Runge-Kutta integrators yield optimal regularization schemes

(to appear in *Inverse Problems*)

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Contents

Inverse and ill-posed problems

$T \in \mathcal{L}(X,Y)$, X, Y real Hilbert spaces, $\mathsf{R}(T)$ non-closed in Y.

For instance: T compact and non-degenerated

Inverse problem: $Tf = g^\varepsilon$

$g^\varepsilon \in Y : \|Tf^+ - g^\varepsilon\|_Y \leq \varepsilon$ and $f^+ \in \mathsf{N}(T)^\perp$

ε noise level

Difficulty: generalized inverse $T^+ : \mathcal{R}(T) \oplus \mathcal{R}(T)^\perp \subset Y \to X$ is unbounded

Regularization of inverse problems

Regularization: $\{\mathcal{R}_n\}_{n\in\mathbb{N}_0}$, $\mathcal{R}_n : Y \to X$ continuous, $\mathcal{R}_n 0 = 0$.
If there is a *parameter choice* $\gamma :]0,\infty[\, \times Y \to \mathbb{N}_0$ such that we have

$$\sup\left\{\|f^+ - \mathcal{R}_{\gamma(\varepsilon,g^\varepsilon)} g^\varepsilon\|_X \;\middle|\; g^\varepsilon \in Y,\ \|Tf^+ - g^\varepsilon\|_Y \le \varepsilon\right\} \longrightarrow 0 \quad \text{as} \quad \varepsilon \to 0$$

for all $f^+ \in \mathsf{N}(T)^\perp$, then $(\{\mathcal{R}_n\}_{n\in\mathbb{N}_0}, \gamma)$ is a regularization scheme for T^+.

Optimality: The regularization scheme $(\{\mathcal{R}_n\}_{n\in\mathbb{N}_0}, \gamma)$ for T^+ is called *(order-)optimal* in $\mathsf{X}_{\mu,\varrho} := (T^*T)^{\mu/2} B_\varrho(0)$, μ, $\varrho > 0$, if

$$\sup\left\{\|f^+ - \mathcal{R}_{\gamma(\varepsilon,g^\varepsilon)} g^\varepsilon\|_X \;\middle|\; g^\varepsilon \in Y,\ \|Tf^+ - g^\varepsilon\|_Y \le \varepsilon,\ f^+ \in \mathsf{X}_{\mu,\varrho}\right\}$$

$$\le C_\mu\, \varepsilon^{\mu/(\mu+1)}\, \varrho^{1/(\mu+1)}.$$

Regularization schemes by filter functions I

$\{F_n\}_{n\in\mathbb{N}_0}$, $F_n : [0, \|T\|^2] \to \mathbb{R}$, piecew. continuous with jump-discontinuities is called regularizing filter if

$$\lim_{n\to\infty} F_n(\lambda) = 1/\lambda \quad \text{and} \quad \lambda|F_n(\lambda)| \le C_F \quad \text{for } \lambda \in]0, \|T\|^2].$$

Candidates for regularization operators: $\mathcal{R}_n := F_n(T^*T)T^* \in \mathcal{L}(Y, X)$

Morozov's discrepancy principle: Choose $\tau > 1$ and set

$$\gamma(\varepsilon, g^\varepsilon) := \min\left\{n \in \mathbb{N}_0 \; : \; \|T\mathcal{R}_n g^\varepsilon - g^\varepsilon\|_Y \le \tau\,\varepsilon\right\}.$$

Remark: $(\{\mathcal{R}_n\}_{n\in\mathbb{N}_0}, \gamma)$ is a regularization scheme for T^+.

Regularization schemes by filter functions II

We have that

$$\sup\{|F_n(\lambda)| \,|\, 0 \leq \lambda \leq \|T\|^2\} = \mathrm{O}(t_n) \quad \text{as } n \to \infty$$

where $\{t_n\}_{n\in\mathbb{N}_0}$ diverges strongly monotone to infinity.

