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A SHORT-TERM RATIONAL KRYLOV METHOD FOR LINEAR INVERSE PROBLEMS*

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Abstract. Motivated by the aggregation method, we present an iterative method for finding approximate solutions of least-squares problems for linear ill-posed problems over (mixed) rational Krylov spaces. The mixed rational Krylov spaces where the solution is sought consist of Tikhonov-regularized solutions mixed with usual Krylov space elements from the normal equations. We present an algorithm based on the Arnoldi–Lanczos iteration, and, as main result, derive the rational CG method, a short-term iteration that, similar as the usual conjugate gradient method, does not requires orthogonalization or saving of the Krylov basis vectors. Some numerical experiments illustrate the performance of the method.

Key words. rational Krylov space, rational conjugate gradient method, aggregation method, short-term recurrence

AMS subject classifications. 65F10, 65F22

1. Introduction.

The setting of this article are linear ill-posed problems stated in Hilbert spaces. That is, given a compact forward operator $A : X \to Y$ between Hilbert spaces X, Y and data $y \in Y$, a standard approach to find (generalized) solutions x of $Ax = y$ is the least-squares method:

$$\min_{x \in X} \|Ax - y\|.$$

In this work, we are particular interested in the case that A represents an ill-posed or ill-conditioned forward operator such that a direct method usually leads to useless solutions, but regularization has to be employed. One of the most popular regularization methods in this case is Tikhonov regularization that calculates an approximate solution of the forward problem by

$$x_\alpha := (A^*A + \alpha I)^{-1} A^* y, \tag{1.1}$$

with $\alpha > 0$ representing a regularization parameter that has to be chosen appropriately. Since this involves solving a linear system, especially in high-dimensional cases, iterative methods are the state-of-the-art, for instance, highly popular are Krylov-space methods (see, e.g., [20]) such as the conjugate gradient (CG) method [17, 28, 32] for the normal equations. We refer to this method (i.e., using the Krylov space $\mathcal{K}(A^*A; A^*y)$ for solving $A^*Ax = A^*y$) as the CGNE method (following [17, 28]), while other authors, e.g., [52], call this the CGNR method and CGNE is then referred to solving the dual normal equations $AA^*z = y$ using the Krylov space $\mathcal{K}(AA^*; Ay)$; a similar name for the CGNE method stated in this article is the CGLS method in [31].

Another quite interesting method, which is also the starting point for our analysis, is the recently proposed *aggregation method* [10], which improves Tikhonov regularization by constructing linear combinations of several x_{α_i} in (1.1) and minimizing the least-squares functional over such combinations. This has, e.g., been successfully used in combination with heuristic parameter choice rules [36], inverse problems in geophysics [53], and in particular in domain adaption in learning [22, 42]. The method has also been suggested independently

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in [33], where also combinations of other regularization methods such as truncated singular value decomposition were considered.

As we will see below (see Section 2), both the CGNE and the aggregation method can be treated in a similar manner, namely as generalized Krylov space methods, where the latter one operates in rational Krylov spaces. Its drawback is, however, that it is non-iterative, and the system matrix is nonsparse in the Krylov basis. To repair this imperfection is one of the main objectives of the current article: In order to alter the aggregation method into a recursive method, we use mixed rational Krylov spaces, which allow for a sparse (in fact, pentadiagonal) representation in this space; see, e.g., [43, 44] and Section 2. Current algorithms in this field use Arnoldi–Lanczos-type method that are based on orthogonalizing vectors with respect to the Krylov basis.

The main novelty of this article is the development of a short-term recursive method, called rational CG (RatCG) method, in mixed Krylov spaces without the need of orthogonalization or saving of the Krylov basis vectors. With respect to the number of iterations to achieve a discrepancy principle, the method requires fewer iterations than almost any existing method on the market (cf. Theorem 2.3), and it is comparable to the aggregation method but with lower complexity involved. Of course, this advantage is gained by an extra effort of solving a Tikhonov-regularized problem in each iteration.

The rational CG method has numerous advantages compared to many traditional regularization schemes: i) since ordinary Tikhonov regularization has to be accompanied with an α-parameter choice [17], several solutions of (1.1) have to be computed anyway, where candidate solutions x_{α_i} not satisfying, e.g., the discrepancy rule are usually discarded; a similar situation arises when using heuristic minimization-based rules [34]. On the contrary, the RatCG method reuses all computed Tikhonov solutions to build up the search space in an (residual-)optimal way and with a rather simple recursion. ii) a similar observation holds for iterated Tikhonov regularization [17, 29]: although its solutions are in a rational Krylov space, compared to the RatCG method, the residuals are usually larger. (iii) Moreover, and in particular, we show that the RatCG method terminates in a discrete setting in finite time in contrast to the methods mentioned in (i) and (ii). (iv) It has a simple short-term recursion in contrast to the aggregation method, requires less memory than the Arnoldi–Lanczos methods, while giving similar results. (v) Compared to CGNE and any usual Krylov space method like the ν-method [7, 27] or Nesterov's iteration [35, 40], the rational CG has always a smaller residual and thus requires fewer iterations to satisfy the discrepancy principle.

A downside of the proposed method is the need of solving linear problems with the system matrix $(A^*A + \alpha_i I)$ multiple times, which implies a higher complexity than simple Krylov methods; however, we will see from the numerical results that the additional overhead is not high, and for some instances even these Krylov space methods can be beaten. As soon as (iterated) Tikhonov regularization or the aggregation method are regarded as valid regularization methods, the RatCG method also has to since it performs better than the former ones.

