taylor expansion of the local error, when $g = 0$:

$$(I - hB)^{-1}(I - hA)^{-1} - e^{h(A+B)} = \frac{1}{2}h^2(A + B)^2 - h^2AB + \mathcal{O}(h^3).$$

As no cancelations can be expected in the general context, the term

$$\sup_{t \in (0, T)} \|ABu(t)\| \quad (3)$$

needs to be moderately bounded in order to achieve (global) first-order convergence. This is an artificial assumption as the evolution equation only relates the time regularity to the full operator $A + B$ and the inhomogeneity g , i.e., the equation offers no information regarding the solutions regularity in terms of (3) being moderately bounded. The above Taylor expansion is of course not valid for unbounded operators, but the same AB term also arises in a more careful error analysis, see the proof of Theorem 4 below.

So what can be done to circumvent this issue? One possibility is to correct for the AB term directly in the splitting scheme. This gives rise to the so-called Douglas–Rachford splitting (DR):

$$u_{n+1} = (I - hB)^{-1}(I - hA)^{-1}((I + h^2AB)u_n + hg(t_n)), \quad (4)$$

which was first introduced in [1]. This is again a first-order scheme, but the local error is now of the form

$$h^2(A + B)^2 + \mathcal{O}(h^3),$$

when $g = 0$. Hence, the artificial assumption regarding the boundedness of the term (3) is no longer required. Furthermore, the DR splitting can be implemented without computing the action of the operator AB , i.e., the computational cost becomes the same as for the Lie splitting. This can be achieved by the variable transformation $u_n = (I - hB)^{-1}v_n$ and rewriting (4) as

$$v_{n+1} = (I - hA)^{-1}((2(I - hB)^{-1} - I)v_n + hg(t_n)) + (I - (I - hB)^{-1})v_n.$$

Note that the DR splitting is closely related to the second-order Peaceman–Rachford splitting (PR), which can be interpreted as a (half) Lie step with the correction term

$$\frac{1}{2}h(A + B) + \frac{1}{4}h^2AB.$$

The DR splitting was proposed by Douglas and Rachford in the mid 1950s for the dimension splitting of the heat equation. Its convergence has also been proven by Lions and Mercier [4] for fully nonlinear dissipative operators. Even so, the DR splittings beneficial error structure and the Lie splittings order reduction has, as far as we know, not been properly analyzed in the literature. The aim of this paper is therefore to derive a rigorous error analysis for these schemes in the setting of linear dissipative operators.

2. Preliminaries

Consider the evolution equation

$$u'(t) = (A + B)u(t) + g(t), \quad u(0) = u_0, \quad (5)$$

where $t \in (0, T]$ and the unbounded operators $A : \mathcal{D}(A) \subseteq X \rightarrow X$ and $B : \mathcal{D}(B) \subseteq X \rightarrow X$ are given on an arbitrary Banach space X with the norm $\|\cdot\|$. The operator norm on X will also be denoted by $\|\cdot\|$. The sum $L = A + B : \mathcal{D}(L) \subseteq X \rightarrow X$ is given the standard domain

$$\mathcal{D}(L) = \mathcal{D}(A) \cap \mathcal{D}(B).$$

Assumption 1. *The operators A , B , and L are all densely defined and m -dissipative in X .*

We recapitulate that an operator L is dissipative if and only if

$$\|(I - hL)u\| \geq \|u\| \quad \text{for all } u \in \mathcal{D}(L) \text{ and } h > 0,$$

and it is m -dissipative if it satisfies in addition the range condition $\mathcal{R}(I - hL) = X$ for all $h > 0$. Hence, it readily follows that the resolvent $(I - hL)^{-1} : X \rightarrow X$ of an m -dissipative operator is nonexpansive on X . Another property of m -dissipative operators is that they generate C_0 semigroups of contractions $\{e^{tL}\}_{t \geq 0}$. A detailed survey of m -dissipative operators and their properties can be found in the monograph [7, Sections 1.4 and 3.3].

