Runge-Kutta integrators yield optimal regularization schemes
(to appear in Inverse Problems)

Andreas Rieder

UNIVERSITÄT KARLSRUHE (TH)
Institut für Wissenschaftliches Rechnen und Mathematische Modellbildung
und
Institut für Praktische Mathematik
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Inverse and ill-posed problems

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

For instance: $T$ compact and non-degenerated

Inverse problem: $T f = g^\epsilon$

$g^\epsilon \in Y : \|T f^+ - g^\epsilon\|_Y \leq \epsilon$ and $f^+ \in N(T)^\perp$

$\varepsilon$ noise level

**Difficulty:** generalized inverse $T^+ : \mathcal{R}(T) \oplus \mathcal{R}(T)^\perp \subset Y \rightarrow X$ 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 \( \gamma : \mathbb{I} \times Y \to \mathbb{N}_0 \) such that we have

\[
\sup \left\{ \| f^+ - \mathcal{R}_{\gamma(\varepsilon, g^\varepsilon)} g^\varepsilon \|_X \mid g^\varepsilon \in Y, \| Tf^+ - g^\varepsilon \|_Y \leq \varepsilon \right\} \to 0 \quad \text{as } \varepsilon \to 0
\]

for all \( f^+ \in \mathbb{N}(T)^\perp \), 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 \( X_{\mu, \varrho} := (T^*T)^{\mu/2} B_2 (0), \mu, \varrho > 0 \), if

\[
\sup \left\{ \| f^+ - \mathcal{R}_{\gamma(\varepsilon, g^\varepsilon)} g^\varepsilon \|_X \mid g^\varepsilon \in Y, \| Tf^+ - g^\varepsilon \|_Y \leq \varepsilon, f^+ \in X_{\mu, \varrho} \right\} \\
\leq C_{\mu} \varepsilon^{\mu/(\mu+1)} \varrho^{1/(\mu+1)}.
\]
Regularization schemes by filter functions I

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

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

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

\[ \gamma(\varepsilon, g^e) := \min \{ n \in \mathbb{N}_0 : \|T\mathcal{R}_n g^e - g^e\|_Y \leq \tau \varepsilon \}. \]

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

\[
\sup_{0 \leq \lambda \leq \|T\|^2} \{|F_n(\lambda)| \} = O(t_n) \quad \text{as } n \to \infty
\]

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

The qualification \( \mu_Q \) of a filter is the largest number such that

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

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

Then, \( \{R_n\}_{n \in \mathbb{N}_0}, \gamma \), \( R_n := F_n(T^*T)T^* \), is an optimal regularization scheme for \( T^+ \) in \( X_{\mu, \varrho} \) for all \( \mu \in ]0, \mu_Q - 1] \) and all \( \varrho > 0 \).
Examples

- Tikhonov-Phillips
  
  \[ F_n(\lambda) = \frac{1}{\lambda + t_n^{-1}}, \quad \mathcal{R}_n = (T^*T + t_n^{-1}I)^{-1}T^*, \quad \mu_Q = 2 \]

- Showalter’s or asymptotic regularization

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

Define \( \mathcal{R}_ng^\varepsilon := u(t_n) \).

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

\[ F_n(\lambda) = \begin{cases} 
1 - \exp(-\lambda t_n) & : \lambda > 0, \\
\frac{\lambda}{t_n} & : \lambda = 0.
\end{cases} \]
Runge-Kutta integrators applied to the evolution equation

\[ u'(t) = T^* \left( g^\varepsilon - Tu(t) \right), \quad u(0) = 0, \]

generate optimal regularization schemes in \( X_{\mu, \varrho} \) for all \( \mu, \varrho > 0 \), when stopped by the discrepancy principle \( (\mu_Q = \infty) \).
Runge-Kutta integrators I

\( \Psi : [0, \infty[ \times W \rightarrow W, \ W \text{ Banach space}, \ w_0 \in W \)

\[ w'(t) = \Psi(t, w(t)), \quad t > 0, \quad w(0) = w_0, \]

Runge-Kutta integrator with \( s \) stages and time steps \( \{\Delta t_n\}_{n \in \mathbb{N}} \subset ]0, \infty[ \):

\[ w_n \approx w(t_n), \quad t_n = \sum_{k=1}^{n} \Delta t_k \]

\[ w_n = w_{n-1} + \Delta t_n \sum_{i=1}^{s} b_i \ k_i(t_{n-1}, w_{n-1}, \Delta t_n), \]

\[ k_i = \Psi \left( t_{n-1} + c_i \Delta t_n, w_{n-1} + \Delta t_n \sum_{j=1}^{s} a_{ij} k_j \right), \quad i = 1, \ldots, s. \]
Runge-Kutta integrators II

Compact representation by *Butcher array*

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

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:**
\[
\begin{array}{c|c}
  0 & 0 \\
  \hline
  1 & 1
\end{array}
\]