Furthermore, we regard the rational CG method just as a first foundation with the prospect of further use and research on rational Krylov spaces for ill-posed problems. At the end of the article, we will discuss some aspects of generalizations and improvements, which we think are worth of consideration. Let us also point out that we do not analyze the regularization properties of the RatCG method but leave this also to future work. Note that even for the usual CGNE method, this is a highly nontrivial task, and it is even more involved in the rational case.

Finally, let us mention some related work in the context of ill-posed problems. Rational Krylov method are well-established in the numerical analysis for well-posed problems; only

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few results exist considering them from a regularization point of view. Grimm [23] has studied regularization properties of such rational CG method, but he uses only constant regularization parameters, whereas we allow varying ones. Compared to Grimm, this makes our algorithm more complicated (we get a three-term recursion in the odd steps), but our method is more flexible and is comparable to the aggregation method. However, the derivation and analysis is also more involved. In several works (see, e.g., [26, 43, 44, 45] and the references in Section 2) a Lanczos-type method for Hermitean and non-Hermitean linear equation is proposed that is essentially identical to the Lanczos method of Algorithm 2 (the precursor of the RatCG method) in this article. Moreover, let us also mention that a short-term recursion for calculating a basis in rational Krylov spaces has been developed [12, 25, 41]. However, the matrix representation there is usually non-sparse, which does not lead to a short-term iterative method. The follow-up of the Lanczos method in Section 3, the RatCG method, is new and the main contribution of this article; we consider this a nontrivial extension of the cited work.

The structure of the article is as follows: In Section 2 we introduce rational Krylov spaces, recall some of their properties, and derive the rational Lanczos method from the sparse representation of the operator in the mixed spaces. Section 3 presents the main algorithm, the RatCG method, which is a low-memory extension of the rational Lanczos method. Some numerical investigations are presented in Section 4.

2. Rational Krylov spaces. In this section we define and discuss the structure of rational Krylov spaces. Rational Krylov spaces have been introduced by Ruhe [47] for eigenvalues computations, and since then a fruitful theory has been developed, mainly in the context of well-posed problems [3, 4, 5, 8, 9, 12, 14, 16, 18, 19, 24, 25, 26, 41, 48, 49, 50, 51, 54]. A similar concept is that of extended Krylov spaces [13].

For notational reasons we introduce the system matrix (or operator) for the normal equations and the corresponding right-hand side:

$$\mathcal{A} := A^*A \qquad \mathrm{y} := A^*y, \qquad \overline{\mathcal{A}} := AA^*\,. \tag{2.1}$$

In the sequel we denote the Hilbert-space inner products in X or Y by $\langle .,. \rangle$. We consider a sequence of pairwise disjoint nonnegative regularization parameters

$$\alpha_1, \ldots \alpha_n, \ldots \qquad \alpha_i > 0, \qquad \alpha_i \neq \alpha_j \quad \text{for } i \neq j. \tag{2.2}$$

For any such α_i, we define the solution x_{α_i} of the associated Tikhonov regularization by (1.1).

Let us start with the motivating method of aggregation proposed in [10] (independently also in [33]) and further developed in [37]. For the aggregation method of [37], one selects a finite number of regularization parameters α_i as in (2.2) and computes the associated Tikhonov regularizations x_{α_i}. The approximate solution of this method is defined as the linear combination $\sum c_i x_{\alpha_i}$ with coefficients c_i that minimize the residual. A similar idea is used in Anderson acceleration [1] but with convex combinations of x_{α_i} instead of linear ones. For the aggregation method, one has to compute and invert the Gramian matrix $G_{i,j} = \langle Ax_{\alpha_i}, Ax_{\alpha_j} \rangle$ of the x_{α_i}. This is a full matrix, and the method is non-recursive, i.e., adding an additional $x_{\alpha_{n+1}}$ to the search space requires (more or less) a full new computation. Also, some precaution in the algorithms has to be taken since the matrix might be ill-conditioned [37]. A version of this method that does not invert the Gramian matrix but computes solutions using the Arnoldi algorithm has been given by Brezinski et al. [8].

Based on this method, let us define the Krylov spaces of interest: With the notation (2.1), the Tikhonov solution x_{α_i} can be written as $f_{\alpha_i}(\mathcal{A})\mathrm{y}$ with

$$f_\alpha(\lambda) = \frac{1}{\lambda + \alpha}.$$

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By definition, the aggregation method minimizes the residual over the rational Krylov space of dimension n

$$\mathcal{R}^n := \operatorname{span}\{f_{\alpha_1}(\mathcal{A})\mathrm{y}, f_{\alpha_2}(\mathcal{A})\mathrm{y}, \dots, f_{\alpha_n}(\mathcal{A})\mathrm{y}\}.$$

Thus, it has a similar structure as the classical conjugate gradient method for the normal equations (CGNE), which minimizes the residual over the usual Krylov space of dimension n

$$\mathcal{K}^n := \operatorname{span}\{\mathrm{y}, \mathcal{A}\mathrm{y}, \mathcal{A}^2\mathrm{y}, \dots, \mathcal{A}^{n-1}\mathrm{y}\}.$$

For the proposed rational CG method in this article, we use mixed rational spaces, defined for even $n = 2k$ and odd $n = 2k+1$ dimensions as follows:

$$\begin{aligned}\mathcal{KR}^{2k} &:= \operatorname{span}\big\{\mathrm{y}, f_{\alpha_1}(\mathcal{A})\mathrm{y}, \mathcal{A}y, f_{\alpha_2}(\mathcal{A}), \mathcal{A}^2y, \dots, f_{\alpha_k}(\mathcal{A})\mathrm{y}\big\}\\ \mathcal{KR}^{2k+1} &:= \operatorname{span}\big\{\mathrm{y}, f_{\alpha_1}(\mathcal{A})\mathrm{y}, \mathcal{A}y, f_{\alpha_2}(\mathcal{A}), \mathcal{A}^2y, \dots, f_{\alpha_k}(\mathcal{A})\mathrm{y}, \mathcal{A}^k y\big\}.\end{aligned}$$