The qualification μ_Q of a filter is the largest number such that

$$\sup_{0\leq\lambda\leq\|T\|^2} \lambda^{\mu/2}\,|1-\lambda\, F_n(\lambda)| = \mathrm{O}\big(t_n^{-\mu/2}\big) \quad \text{as } n \to \infty \ \text{ for all } \mu \in \,]0, \mu_\mathsf{Q}].$$

Theorem: $\{F_n\}_{n\in\mathbb{N}_0}$ as above with $t_n/t_{n+1} \geq \vartheta > 0$ and $\mu_Q > 1$, γ discr. principle, $\tau > \sup\{|1-\lambda F_n(\lambda)| \,|\, n \in \mathbb{N}_0,\ 0 \leq \lambda \leq \|T\|^2]\} \geq 1$.

Then, $(\{\mathcal{R}_n\}_{n\in\mathbb{N}_0}, \gamma)$, $\mathcal{R}_n := F_n(T^*T)T^*$, is an optimal regularization scheme for T^+ in $\mathsf{X}_{\mu,\varrho}$ for all $\mu \in \,]0, \mu_\mathsf{Q} - 1]$ and all $\varrho > 0$.

Examples

- Tikhonov-Phillips

  $F_n(\lambda) = 1/(\lambda + t_n^{-1}), \quad \mathcal{R}_n = (T^*T + t_n^{-1} I)^{-1} T^*, \quad \mu_{\mathsf{Q}} = 2$

- Showalter's or asymptotic regularization

$$u'(t) = T^*\big(g^\varepsilon - Tu(t)\big), \quad u(0) = 0,$$

Define $\mathcal{R}_n g^\varepsilon := u(t_n).$

We have $\mu_Q = \infty$ and $\mathcal{R}_n = F_n(T^*T)T^*$ where

$$F_n(\lambda) = \begin{cases} \dfrac{1 - \exp(-\lambda\, t_n)}{\lambda} & : \quad \lambda > 0, \\ t_n & : \quad \lambda = 0. \end{cases}$$

Sneak preview: Conclusion of the talk

Runge-Kutta integrators applied to the evolution equation

$$u'(t) = T^*\big(g^\varepsilon - Tu(t)\big), \quad u(0) = 0,$$

generate optimal regularization schemes in $\mathsf{X}_{\mu,\varrho}$ for all $\mu,\ \varrho > 0$, when stopped by the discrepancy principle ($\mu_Q = \infty$).

Runge-Kutta integrators I

$\Psi : [0,\infty[\times W \to W$, W Banach space, $w_0 \in W$

$$w'(t) = \Psi\big(t, w(t)\big), \quad t > 0, \quad w(0) = w_0,$$

Runge-Kutta integrator with s stages and time steps $\{\Delta \mathsf{t}_n\}_{n\in\mathbb{N}} \subset]0,\infty[$:

$$w_n \approx w(t_n), \quad t_n = \sum_{k=1}^{n} \Delta \mathsf{t}_k$$

$$w_n = w_{n-1} + \Delta \mathsf{t}_n \sum_{i=1}^{s} b_i\, k_i(t_{n-1}, w_{n-1}, \Delta \mathsf{t}_n),$$

$$k_i = \Psi\Big(t_{n-1} + c_i \Delta \mathsf{t}_n,\ w_{n-1} + \Delta \mathsf{t}_n \sum_{j=1}^{s} a_{ij} k_j\Big), \quad i = 1, \ldots, s.$$

Runge-Kutta integrators II

Compact representation by *Butcher array*

$$\begin{array}{c|c} c & A \\ \hline & b^t \end{array} \quad = \quad \begin{array}{c|ccc} c_1 & a_{11} & \cdots & a_{1s} \\ \vdots & \vdots & \vdots & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

RK is called explicit if A is strictly lower triangular, otherwise implicit.

RK is called consistent if $\sum_{i=1}^{s} b_i = 1$.

explicit Euler: $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$ implicit Euler: $\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$

Runge-Kutta integrators seen as regularizations I

Application of RK to Showalter's ODE yields

$$w_n = R(-\Delta \mathsf{t}_n\, T^*T) w_{n-1} + \Delta \mathsf{t}_n\, Q(-\Delta \mathsf{t}_n\, T^*T) T^* g^\varepsilon, \quad w_0 = 0,$$

where

$$R(z) = \frac{\det(I - z\,A + z\mathbb{1}b^t)}{\det(I - z\,A)}, \quad Q(z) = \frac{R(z) - 1}{z}.$$

