Relaxation Runge-Kutta Methods and Entropy Stability

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Introduction

Why do we want entropy stabile methods?

ODE

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}u(t) &= f(t, u(t)), \quad t \in (0, T)\\ u(0) &= u^0\end{aligned}$$

$u \in \mathcal{H}$ real Hilbert space with the inner product $\langle \cdot, \cdot \rangle$, inducing the norm $\|\cdot\|$.

Entropy

$$\eta : \mathcal{H} \to \mathbb{R}$$

smooth convex function in time.

E.g. entropy, energy or momentum.

Entropy 2

$$\frac{\mathrm{d}}{\mathrm{d}t}\eta(u(t)) = \left\langle \eta'(u(t)), f(t, u(t)) \right\rangle .$$

Entropy dissipative:

$$\left\langle \eta'(u(t)), f(t, u(t)) \right\rangle \leq 0, \quad \forall u \in \mathcal{H}, t \in [0, T],$$

Entropy conservative:

$$\left\langle \eta'(u(t)), f(t, u(t)) \right\rangle = 0, \quad \forall u \in \mathcal{H}, t \in [0, T].$$

Classic Runge-Kutta

Butcher tableau

$$
\begin{array}{c|c}
c & A \\
\hline
 & b^{\mathrm{T}}
\end{array}, \qquad A \in \mathbb{R}^{s\times s} \text{ and } b, c \in \mathbb{R}^s
$$

Scheme

$$
\begin{aligned}
y_i &= u^n + \Delta t \sum_{j=1}^{s} a_{i,j} f(t_n + c_j \Delta t, y_j), \quad i = 1, \dots, s \\
u^{n+1} &= u^n + \Delta t \sum_{i=1}^{s} b_i f(t_n + c_i \Delta t, y_i).
\end{aligned}
$$

We introduce the notation

$$
f_i = f(t_n + c_i \Delta t, y_i), \qquad f_0 = f(t_n, u^n).
$$

Relaxation Runge-Kutta

$$u_\gamma^{n+1} = u^n + \gamma_n \Delta t \sum_{i=1}^{s} b_i f_i,$$

with $\gamma_n \in \mathbb{R}$.

Relaxed Runge-Kutta, RRK, interprets $u_\gamma^{n+1} \approx u(t_n + \gamma \Delta t)$.

The incremental direction technique, or IDT-method, interprets $u_\gamma^{n+1} \approx u(t_n + \Delta t)$.

Relaxation Runge-Kutta 2

We choose γ_n fulfilling

$$\eta(u_\gamma^{n+1}) - \eta(u^n) = \gamma \Delta t \sum_{i=1}^{s} b_i \left\langle \eta'(y_i), f_i \right\rangle ,$$

by finding a root of

$$r(\gamma) = \eta(u^n + \gamma_n \Delta t \sum_{i=1}^{s} b_i f_i) - \eta(u^n) - \gamma \Delta t \sum_{i=1}^{s} b_i \left\langle \eta'(y_i), f_i \right\rangle .$$

Properties of r

- $r(\gamma)$ is convex
- $r(0) = 0$

Existence of a solution

Lemma

Let a Runge-Kutta method be given such that $\sum_{i=1}^{s} b_i a_{i,j} > 0$*. If* $n''(u^n)(f_0, f_0) > 0$ *then* $r'(0) < 0$ *for sufficiently small* $\Delta t > 0$*.*

Note that $\sum_{i=1}^{s} b_i a_{i,j} > 0$ is a reasonable assumption.

Proof.

By definition of r we have that

$$r'(0) = \eta'(u^n) \cdot \left(\Delta t \sum_{i=1}^{s} b_i f_i \right) - \Delta t \sum_{i=1}^{s} b_i \left\langle \eta'(y_i), f_i \right\rangle$$
$$= -\Delta t^2 \sum_{i,j=1}^{s} b_i a_{i,j} \int_0^1 \eta'' \left(u^n + v \Delta t \sum_{k=1}^{s} a_{i,k} f_k \right) (f_i, f_j) \, \mathrm{d}v.$$

With Taylor expansions of $f_i, f_j = f_0 + \mathcal{O}(\Delta t)$,

$$r'(0) = -\Delta t^2 \sum_{i,j=1}^{s} b_i a_{i,j} \int_0^1 \eta'' \left(u^n + v \Delta t \sum_{k=1}^{s} a_{i,k} f_k \right) (f_0, f_0) \, \mathrm{d}v + \mathcal{O}(\Delta t^3)$$

Thus, with the given assumptions, $r'(0) < 0$. $\square$

Existence of a solution, cont.