Hence,

$$\mathcal{KR}^n = \begin{cases}\mathcal{R}^k \cup \mathcal{K}^k & n = 2k,\\ \mathcal{R}^k \cup \mathcal{K}^{k+1} & n = 2k+1.\end{cases}$$

Thus, we mix the ordinary and the rational Krylov spaces. The reason for this is the sparsity of the system matrix; cf. Theorem 2.8. For an odd iteration index $n = 2k+1$, we add an element from the ordinary Krylov space $\mathcal{K}$. We refer to this as "Krylov step". For an even $n = 2k$, we add an element from the rational Krylov space, and we refer to such an iteration index as "rational step".

We can now state the various approximate solutions of the different methods in a common framework: The n-th iteration of the CGNE method is uniquely defined [17, 28] as

$$x_{\mathcal{K},n} := \operatorname*{argmin}_{x\in\mathcal{K}^n} \|Ax - y\|. \tag{2.3}$$

The acceleration method of [10] computes

$$x_{\mathcal{R},n} := \operatorname*{argmin}_{x\in\mathcal{R}^n} \|Ax - y\|. \tag{2.4}$$

In analogy to the above, we define the approximate solution that is computed in this paper by

$$x_{\mathcal{KR},n} := \operatorname*{argmin}_{x\in\mathcal{KR}^n} \|Ax - y\|. \tag{2.5}$$

Algorithm 3 below provides a recursive method, called RatCG, that computes these minimizers recursively. The superiority of the mixed spaces (2.5) over (2.4) lies in the obtained sparse matrix structure. The advantage over the pure Krylov method $x_{\mathcal{K},n}$ is in the additional inclusion of the x_{α_i} into the basis.

2.1. Some rational representation. Before we develop the method, we study some well-known representations of the Krylov spaces by rational functions: Note that the above-defined spaces $\mathcal{R}^n, \mathcal{K}^n, \mathcal{KR}^n$ could all be treated in one common framework as being rational Krylov spaces, where the usual Krylov spaces are obtained by setting $\alpha \to \infty$. For the sake of comparison, however, we develop the representation for the three spaces separately.

Denote by $\mathcal{P}^n$ the space of all polynomials of degree less than n. (We denote by $\lfloor . \rfloor$ the floor function, i.e., the rounding to the next smaller integer). The following representation

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of the spaces by rational functions is well known and was obtained by Ruhe [47]; see also, e.g., [2, 14, 25, 26]:

PROPOSITION 2.1. *The Krylov spaces defined above have the following representation:*

$$\begin{aligned}
\mathcal{K}^n &= p_{n-1}(\mathcal{A})\mathrm{y}, && && p_{n-1}\in\mathcal{P}^{n-1},\\
\mathcal{R}^n &= r_{n-1}(\mathcal{A})\mathrm{y}, && r_n(x)=\frac{p_{n-1}(x)}{\Pi_{i=1}^n(x+\alpha_i)}, && p_{n-1}\in\mathcal{P}^{n-1},\\
\mathcal{KR}^n &= s_{n-1}(\mathcal{A})\mathrm{y}, && s_{n-1}(x)=\frac{p_{n-1}(x)}{\Pi_{i=1}^k(x+\alpha_i)}, && p_{n-1}\in\mathcal{P}^{n-1}, k=\lfloor\frac{n}{2}\rfloor.
\end{aligned}$$

For each of the above Krylov spaces, we define the residual spaces of the normal equations (recall our notation $\mathcal{A}x-\mathrm{y}=A^*Ax-A^*y$):

$$\mathcal{Q}_{\mathcal{X}} := \operatorname{span}\{\mathcal{A}x-\mathrm{y}|x\in\mathcal{X}\},\qquad \mathcal{X}\in\{\mathcal{K}^n,\mathcal{R}^n,\mathcal{KR}^n\}. \tag{2.6}$$

Let $\mathcal{P}_1^n$ be the space of polynomials $p_n(x)$ of degree at most n that satisfy

$$p_n(0)=1.$$

In a similar way as before, the representations for the residuals is valid:

PROPOSITION 2.2. *Let $\mathcal{Q}_{\mathcal{K}^n}$. $\mathcal{Q}_{\mathcal{R}^n}$, $\mathcal{Q}_{\mathcal{KR}^n}$ be the residual spaces in (2.6). Then*

$$\begin{aligned}
\mathcal{Q}_{\mathcal{K}^n} &= p_n(\mathcal{A})\mathrm{y}, && && p_n\in\mathcal{P}_1^n,\\
\mathcal{Q}_{\mathcal{R}^n} &= r_n(\mathcal{A})\mathrm{y}, && r_n(x)=\frac{p_n(x)}{\Pi_{i=1}^n(\frac{x}{\alpha_i}+1)}, && p_n\in\mathcal{P}_1^n,\\
\mathcal{Q}_{\mathcal{KR}^n} &= s_n(\mathcal{A})\mathrm{y}, && s_n(x)=\frac{p_n}{\Pi_{i=1}^k(\frac{x}{\alpha_i}+1)}, && p_n\in\mathcal{P}_1^n, k=\lfloor\frac{n}{2}\rfloor.
\end{aligned}$$