Assumption 2. *The solution and the inhomogeneity satisfy $u \in \mathcal{C}^2([0, T]; X)$ and $g \in \mathcal{C}^1([0, T]; X)$.*

With this assumption one also has that $u \in \mathcal{C}^1([0, T]; \mathcal{D}(L))$, which follows from the relation

$$u'(t) = (I - L)^{-1}(u'(t) - u''(t) + g'(t)).$$

For a sectorial operator L the regularity assumption $u \in \mathcal{C}^2([0, T]; X)$ is fulfilled if

$$u_0 \in \mathcal{D}(L), \quad Lu_0 + g(0) \in \mathcal{D}(L), \quad \text{and} \quad g \in \mathcal{C}^{1+\theta}([0, T]; X), \quad (6)$$

for some $\theta > 0$; for its proof we refer to [5]. Hence, in the sectorial case Assumption 2 can be stated in terms of the regularity for the known quantities u_0 and g .

By employing the variation-of-constants formula, the solution of the evolution equation (5) can be written as

$$u(t) = e^{tL}u_0 + \int_0^t e^{(t-\tau)L}g(\tau) \, d\tau,$$

and at time $t_{n+1} = t_n + h$, with a step size $h > 0$, we have the representation

$$u(t_{n+1}) = e^{hL}u(t_n) + \int_0^h e^{(h-s)L}g(t_n + s) \, ds.$$

A Taylor expansion of $g(t_n + s)$ at t_n then yields that

$$u(t_{n+1}) = e^{hL}u(t_n) + \int_0^h e^{(h-s)L} \left(g(t_n) + \int_{t_n}^{t_n+s} g'(\tau) \, d\tau \right) ds.$$

This expansion motivates the introduction of the operator $\lambda_j : X \rightarrow X$ defined as

$$\lambda_j = \frac{1}{h^j} \int_0^h e^{(h-s)L} \frac{s^{j-1}}{(j-1)!} \, ds, \quad j \geq 1,$$

and $\lambda_0 = e^{hL}$. The operators λ_j are related by the recurrence relations

$$\lambda_j = \frac{1}{j!} I + hL\lambda_{j+1}, \quad j \geq 0, \quad (7)$$

which follows by integration by parts. With this notation we get the following representation of the solution at time $t = t_{n+1}$:

$$u(t_{n+1}) = \lambda_0 u(t_n) + h\lambda_1 g(t_n) + R_{2,n}(h), \quad (8)$$

with the remainder

$$R_{2,n}(h) = \int_0^h e^{(h-s)L} \left(\int_{t_n}^{t_n+s} g'(\tau) \, d\tau \right) ds.$$

3. Convergence analysis

The convergence analysis for the Lie and DR splittings follow along the same lines, and we therefore start off with a new proof of the Lie splitting's first-order convergence. To this end, consider the operators

$$a = hA, \quad b = hB, \quad \ell = hL, \quad \alpha = (I - a)^{-1}, \quad \text{and} \quad \beta = (I - b)^{-1}.$$

By definition $a\alpha = \alpha a$ on $\mathcal{D}(A)$ and as the domain $\mathcal{D}(A)$ is assumed to be dense in X one can interpret the bounded operator $a\alpha : X \rightarrow X$ as the extension of $\alpha a : \mathcal{D}(A) \subseteq X \rightarrow X$ to all of X and in particular $\|\alpha a\| = \|a\alpha\|$. Hence, hereafter no distinction will be made between the operators $a\alpha$ and αa . The same holds for the operator pairs $(b\beta, \beta b)$ and $(\ell\lambda_j, \lambda_j\ell)$, for $j \geq 1$. We furthermore observe that the commutator relation below is valid on $\mathcal{D}(B)$:

$$\beta b\alpha = \beta\alpha b + \beta b a\alpha - \beta\alpha a b. \quad (9)$$

With this in place, we can derive a consistency result for the Lie splitting in the homogeneous case:

Lemma 3. *Under Assumption 1 the following equalities hold on $\mathcal{D}(L)$:*

$$\beta\alpha - \lambda_0 = h(\beta\alpha - \lambda_1)L - h^2\beta\alpha AB \quad \text{and} \quad \beta\alpha - \lambda_1 = h\beta(E_1 + E_2L),$$

where E_1 and E_2 are bounded linear operators on X .