**implicit Euler:**
\[
\begin{array}{c|c}
  1 & 1 \\
  \hline
  1 & 1
\end{array}
\]
Runge-Kutta integrators seen as regularizations I

Application of RK to Showalter’s ODE yields

\[ w_n = R(-\Delta t_n T^*T)w_{n-1} + \Delta t_n Q(-\Delta t_n T^*T)T^*g^\varepsilon, \quad w_0 = 0, \]

where

\[ R(z) = \frac{\det(I - zA + zIb^t)}{\det(I - zA)}, \quad Q(z) = \frac{R(z) - 1}{z}. \]

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

Lemma: We have that

\[ w_n = R_n g^\varepsilon = F_n(T^*T)T^*g^\varepsilon \quad \text{with} \quad F_n(\lambda) = \frac{1 - \prod_{k=1}^n R(-\Delta t_k \lambda)}{\lambda}. \]
Runge-Kutta integrators seen as regularizations II

**Theorem 1:** To any consistent RK there is a maximal $\Delta t_{\text{max}}$ such that for any $0 < \Delta t_{\text{min}} < \Delta t_{\text{max}}$ the family $\{F_n\}_{n \in \mathbb{N}_0}$ with $\{\Delta t_n\}_{n \in \mathbb{N}} \subset [\Delta t_{\text{min}}, \Delta t_{\text{max}}]$ 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

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

then the above statement holds without a restriction on the magnitude of $\Delta t_{\text{max}}$.

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

**Proof:** $R(z) = \exp(z) + O(z^2) = 1 + z + O(z^2)$ as $z \to 0$. 
Examples

- **Explicit Euler:** \( R(z) = 1 + z \),
  \[
  \begin{pmatrix}
  0 & 0 \\
  1 & 1
  \end{pmatrix},
  \Delta t_{\text{max}} = \frac{2}{\|T\|^2}
  \]
  \[
  w_n = (I - \Delta t_n T^* T)w_{n-1} + \Delta t_n T^* g^\varepsilon = w_{n-1} + \Delta t_n T^* (g^\varepsilon - Tw_{n-1})
  \]
  This is the well-known Landweber iteration.

- **Implicit Euler:** \( R(z) = \frac{1}{1 - z} \),
  \[
  \begin{pmatrix}
  1 & 1 \\
  1 & 1
  \end{pmatrix},
  \text{no restriction on } \Delta t_{\text{max}}
  \]
  \[
  w_n = (I + \Delta t_n T^* T)^{-1} w_{n-1} + \Delta t_n (I + \Delta t_n T^* T)^{-1} T^* g^\varepsilon
  \]
  \[
  = (I + \Delta t_n T^* T)^{-1} (w_{n-1} + \Delta t_n T^* g^\varepsilon).
  \]
  This iteration is also known as nonstationary iterated Tikhonov-Phillips regularization.
Selection of the step sizes

Since

$$\|f^+ - \mathcal{R}_n T f^+\|_X \leq C_Q \varrho \left( \sum_{j=1}^n \Delta t_j \right)^{-\mu/2}$$

for any \( f^+ \in X_{\mu, \varrho} \)

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 \( q := \frac{\|T\mathcal{R}_{\gamma(\varepsilon, g^\varepsilon)} g^\varepsilon - g^\varepsilon\|_Y}{\tau \varepsilon} \).

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.

In above experiments:

\[ q = q_t \geq 0.96 \] lead to comparable reconstruction errors.
Generalization to inconsistent RK

**Observation:** Theorems 1 and 2 remain valid under

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

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 $T(f) = g^\epsilon$ means: solve

$$u'(t) = T'(u(t))^* \left( g^\epsilon - T(u(t)) \right), \quad u(0) = u_0,$$

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

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 \(\Delta t_{\text{max}}\)),
2. \(R'(0) \gg 1\) (good damping of contributions of small spectral values).
A synthetic scheme: SYNTH

\[
\begin{array}{ccc}
1 & 1 & R(z) = \frac{1 + \theta z}{(1 - z)^2} \\
2 + \theta & 1 + \theta & 1 \\
1 + \theta & 1 & \\
\end{array}
\]

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

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

The generated iteration reads

\[
w_n = (I + \Delta t_n T^*T)^{-2} \left( (I - \theta \Delta t_n T^*T) w_{n-1} + \Delta t_n ((2 + \theta)I + \Delta t_n T^*T) T^*y \right).
\]
Theorem 3: To any \( \theta \in [0, 1] \) there is a family \( \{Q_n\} \subset \mathcal{L}(Y) \) converging point-wise to 0 such that

\[
T w_n^S - g^e = Q_n (T w_n^E - g^e).
\]

Here, \( \{w_n^E\} \) and \( \{w_n^S\} \) denote the sequences generated by impl. Euler and SYNTH, respectively, for a joint constant time step \( \Delta t \).

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