A consequence is the following useful result: Let $n=2k$, i.e., a rational step. Then

$$(\mathcal{A}+\alpha_k I)^{-1}\mathcal{Q}_{\mathcal{KR}^{n-1}}\subset\mathcal{KR}^n,\qquad (\mathcal{A}+\alpha_k I)^{-1}\mathcal{KR}^{n-1}\subset\mathcal{KR}^n. \tag{2.7}$$

For a Krylov step $n=2k+1$ we have

$$\mathcal{A}\mathcal{Q}_{\mathcal{KR}^{n-1}}\subset\mathcal{KR}^n,\qquad \mathcal{AKR}^{n-1}\subset\mathcal{KR}^n.$$

Note that the same representation holds for the least-squares residual $Ax-y$ but with $\mathcal{A}$ replaced by $\overline{\mathcal{A}}$ (cf. Definition 2.1) and y replaced by y. This follows since

$$Af(\mathcal{A})\mathrm{y}-y=(\overline{\mathcal{A}}f(\overline{\mathcal{A}})-1)y.$$

As a further consequence, we can bound the residual for the various rational Krylov methods by that of the standard Krylov methods:

THEOREM 2.3. *Let $x_{\mathcal{K},n}$, $x_{\mathcal{R},n}$, and $x_{\mathcal{KR},n}$ be defined as in (2.3), (2.4), and (2.5), respectively. Then,*

$$\|Ax_{\mathcal{R},n}-y\|\le\|Ax_{\mathcal{KR},n}-y\|\le\|Ax_{\mathcal{K},n}-y\|,$$

and

$$\|Ax_{\mathcal{K},n}-y\|\le\Pi_{i=1}^k\left(\tfrac{\|\overline{\mathcal{A}}\|}{\alpha_i}+1\right)\|Ax_{\mathcal{KR},n}-y\|\le\Pi_{i=1}^n\left(\tfrac{\|\overline{\mathcal{A}}\|}{\alpha_i}+1\right)\|Ax_{\mathcal{R},n}-y\|.$$

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Proof. We have with the notation in Proposition 2.2 and by the definition of $x_{\mathcal{K},n}$,

$$\begin{aligned}\|Ax_{\mathcal{R},n} - y\| &= \inf_{p_n \in \mathcal{P}_1^n} \|\Pi_{i=1}^n (\tfrac{\overline{\mathcal{A}}}{\alpha_i} + I)^{-1} p_n(\overline{\mathcal{A}}) y\| \\ &\le \Pi_{i=1}^n \|(\tfrac{\overline{\mathcal{A}}}{\alpha_i} + I)^{-1}\| \inf_{p_n \in \mathcal{P}_1^n} \|p_n(\overline{\mathcal{A}}) y\| \\ &\le \inf_{p_n \in \mathcal{P}_1^n} \|p_n(\overline{\mathcal{A}}) y\| = \|Ax_{\mathcal{K},n} - y\|.\end{aligned}$$

The result for $x_{\mathcal{KR},n}$ is obtained in a similar way and so are the opposite directions of the estimates. ∎

Hence, the rational methods are always better with respect to the residual than any ordinary Krylov space method. As a further immediate consequence, it follows that n-dimensional least-squares problems (or more general, any n-dimensional symmetric positive definite linear problem) can be solved by rational Krylov method in at most n steps, assuming exact arithmetic. In fact, since $\|Ax_{\mathcal{K},n} - y\|$ vanishes after at most n steps, we obtain:

COROLLARY 2.4. *Let $\mathcal{A} \in \mathbb{R}^{n\times n}$ be symmetric positive definite, and let $x \in \mathbb{R}^n$ be the solution of $\mathcal{A}x = \mathrm{y}$ for some $\mathrm{y} \in \mathbb{R}^n$. Then in at most n steps we have $x_{\mathcal{R},n} = x$ and $x_{\mathcal{KR},n} = x$.*

Note that this result does of course not hold for ordinary Tikhonov regularization with parameter search, where a stopping criterion is tested with various x_{α_i} for different parameters α_i: even in the discrete case with an unpleasant choice of the α_i, there is no upper bound for the number of Tikhonov regularizations to be solved. Neither does this result hold for iterative Tikhonov regularization, whose solutions are also in $\mathcal{R}$ but usually terminate not finitely for exact data.

As for the Krylov methods, we have to take care of the (rare) occasion of a breakdown:

DEFINITION 2.5. *Let $\mathcal{X}$ be any of the Krylov spaces $\mathcal{X} \in \{\mathcal{K}^n, \mathcal{R}^n, \mathcal{KR}^n\}$. We say that the respective space $\mathcal{X}$ does not break down at step n if*

$$\dim \mathcal{X} = n.$$

The criterion for breakdown is well-known in the Krylov space case and can be extend to the rational cases. The next proposition follows from [47, Section 4]; see, also [3, Eq. (2.1)].