Proof. The first assertion follows by the relations (7) and (9) together with the equality

$$\begin{aligned} \beta\alpha - \lambda_0 &= \beta\alpha - I - \lambda_1\ell \\ &= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha) - \lambda_1\ell \\ &= \beta\alpha a + \beta b\alpha - \beta b a\alpha - \lambda_1\ell \\ &= \beta\alpha a + (\beta\alpha b + \beta b a\alpha - \beta\alpha a b) - \beta b a\alpha - \lambda_1\ell \\ &= \beta\alpha\ell - \lambda_1\ell - \beta\alpha a b \\ &= h(\beta\alpha - \lambda_1)L - h^2\beta\alpha AB. \end{aligned}$$

The second assertion is also a consequence of (7):

$$\begin{aligned} \beta\alpha - \lambda_1 &= \beta(\alpha - (I - b)\lambda_1) \\ &= \beta((I + a\alpha) - \lambda_1 + b\lambda_1) \\ &= h\beta(-\lambda_2L + \alpha A + B\lambda_1) \\ &= h\beta(E_1 + E_2L), \end{aligned}$$

where the last equality follows by the observation that $A(I-L)^{-1}$ and $B(I-L)^{-1}$ are both bounded operators on X , as the operators A and B are closed. \square

In this short notation the Lie splitting applied to (5) reads

$$u_{n+1} = \beta\alpha(u_n + hg(t_n)). \quad (10)$$

Its convergence is now a mere matter of writing out the error recursion.

Theorem 4. *If Assumptions 1 and 2 hold and the exact solution of (5) is an element of $\mathcal{C}([0, T]; \mathcal{D}(AB))$, then the Lie splitting (10) is first-order convergent, i.e., the global error satisfies the bound*

$$\|u_n - u(t_n)\| \leq Ch, \quad 0 \leq t_n \leq T,$$

with a constant C that can be chosen uniformly on $[0, T]$, independently of n and h .

Proof. Subtracting the exact solution (8) from the numerical scheme (10) and employing Lemma 3 yields the following expansion of the global error $e_{n+1} = u_{n+1} - u(t_{n+1})$:

$$\begin{aligned} e_{n+1} &= \beta\alpha e_n + (\beta\alpha - \lambda_0)u(t_n) + h(\beta\alpha - \lambda_1)g(t_n) - R_{2,n}(h) \\ &= \beta\alpha e_n + h(\beta\alpha - \lambda_1)(Lu(t_n) + g(t_n)) - h^2\beta\alpha ABu(t_n) - R_{2,n}(h) \\ &= \beta\alpha e_n + h^2\beta(E_1 + E_2L)u'(t_n) - h^2\beta\alpha ABu(t_n) - R_{2,n}(h). \end{aligned}$$

We next solve the above error recursion and obtain that

$$e_n = \sum_{k=0}^{n-1} (\beta\alpha)^{n-1-k} \left(h^2\beta((E_1 + E_2L)u'(t_k) - \alpha ABu(t_k)) - R_{2,k}(h) \right). \quad (11)$$

The first-order convergence is now obtained as Assumption 1 implies stability, i.e., $\|(\beta\alpha)^k\| \leq 1$, the term $ABu(t)$ is bounded as the exact solution is assumed to be in $\mathcal{C}([0, T]; \mathcal{D}(AB))$, and Assumption 2 yields that $\|R_{2,k}(h)\| \leq Ch^2$, where the constant C is uniform with respect to k . \square