R stability function (polynomial/rational function for explicit/implicit RK)

Lemma: We have that

$$w_n = \mathcal{R}_n g^\varepsilon = F_n(T^*T) T^* g^\varepsilon \quad \text{with } F_n(\lambda) = \frac{1 - \prod_{k=1}^n R(-\Delta \mathsf{t}_k\, \lambda)}{\lambda}.$$

Runge-Kutta integrators seen as regularizations II

Theorem 1: To any consistent RK there is a maximal Δt_{max} such that for any $0 < \Delta t_{min} < \Delta t_{max}$ the family $\{F_n\}_{n\in\mathbb{N}_0}$ with $\{\Delta t_n\}_{n\in\mathbb{N}} \subset [\Delta t_{min}, \Delta t_{max}[$ constitutes a filter having infinite qualification.

In other words: RK integrators with sufficiently small step sizes bounded away from zero yield optimal regularization schemes in $X_{\mu,\varrho}$ for all $\mu,\ \varrho > 0$ when stopped by the discrepancy principle.

Theorem 2: If the consistent RK additionally satisfies

$$|R(-z)| < 1 \quad \text{for all } z > 0,$$

then the above statement holds without a restriction on the magnitude of Δt_{max}.

Remark: The add. requirement in Th. 2 can only be satisfied by implicit RKs.

Proof: $R(z) = \exp(z) + \mathrm{O}(z^2) = 1 + z + \mathrm{O}(z^2)$ as $z \to 0$.

Examples

- Explicit Euler: $R(z) = 1 + z$, $\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$, $\Delta t_{\text{max}} = \dfrac{2}{\|T\|^2}$

$$w_n = (I - \Delta t_n T^* T) w_{n-1} + \Delta t_n T^* g^\varepsilon = w_{n-1} + \Delta t_n T^* (g^\varepsilon - T w_{n-1})$$

  This is the well-known Landweber iteration.

- Implicit Euler: $R(z) = \dfrac{1}{1-z}$, $\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$, no restriction on Δt_{max}

$$\begin{aligned} w_n &= (I + \Delta t_n T^* T)^{-1} w_{n-1} + \Delta t_n (I + \Delta t_n T^* T)^{-1} T^* g^\varepsilon \\ &= (I + \Delta t_n T^* T)^{-1} (w_{n-1} + \Delta t_n T^* g^\varepsilon). \end{aligned}$$

  This iteration is also known as nonstationary iterated Tikhonov-Phillips regularization.

Selection of the step sizes

Since

$$\|f^+ - \mathcal{R}_n T f^+\|_X \le C_Q\, \varrho \left(\sum_{j=1}^{n} \Delta \mathrm{t}_j \right)^{-\mu/2} \quad \text{for any } f^+ \in \mathrm{X}_{\mu,\varrho}$$

large step sizes are attractive!
On the other side: If the last time step is too large the discrepancy principle might be over-satisfied, that is,

$$\|T\mathcal{R}_{\gamma(\varepsilon,g^\varepsilon)} g^\varepsilon - g^\varepsilon\|_Y \ll \tau\,\varepsilon,$$

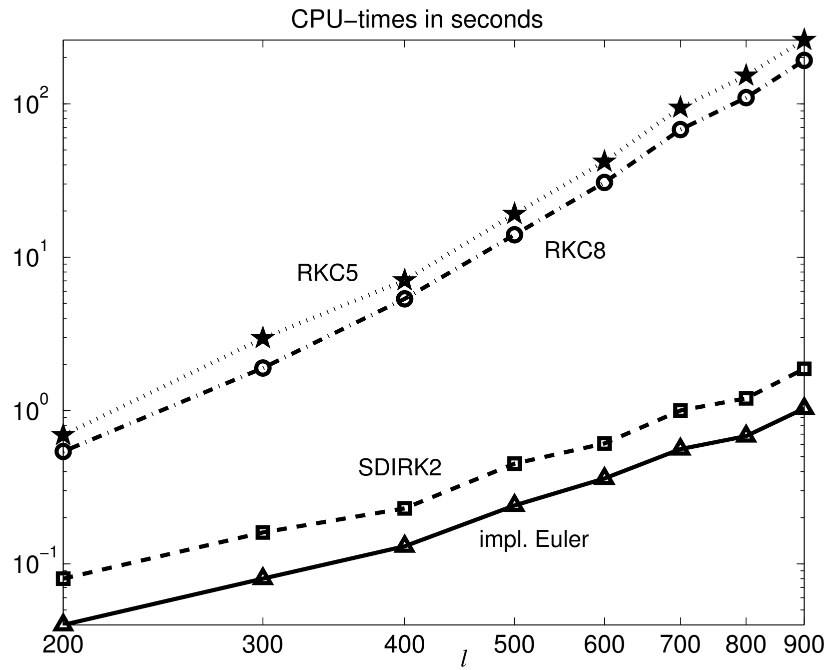
and the noise gets amplified.