PROPOSITION 2.6. *Let n_{bd} be the smallest iteration number where one of the Krylov spaces $\mathcal{X} \in \{\mathcal{K}^n, \mathcal{R}^n, \mathcal{KR}^n\}$ breaks down, i.e., $n_{bd} - 1 = \dim \mathcal{X} < n_{bd}$. Then $n = n_{bd}$ if and only if y can be written as a linear combination of $n-1$ eigenvectors of $\mathcal{A}$.*

2.2. Arnoldi method and Arnoldi relation. We now construct an orthonormal basis for $\mathcal{KR}^n$ by orthonormalizing the basis elements in the definition by a (modified) Gram–Schmidt method, which yields a pentadiagonal representation of the operator $\mathcal{A}$. The method is stated in Algorithm 1. For the usual case $\mathcal{K}^n$ this is exactly the standard Arnoldi method. For the rational case, Algorithm 1 has been introduced by Ruhe [47]. Let us stress that in this method and as proposed by Ruhe [47], the next element in the Krylov space $\mathcal{KR}$ is given by either $(\mathcal{A} + \alpha_k I)^{-1} q_{i-1}$ or $\mathcal{A} q_{i-1}$ and not—as one would at first guess by the definition of $\mathcal{KR}$—by $(\mathcal{A} + \alpha_k I)^{-1}\mathrm{y}$ or $\mathcal{A}^k \mathrm{y}$.

We have written the algorithm with a usual Gram–Schmidt orthgonalization, but the modified Gram–Schmidt method is suited as well (and recommended) since they are mathematically equivalent, but the latter is numerically more stable.

The algorithm is *well-defined* as long as $\|\tilde{q}_i\| \neq 0$ such that the normalization step can be performed [47, 48, 49, 50]:

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Algorithm 1 Arnoldi method for $\mathcal{KR}$.

1: $q_1 := \frac{y}{\|y\|}$
2: **for** $i = 1 \dots N$ **do**
3: $v_i = \begin{cases} (\mathcal{A} + \alpha_k I)^{-1} q_{i-1} & n = 2k \\ \mathcal{A} q_{i-1} & n = 2k+1 \end{cases}$
4: $\tilde{q}_i := v_i - \sum_{j=1}^{j-1} \langle v_i, q_j \rangle q_j$ # Gram–Schmidt step
5: $q_i = \frac{\tilde{q}_i}{\|\tilde{q}_i\|}$ # normalization step
6: **end for**

PROPOSITION 2.7. *The iterations in Algorithm 1 are well defined as long as the Krylov space $\mathcal{KR}$ does not break down up to dimension $n \le N$. Moreover, in this case, the vectors $(q_i)_{i=1}^n$ build an orthonormal basis for $\mathcal{KR}^n$.*

The main motivation for mixed rational Krylov spaces, in contrast to rational ones, is the sparse representation of the system matrix in the $\mathcal{KR}$-basis: The following structure result has been stated explicitly by Pranić and Reichel and coworkers [43, 44, 45]. It is based on orthogonality relations of rational functions; see, e.g., [11, Chpt. 11], [9, 12].

THEOREM 2.8. *Assume that the Arnoldi method in Algorithm 1 does not break down up to an index N yielding the orthogonal basis q_i. Then the matrix*

$$T_{i,j} := \langle q_i, \mathcal{A} q_j \rangle_{i,j=1,N}$$

is pentadiagonal and satisfies

$$\begin{aligned} T_{m,2k} &= 0 \quad \text{for } m = 2k+2, \dots, N, \\ T_{m,2k+1} &= 0 \quad \text{for } m = 2k+3, \dots, N. \end{aligned}$$

As an illustration, the matrix T has the following form. Denote by $Q_n : \mathbb{R}^n \to \mathcal{X}$ the following operator that produces linear combinations of the vectors q_i:

$$Q_n = [q_1 \cdots q_n]. \tag{2.8}$$

Then the resulting matrix T has the following structure (compare [44, Eq. (2.18)]):

$$T = Q_n^T \mathcal{A} Q_n = \begin{bmatrix} \kappa_1 & \beta_2 & \gamma_3 & & & & & \\ \beta_2 & \kappa_2 & \beta_3 & & & & & \\ \gamma_3 & \beta_3 & \kappa_3 & \beta_4 & \gamma_5 & & & \\ & & \beta_4 & \kappa_4 & \beta_5 & & & \\ & & \gamma_5 & \beta_5 & \kappa_5 & \beta_6 & \gamma_7 & \\ & & & & \beta_6 & \kappa_6 & \beta_7 & \\ & & & & \gamma_7 & \beta_7 & \kappa_7 & \dots \\ & & & & & \dots & \dots & \dots \end{bmatrix}. \tag{2.9}$$

That is, a pentadiagonal matrix with zeros in the second diagonal at even indices. One may as well view this as a block-tridiagonal matrix consisting of 2×2 blocks with rank-1 off-diagonal blocks.

We note that a corresponding representation can also be established for the non-symmetric case [45], where the matrix T has generalized Hessenberg form with several subdiagonals; see, e.g., equation (18) ibid. This sparse structure is the main motivation for the mixed rational Krylov spaces; adding elements of the ordinary Krylov space $\mathcal{K}$ creates zeros below the subdiagonals. On the contrary, the representation in the pure rational space $\mathcal{R}$ is usually full.

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2.3. The rational Lanczos method. Based on the Arnoldi relations, we can now solve the least-squares problem by exploiting the structure of T. The algorithmic steps are determined by the previous results: At first compute an orthogonal basis by the Arnoldi method, Algorithm 1. Secondly, in this basis, the normal equations are given by a pentadiagonal matrix by Theorem 2.8, which can be solved recursively. As a result we obtain the rational Lanczos method, which is the analogue of the usual Lanczos method for "ordinary" Krylov space methods for solving linear equations [52, Chpt. 6.7]. The latter method is based on a tridiagonal structure and leads to a three-term recursion, which can be considered a precursor of the CG method; see [52]. The rational method in this section is essentially identical to that of Pranić and Reichel [43, 44, 45] (see also [25, 26]), although there the recursion for the pentadiagonal matrix has not been elaborated. The result in this section serve as a preliminary study for the rational CG method in Section 3.