Lemma

Let a Runge-Kutta method be given such that $\sum_{i,j=1}^{s} b_i(a_{i,j} - b_j) < 0$*. If* $\eta''(u^n)(f_0, f_0) > 0$ *then* $r'(1) > 0$ *for sufficiently small* $\Delta t > 0$*.*

Note that the assumption $\sum_{i,j=1}^{s} b_i(a_{i,j} - b_j) < 0$ is also reasonable.

Proof.

By the definition of $r(\gamma)$ we have that

$$r'(1) = -\Delta t^2 \sum_{i,j=1}^{s} b_i \left(a_{i,j} - b_j\right) \int_0^1 \eta'' \left(u^{n+1} + \Delta t \sum_{k=1}^{s} \left(a_{i,k} - b_k\right) f_k\right) \left(f_i, f_j\right) \mathrm{d}v$$

With Taylor expansions of $f_i, f_j = f_0 + \mathcal{O}(\Delta t)$,

$$r'(1) = -\Delta t^2 \sum_{i,j=1}^{s} b_i \left(a_{i,j} - b_j\right) \int_0^1 \eta'' \left(u^{n+1} + \Delta t \sum_{k=1}^{s} \left(a_{i,k} - b_k\right) f_k\right) \left(f_0, f_0\right) \mathrm{d}v + \mathcal{O}(\Delta t^3)$$

Thus, with the given assumptions, $r'(1) > 0$. □

Existence of a solution, cont.

Theorem

Assume that the Runge-Kutta method satisfies $\sum_{i,j=1}^{s} b_i a_{i,j} > 0$ and $\sum_{i,j=1}^{s} b_i(a_{i,j} - b_j) < 0$. If $\eta''(u^n)(f_0, f_0) > 0$ then r has a positive root for sufficiently small $\Delta t > 0$.

Proof.

Since $r(0) = 0$ and $r'(0) < 0$ we have that $r(\gamma) < 0$ for small $\gamma > 0$. Because $r'(1) > 0$ and r is convex we have that r' is monotone. Thus, there must be a positive root of r. □

Accuracy

Theorem

Let a given RK-method be of order p. Consider the IDT and RRK methods based on them and suppose that $\gamma_n = 1 + \mathcal{O}(\Delta t^{p-1})$, *then*

1. *The IDT method interpreting* $u_\gamma^{n+1} \approx u(t_n + \Delta t)$ *has order* $p - 1$.
2. *The RRK method interpreting* $u_\gamma^{n+1} \approx u(t_n + \gamma \Delta t)$ *has order* p.

Accuracy 2

Theorem

Let $\mathcal{W}$ be a Banach space, $\Phi : [0, T] \times \mathcal{H} \to \mathcal{W}$ a smooth function and b_i, c_i coefficients of a Runge-Kutta method of order p. Then

$$\sum_{i=1}^{s} b_i \Phi(t_n + c_i \Delta t, y_i) = \sum_{i=1}^{s} b_i \Phi(t_n + c_i \Delta t, u(t_n + c_i \Delta t)) + \mathcal{O}(\Delta t^p).$$

Corollary

If η is smooth and the given Runge-Kutta method is p-order accurate, $r(\gamma = 1) = \mathcal{O}(\Delta t^{p+1})$.

Accuracy 3

Theorem

Assume there exists a positive root γ_n of r. Consider the IDT/RRK methods based on a given Runge-Kutta method that is p-order accurate. Then

1. *The IDT method interpreting $u_\gamma^{n+1} \approx u(t_n + \Delta t)$ has order $p - 1$.*
2. *The RRK method interpreting $u_\gamma^{n+1} \approx u(t_n + \gamma\Delta t)$ has order p.*

Proof.