Therefore, step size control by monitoring of $q := \dfrac{\|T\mathcal{R}_{\gamma(\varepsilon,g^\varepsilon)} g^\varepsilon - g^\varepsilon\|_Y}{\tau\,\varepsilon}$.
Accept $\mathcal{R}_{\gamma(\varepsilon,g^\varepsilon)} g^\varepsilon$ as approximate solution when $q \approx 1$.

Otherwise, reduce last time step.

Numerical experiments: Integral equation of the 1. kind

- Discretization by projection method and
- discretization effects are taken into account.



integrator	Δt
RKC5	529
RKC8	1128
impl. Euler	$l^{3/2}$
SDIRK2	$l^{3/2}$

In above experiments:

$q = q_l \geq 0.96$ lead to comparable reconstruction errors.

Generalization to inconsistent RK

Observation: Theorems 1 and 2 remain valid under

$$R(z) = 1 + c\,z + \mathrm{O}(z^2) \quad \text{as } z \to 0 \text{ for } c > 1,$$

that is, RK-integrators may be inconsistent.

Question: Can we use this additional freedom to construct schemes which converge faster than the implicit Euler scheme?

Answer: YES!

Outlook: Non-linear Problems

Asymptotic regularization in the non-linear case $T(f) = g^\varepsilon$ means: solve

$$u'(t) = T'\big(u(t)\big)^*\Big(g^\varepsilon - T\big(u(t)\big)\Big), \quad u(0) = u_0,$$

and set $\mathcal{R}_n g^\varepsilon := u(t_n)$.

The application of integrators to the above ODE generates a variety of new potential regularization schemes.

Manuscript for download:

`www.mathematik.uni-karlsruhe.de/~rieder`

Inconsistent RK can do better

Desired properties of a synthetic scheme:

1. $|R(-z)| < 1$ for $z > 0$ and $|R(\infty)| < 1$ (no restriction on Δt_{max}),
2. $R'(0) \gg 1$ (good damping of contributions of small spectral values).

A synthetic scheme: SYNTH

$$\begin{array}{c|cc} 1 & 1 & \\ 2+\theta & 1+\theta & 1 \\ \hline & 1+\theta & 1 \end{array} \qquad R(z) = \frac{1+\theta\, z}{(1-z)^2}$$

For $\theta \in \big[0, 2(1+\sqrt{2})\big[$ the desired properties are satisfied with

$$R'(0) = 2+\theta \quad \text{and} \quad |R(\infty)| = 0.$$

The generated iteration reads

$$w_n = (I + \Delta\mathrm{t}_n T^*T)^{-2}\Big(\big(I - \theta\Delta\mathrm{t}_n T^*T\big) w_{n-1} + \Delta\mathrm{t}_n\big((2+\theta)I + \Delta\mathrm{t}_n T^*T\big)T^*y\Big).$$

Impl. Euler vs. SYNTH

Theorem 3: To any $\theta \in [0,1]$ there is a family $\{Q_n\} \subset \mathcal{L}(Y)$ converging pointwise to 0 such that

$$Tw_n^{\mathsf{S}} - g^{\varepsilon} = Q_n(Tw_n^{\mathsf{E}} - g^{\varepsilon}).$$

Here, $\{w_n^{\mathsf{E}}\}$ and $\{w_n^{\mathsf{S}}\}$ denote the sequences generated by impl. Euler and SYNTH, respectively, for a joint constant time step Δt.

Consequence:

We expect the discrepancy principle to stop SYNTH earlier than impl. Euler.

CPU-timing: Impl. Euler vs. SYNTH