For simplicity of notation we now assume a finite-dimensional case with $\mathcal{A}$ given by a symmetric $N \times N$ matrix and y a given vector in $\mathbb{R}^N$. Let e_n be the standard basis vectors with 1 at position n and zero elsewhere

$$e_n := (0, \dots, 0, 1, 0, \dots 0)^T.$$

Assume that the Arnoldi method does not break down up to the index N. We define the matrix (respectively operators)

$$T_n = Q_n^T \mathcal{A} Q_n = (T_{i,j})_{i,j=1,n},$$

with Q_n from (2.8), and we set $Q = Q_N$. It follows that

$$Q^T \mathrm{y} = \beta e_1,$$

where e_1 is the first unit vector and $\beta \in \mathbb{R}$.

Recall the pentadiagonal structure of T_n; we denote the scalar entries by the Greek letters

$$\beta_n, \gamma_n, \kappa_n$$

as follows: In case of a rational step $n = 2k$:

$$T_n = \begin{bmatrix} T_{n-1} & \begin{matrix} 0 \\ \beta_n \end{matrix} \\ \begin{matrix} 0 & \beta_n \end{matrix} & \kappa_n \end{bmatrix}. \tag{2.10}$$

In case of a Krylov step $n = 2k+1$ we have

$$T_n = \begin{bmatrix} & & 0 \\ & T_{n-1} & \gamma_n \\ & & \beta_n \\ 0 & \gamma_n & \beta_n & \kappa_n \end{bmatrix} = \begin{bmatrix} & T_{n-2} & & 0 & 0 \\ & & & \beta_{n-1} & \gamma_n \\ 0 & \beta_{n-1} & & \kappa_{n-1} & \beta_n \\ 0 & \gamma_n & & \beta_n & \kappa_n \end{bmatrix}. \tag{2.11}$$

Algorithm 2 requires two iterates x_n, p_n in the original Hilbert space X (more precisely in $\mathcal{KR}$) and their coefficients $c_n, d_n \in \mathbb{R}^n$.

By orthogonality, the normal equation $\mathcal{A}x = \mathrm{y}$ translates to $Tc = \beta e_1$, where $x = Qc$. Finding the least-squares minimizer x_n in the Krylov space $\mathcal{KR}^n$ translates to $Q_n^T \mathcal{A} x_n = Q_n^T \mathrm{y}$ or

$$T_n c_n = \beta e_1 \qquad \text{with} \qquad x_n = Q_n c_n. \tag{2.12}$$

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To obtain a recursion, as in [52, Chpt. 6.7] for the usual Lanczos method, we define an additional coefficient vector d_n for p_n:

$$T_n d_n := e_n \qquad p_n = Q_n d_n. \tag{2.13}$$

By recursively solving the pentadiagonal structure, we obtain the following recursion:

PROPOSITION 2.9. *Let x_n be the least-squares solution in the mixed Krylov space $\mathcal{KR}^n$. Let $\beta_n, \gamma_n, \kappa_n$ be the entries of T_n as above. Let Q_n, p_n, q_n be defined above. Then the following recursion holds:*

$$x_n = x_{n-1} + \xi_n p_n, \tag{2.14}$$

$$p_n = \begin{cases} \sigma_n p_{n-1} + \tau_n q_n & n = 2k, \\ \sigma_n p_{n-1} + \eta_n p_{n-2} + \tau_n q_n & n = 2k+1, \end{cases} \tag{2.15}$$

where the scalars $\tau_n, \sigma_n, \eta_n \in \mathbb{R}$ satisfy

Case $n = 2k$:

$$\begin{aligned} \xi_n &= -\beta_n x_{n-1}^T q_{n-1}, \\ \begin{bmatrix} \tau_n \\ \sigma_n \end{bmatrix} &= \begin{bmatrix} 1 & \beta_n \\ \beta_n \tau_{n-1} & \gamma_n \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \end{aligned} \tag{2.16}$$

Case $n = 2k+1$

$$\begin{aligned} \xi_n &= -\gamma_n x_{n-1}^T q_{n-2} - \beta_n x_{n-1}^T q_{n-1}, \\ \begin{bmatrix} \sigma_n \\ \tau_n \\ \eta_n \end{bmatrix} &= \begin{bmatrix} 0 & \gamma_n & 1 \\ 1 & \beta_n & \tau_{n-2}\beta_{n-1} \\ \beta_n \tau_{n-1} + \gamma_n \sigma_{n-1} \tau_{n-2} & \kappa_n & \tau_{n-2}\gamma_n \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \end{aligned} \tag{2.17}$$

Proof. We use the following notation: For a coefficient vector $g_n \in \mathbb{R}^n$ we denote by $g_{n;k}$ its k-th entry. To start the proof, we verify that the following recursion with some $\xi_n \in \mathbb{R}$ is valid:

$$c_n = \begin{bmatrix} c_{n-1} \\ 0 \end{bmatrix} + \xi_n d_n. \tag{2.18}$$

Applying Q_n to this identity then leads to the x_n-recursion (2.14).

Indeed, in case of a rational step $n = 2k$, we plug in (2.18) into (2.12). Noting that $T_{n-1}c_{n-1} = \beta e_1$ and $T_n d_n = e_n$, yields

$$\begin{bmatrix} 0 \\ \beta_n c_{n-1;n-1} \end{bmatrix} + \xi_n e_n = 0,$$

which leads to $\xi_n = -\beta_n c_{n-1;n-1} = -\beta_n c_{n-1}^T e_{n-1}$, and by the orthogonality of Q_n translates to the formula for ξ_n.