We have that $r(1) = \mathcal{O}(\Delta t^{p+1})$ and $r'(1) = c\Delta t^2 + \mathcal{O}(\Delta t^3)$ for some $c > 0$. Thus there is a root $\gamma_n = 1 + \mathcal{O}(\Delta t^{p-1})$ of r. Applying to earlier theorem yield the desired result. $\square$

Numerical Examples

Notes regarding the experiments:

- Last iterative step
- $\Delta t \to 1$
- Chosen methods

Problem 1 - Conserved exponential entropy

First we consider the system

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} u_1(t) \\ u_2(t) \end{bmatrix} = \begin{bmatrix} -\exp(u_2(t)) \\ \exp(u_1(t)) \end{bmatrix}, \qquad u^0 = \begin{bmatrix} 1 \\ 0.5 \end{bmatrix},$$

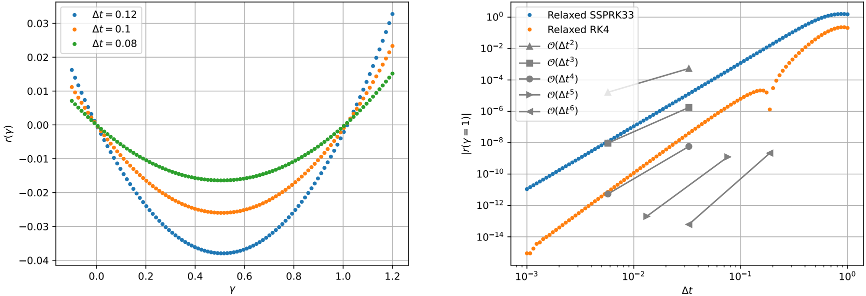
with exponential entropy

$$\eta(u) = \exp(u_1) + \exp(u_2), \qquad \eta'(u) = \begin{bmatrix} \exp(u_1) \\ \exp(u_2) \end{bmatrix},$$

and analytic solution

$$u(t) = \left(\log\left(\frac{\mathrm{e} + \mathrm{e}^{3/2}}{\sqrt{\mathrm{e}} + \mathrm{e}^{(\sqrt{\mathrm{e}}+\mathrm{e})t}} \right), \log\left(\frac{\mathrm{e}^{(\sqrt{\mathrm{e}}+\mathrm{e})t}(\sqrt{\mathrm{e}} + \mathrm{e})}{\sqrt{\mathrm{e}} + \mathrm{e}^{(\sqrt{\mathrm{e}}+\mathrm{e})t}} \right) \right)^{\mathrm{T}}.$$

Problem 1, cont.

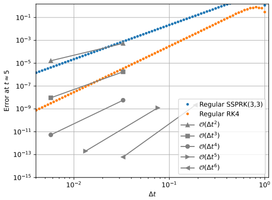


(a) $r(\gamma)$ for SSPRK(3,3)

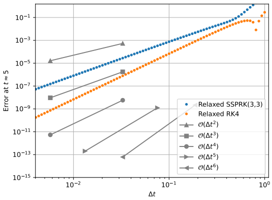
(b) $|r(\gamma = 1)|$ for some RK methods

Figure: Numerical results for r at the first time step of problem 1.

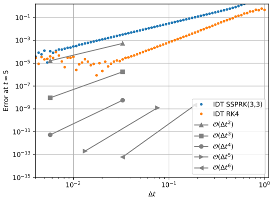
Problem 1, cont.



(a) Classic methods



(b) RRK Methods



(c) IDT methods

Figure: Convergence study for problem 1.