Remark. The somehow artificial condition $u \in \mathcal{C}([0, T]; \mathcal{D}(AB))$ can be played back to the data. The identity $ABu(t_n) = ABL^{-2}Lu'(t_n) - ABL^{-1}g(t_n)$ motivates us to consider the following conditions:

$$\mathcal{D}(L^2) \subseteq \mathcal{D}(AB), \quad g \in \mathcal{C}([0, T]; \mathcal{D}(ABL^{-1})). \quad (12)$$

The proof of Theorem 4 shows that the Lie splitting is again first-order convergent if Assumption 1 and the conditions (6) and (12) hold. We note, however, that (12) imposes unnatural boundary conditions on g , in general.

For the DR splitting, which in the above notation becomes

$$u_{n+1} = \beta\alpha((I + ab)u_n + hg(t_n)), \quad (13)$$

we may conduct the same line of reasoning without the presence of the term $ABu(t)$ in the error expansion, to the price of a slight restriction on the operators A and B .

Theorem 5. *If Assumptions 1 and 2 hold and the two operators $(I + a)\alpha$ and $(I + b)\beta$ are nonexpansive, then the Douglas–Rachford splitting (13) is first-order convergent.*

Proof. For the DR splitting, we obtain an error recursion of the form

$$\begin{aligned} e_{n+1} &= \beta\alpha(I + ab)e_n + (\beta\alpha(I + ab) - \lambda_0)u(t_n) + h(\beta\alpha - \lambda_1)g(t_n) - R_{2,n}(h) \\ &= \beta\alpha(I + ab)e_n + h(\beta\alpha - \lambda_1)(Lu(t_n) + g(t_n)) - R_{2,n}(h) \\ &= \beta\alpha(I + ab)e_n + h^2\beta(E_1 + E_2L)u'(t_n) - \beta(I - hB)R_{2,n}(h), \end{aligned}$$

which yields the global error representation

$$e_n = \sum_{k=0}^{n-1} (\beta\alpha(I + ab))^{n-1-k} \beta(h^2(E_1 + E_2L)u'(t_k) - R_{2,k}(h) + hBR_{2,k}(h)).$$

The stability now follows as the operator

$$(\beta\alpha(I + ab))^k \beta = \beta(\alpha(I + ab)\beta)^k = \beta\left(\frac{1}{2}\alpha(I + a)(I + b)\beta + \frac{1}{2}I\right)^k$$

is itself nonexpansive whenever the operators $(I + a)\alpha$ and $(I + b)\beta$ are nonexpansive. What remains to prove is that the new remainder term $hBR_{2,k}(h)$ is again bounded by Ch^2 . This holds as

$$\begin{aligned} \|LR_{2,k}(h)\| &= \left\| \int_0^h Le^{(h-s)L} \int_{t_k}^{t_k+s} g'(\tau) d\tau ds \right\| \\ &= \left\| g(t_k) - g(t_k + h) + \int_0^h e^{(h-s)L} g'(t_k + s) ds \right\| \leq Ch \end{aligned}$$

and by once more noting that $B(I - L)^{-1}$ is a bounded operator. \square

Remark. The assumption that $(I + a)\alpha$ is nonexpansive for an m -dissipative operator a is always valid if X is a Hilbert space, as

$$\begin{aligned} \|(I + a)v\|^2 &= \|v\|^2 + 2\operatorname{Re}(av, v) + \|av\|^2 \\ &\leq \|v\|^2 - 2\operatorname{Re}(av, v) + \|av\|^2 = \|(I - a)v\|^2, \end{aligned}$$

where (\cdot, \cdot) denotes the inner product on X . However, this is not in general true for an m -dissipative operator on an arbitrary Banach space X . Furthermore, the PR splitting, which is of classical order two, is first-order convergent under the hypotheses of Theorem 5. It is also of order two under additional assumptions derived in [6, Section 4].