In case of a Krylov step, $n = 2k+1$ (with $n > 1$), we similarly use the equation $T_n c_n = \beta e_n$, and, noting $T_n d_n = e_n$, we obtain the condition

$$\xi_n = -\gamma_n c_{n-1;n-2} - \beta_n c_{n-1;n-1} = -\gamma_n c_{n-1}^T e_{n-2} - \beta_n c_{n-1}^T e_{n-1}.$$

This gives the second formula for ξ_n.

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In the next step, we derive a recursion for d_n, which leads to that for p_n. Assume again a rational step $n = 2k$. Note that d_n is a vector in $\mathbb{R}^n$. We verify that numbers $\sigma_n, \tau_n \in \mathbb{R}$ exists such that

$$d_n = \sigma_n \begin{bmatrix} d_{n-1} \\ 0 \end{bmatrix} + \tau_n e_n, \qquad \text{i.e.,} \qquad d_n = \begin{bmatrix} * \\ \sigma_n \tau_{n-1} \\ \tau_n \end{bmatrix}.$$

The defining equation for d_n, (2.13), yields the condition for τ_n, σ_n (noting (2.10) and that $T_{n-1} d_{n-1} = e_{n-1}$)

$$\begin{bmatrix} 0 \\ \sigma_n \\ \sigma_n \beta_n d_{n-1;n-1} \end{bmatrix} + \tau_n \begin{bmatrix} 0 \\ \beta_n \\ \kappa_n \end{bmatrix} = e_n,$$

which can be resolved to the formula (2.16) (recall that $d_{n-1;n-1} = \tau_{n-1}$).

In a Krylov step $n = 2k + 1$, the recursion for d_n is now more involved as we need a two-step recursion. Indeed, we make the ansatz

$$d_n = \sigma_n \begin{bmatrix} d_{n-1} \\ 0 \end{bmatrix} + \tau_n e_n + \eta_n \begin{bmatrix} d_{n-2} \\ 0 \\ 0 \end{bmatrix}, \quad \text{i.e.,} \quad d_n = \begin{bmatrix} \eta_n \tau_{n-2} \\ \sigma_n \tau_{n-1} \\ \tau_n \end{bmatrix},$$

with parameter σ_n, η_n, τ_n, and plug this into (2.13). The last three rows yield a linear equation for the coefficients σ_n, τ_n, η_n:

$$\sigma_n \begin{bmatrix} 0 \\ 1 \\ \beta_n d_{n-1;n-1} + \gamma_n d_{n-1;n-2} \end{bmatrix} + \tau_n \begin{bmatrix} \gamma_n \\ \beta_n \\ \kappa_n \end{bmatrix} + \eta_n \begin{bmatrix} 1 \\ d_{n-2;n-2} \beta_{n-1} \\ d_{n-2;n-2} \gamma_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix},$$

which leads to (2.17) . □

The recursion starts at $n = 1$ by a direct calculation of

$$x_1 = \frac{\langle \mathrm{y}, \mathrm{y} \rangle}{\langle \mathcal{A}\mathrm{y}, \mathrm{y} \rangle} \mathrm{y}, \qquad q_1 = \frac{\mathrm{y}}{\|\mathrm{y}\|}, \qquad \tau_1 = \frac{\langle \mathrm{y}, \mathrm{y} \rangle}{\langle \mathcal{A}\mathrm{y}, \mathrm{y} \rangle}, \qquad p_1 = \tau_1 q_1.$$

We note that the rational step above for p_n is valid for $n = 2$. Also, the 2×2 matrix in the calculation of τ_n, σ_n can easily be inverted leading to the formulae

$$\tau_n = \frac{1}{\kappa_n - \beta_n^2 \tau_{n-1}}, \qquad \sigma_n = -\tau_n \beta_n.$$

The full method for calculating least-squares solutions in $\mathcal{KR}$ is now presented in Algorithm 2 as a pseudo-Matlab code. The routine GramSchmid(v, Q) there means an orthgonalization *and* normalization step as in the calculation of q_i via $\tilde{q}_i$ in the Arnoldi method in Algorithm 1.

This algorithm is the implementation of the formulas defined above, and it is well-defined as long as the Krylov space $\mathcal{KR}$ does not break down. The involved divisions or matrix inversions (e.g., M^{-1}) are well-defined in case of non-breakdown in exact arithmetic because T_n is then always invertible, and the formulas are derived from solving (2.13).

As in the standard case for $\mathcal{K}$, the iterations of Algorithm 2 satisfy certain orthogonality relations:

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Algorithm 2 Lanczos Algorithm for $\mathcal{KR}$.