Problem 2 - Dissipated exponential entropy

Consider the ODE

$$\frac{\mathrm{d}}{\mathrm{d}t}u(t) = -\exp(u(t)), \qquad u^0 = 0.5,$$

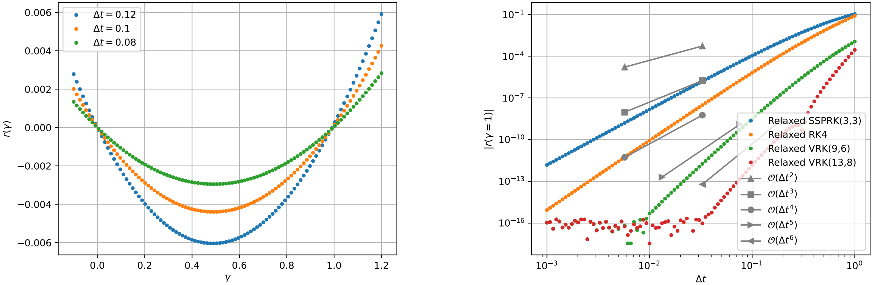
with the exponential entropy

$$\eta(u) = \exp(u), \qquad \eta'(u) = \exp(u),$$

and analytical solution

$$u(t) = -\log(\mathrm{e}^{-1/2} + t).$$

Problem 2, cont.



(a) $r(\gamma)$ for SSPRK(3,3)

(b) $|r(\gamma = 1)|$ for some RK methods

Figure: Numerical results for r at the first time step of problem 2.

Problem 2, cont.

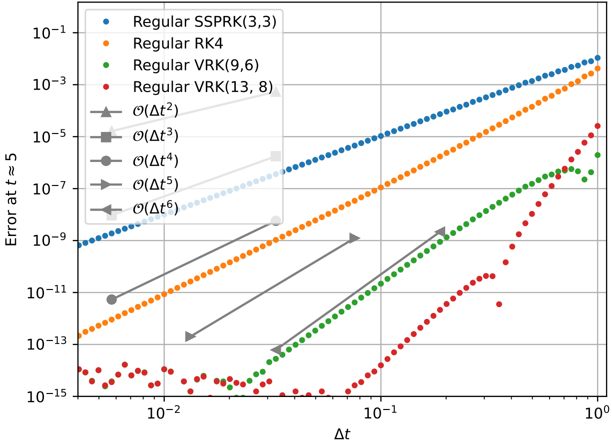


Figure: Convergence study for problem 2, classic methods.

Problem 2, cont.

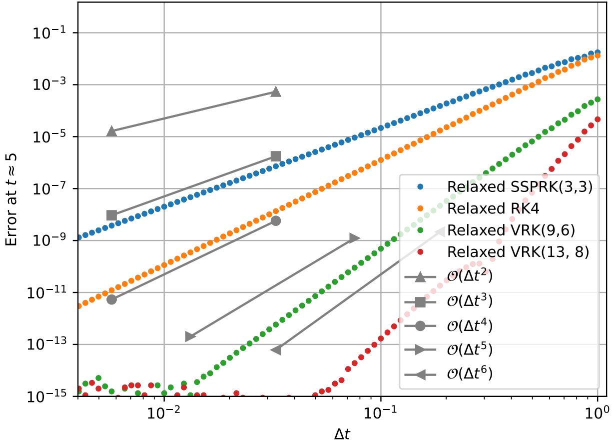


Figure: Convergence study for problem 2, relaxed methods.

Problem 2, cont.

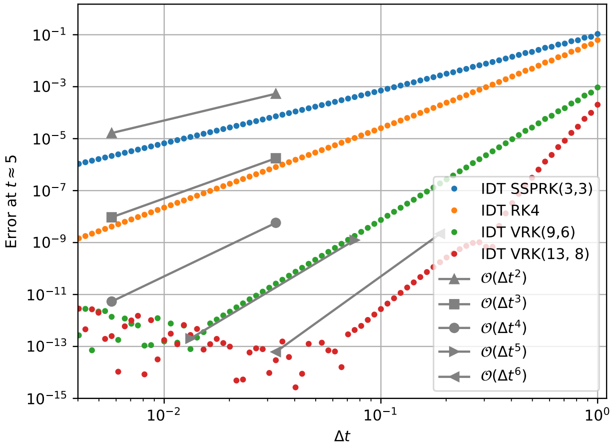


Figure: Convergence study for problem 2, IDT methods.

Conclusion

- Simple
- Cheap
- Physically correct
- Requires η