4. Numerical experiments

We will next illustrate the order reduction of the Lie splitting, as well as the far superior performance of the DR/PR splittings. To this end, we consider the dissipative case where A is the Laplace operator equipped with Dirichlet boundary conditions on the interval $\Omega = (0, 1)$ and B is the operator given by multiplication with a fixed negative function $q : \Omega \rightarrow \mathbb{R}^-$. The operators A and B are m -dissipative if we set $X = L^2(\Omega)$, $q \in X$, $\mathcal{D}(A) = H^2(\Omega) \cap H_0^1(\Omega)$ and $\mathcal{D}(B) = \{u \in X : Bu \in X\}$, respectively. As the function q may have singularities of the form $|x - \alpha|^{-(1-\varepsilon)/2}$, $0 \leq \alpha \leq 1$, any continuous solution $u(t)$ which does not vanish at the singularities of q will give rise to a term $Bu(t)$ in $X \setminus \mathcal{C}(\overline{\Omega})$, i.e., $Bu(t)$ is not an element of $\mathcal{D}(A) \subset \mathcal{C}(\overline{\Omega})$ and $ABu(t)$ is therefore not well defined in X . With these considerations in mind, we choose

$$q(x) = -750 \sum_{j=1}^{30} |x - \alpha_j|^{-(1-\varepsilon)/2},$$

where the points α_j are equally spaced between π^{-2} and $1 - \pi^{-2}$ and $\varepsilon = 1/20$.

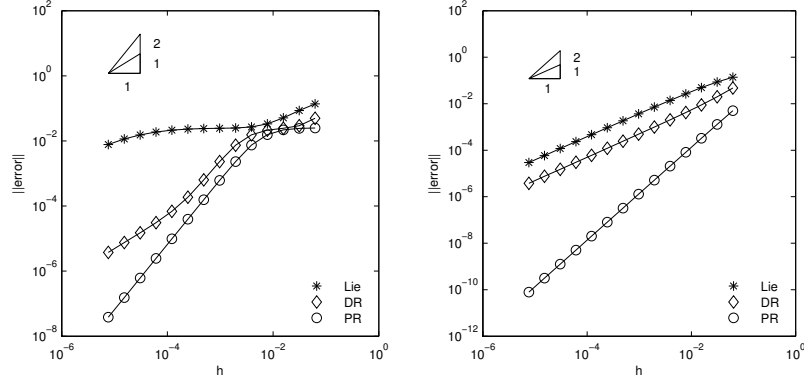


Figure 1: Discrete L^2 -errors at time $t = 1$ for the splitting schemes with $M = 5000$ spatial grid points. In the left graph A is the Dirichlet Laplacian and B is the multiplication operator. The operators have been interchanged in the experiment of the right graph.

We furthermore prescribe the solution

$$u(t, x) = x(1 - x)(e^t - 1)$$

by a suitable choice of the inhomogeneity g and the operator A is discretized by standard central differences over the equidistant grid $\Omega_{\Delta x}$ with M grid points and $\Delta x = 1/(M + 1)$. Note that no spatial error is introduced as the exact solution is a second order polynomial in the spatial variable x .

The global errors at time $t = 1$ for the Lie, DR and PR splittings are presented in the left graph of Figure 1 for varying time step sizes h and $M = 5000$ grid points in space. As seen from the graph, the global error decreases very slowly for the Lie splitting, and the error virtually comes to a halt for time step sizes in the range 10^{-2} to 10^{-4} . The scheme is in other words of no practical use in this rather trivial situation. The resulting global errors for the DR and PR splittings schemes display convergence orders between one and two. Hence, the previous lack of convergence for the Lie splitting is no longer present for the DR and PR methods.

To further illustrate that the order reduction is caused by the term $ABu(t)$, we conduct the same experiment by interchanging the operators A and B with each other in the splitting schemes. The term $BAu(t)$ is then well defined and the classical convergence orders are obtained for all schemes, as seen in the right graph of Figure 1.

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