$\mathcal{A} = A^*A$, $\mathrm{y} = A^*y$
$\tau = \frac{\langle \mathrm{y},\mathrm{y}\rangle}{\langle \mathcal{A}\mathrm{y},\mathrm{y}\rangle}$, $Q(:,1) = \frac{\mathrm{y}}{\|\mathrm{y}\|}$, $p = \tau Q(:,1)$, $x = \frac{\langle \mathrm{y},\mathrm{y}\rangle}{\langle \mathcal{A}\mathrm{y},\mathrm{y}\rangle}\mathrm{y}$
for $n = 2 \ldots \mathrm{MAXIT}$ **do**
  if n is even **then** # Rational step
    $k := \frac{n}{2}$
    $v = (\mathcal{A} + \alpha_k I)^{-1} Q(:, n-1)$
    $q = \mathrm{GramSchmid}(v, Q)$ (by Algorithm 1)
    $Q(:,n) = q$
    $\kappa = q^T \mathcal{A} q$, $\beta = Q(:,n-1)^T \mathcal{A} q$ # Entries of T
    $\tau_{old} = \tau$
    $\tau = 1/(\kappa - \tau\beta^2) \quad \sigma = -\tau\beta$ # Coef. for p rec.
    $p_{old} = p$
    $p = \sigma p + \tau q$ # Update p
    $\xi = -\beta x^T Q(:,n-1)$ # Coef. for x rec.
    $x = x + \xi p$ # Update x
  else # Krylov step
    $v = \mathcal{A} Q(:,n-1)$
    $q = \mathrm{GramSchmid}(v, Q)$
    $Q(:,n) = q$
    $\beta_{old} = \beta$
    $\kappa = q^T \mathcal{A} q$,
    $\beta = Q(:,n-1)^T \mathcal{A} q$, # T-Entries
    $\gamma = Q(:,n-2)^T \mathcal{A} q$
    $M = \begin{bmatrix} 0 & \gamma & 1 \\ 1 & \beta & \tau_{old}\beta_{old} \\ \beta\tau + \gamma\sigma\tau_{old} & \kappa & \tau_{old}\gamma \end{bmatrix}$
    $\tau_{old} = \tau$
    $\begin{bmatrix} \sigma \\ \tau \\ \eta \end{bmatrix} = M^{-1} \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$ # Coef. for p rec.
    $p_{new} = \sigma p + \eta p_{old} + \tau Q(:,n)$ # Update p
    $p_{old} = p$
    $p = p_{new}$
    $\xi = -\gamma x^T Q(:,n-2) - \beta x^T Q(:,n-1)$ # Coef. for x rec.
    $x = x + \xi p$ # Update x
  end if
end for

PROPOSITION 2.10. *Define $p_n := p$ in Algorithm 2 at iteration n. Then*

$$\langle \mathcal{A} p_n, p_k \rangle = 0 \qquad \text{for } n \neq k.$$

Proof. Note that by construction $p_n = Q_n T_n^{-1} e_n$. Since $T_n = Q_n^T \mathcal{A} Q_n$, we have that $Q_n^T \mathcal{A} Q_n d_n = e_n$ and hence $Q_n^T \mathcal{A} p_n = e_n$. As a consequence we have the relation $\mathcal{A} p_n = q_n + \mathrm{span}\{q_j, j > n\}$. Thus, for $k < n$,

$$\langle \mathcal{A} p_n, p_k \rangle = \langle q_n + \mathrm{span}\{q_j, j > n\}, p_k \rangle = 0$$

since $p_k \in \mathrm{span}\{q_1, \ldots, q_k\}$ and the orthogonality of the q_i holds. By symmetry, the results holds also for $k > n$. ∎

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This means that the matrix $\langle \mathcal{A}p_i, p_j \rangle$, $i, j = 1 \ldots, N$, is diagonal.

PROPOSITION 2.11. *Consider the residual for the normal equations*

$$r_n = \mathcal{A}x_n - \mathrm{y}$$

for the iterations $x_n = x$ in Algorithm 2 at iteration n. The Gramian matrix for the residual vectors has the following nonzero entries:

$$R_{i,j} := \langle r_i, r_j \rangle = \begin{bmatrix} * & * & & & & & \\ * & * & & & & & \\ & & * & * & & & \\ & & * & * & & & \\ & & & & * & * & \\ & & & & * & * & \end{bmatrix},$$

i.e., it is tridiagonal with additional zeros in the lower off-diagonals for even and in the upper off-diagonal for odd indices. Moreover, we have

$$\langle r_n, p_i \rangle = 0, \quad \textit{for all } i = 1, \ldots, n. \tag{2.19}$$

Proof. Let $\tilde{c}_n \in \mathbb{R}^N$ be a vector with values c_n at position $1, \ldots, n$ and 0 at the rest. By the structure (2.9), (2.10), (2.11), it follows for a rational step that

$$\tilde{r}_n := T\tilde{c}_n - \beta e_1 = \beta_{n+1} e_{n+1}, \qquad \text{for } n = 2k, \tag{2.20}$$

while in a Krylov step

$$\tilde{r}_n := T\tilde{c}_n - \beta e_1 = \beta_{n+1} e_{n+1} + \gamma_{n+2} e_{n+1}, \qquad \text{for } n = 2k+1. \tag{2.21}$$

Thus, in case of $n = 2k$, $\tilde{r}_n^T \tilde{r}_{n+1} = 0$, which results in the 0 in the first off-diagonals. In any case we have $\tilde{r}_n^T \tilde{r}_{n+k} = 0$ for $k \geq 2$. The claimed matrix structure is now verified by the observation that $r_n = Q\tilde{r}_n$ and the orthogonality of Q.

Identity (2.19) follows since d_i is a vector of length i, hence $p_i \in \mathcal{KR}^i$, while $\tilde{r}_n$ has zero entries in the first n components. Thus r_n is orthogonal to $\mathcal{KR}^n$ and hence to all p_i. ∎

3. The rational CG method. The disadvantage of the previous Lanczos method in Algorithm 2 is that the orthogonal vectors q_i have to be saved, and thus the memory requirement might get large. A second drawback is that the orthogonalization might become contaminated by rounding errors and thus inexact.

In this section we state an equivalent algorithm that avoids saving the q_i and the Gram–Schmidt orthogonalization, and it is directly based on one- and two-step recurrence relations for the vectors p_n and x_n (the x_n have the same meaning as in the previous section while the p_n can differ by a scalar). The derivation is analogous to (but more involved than) the derivation of the CG method from the D-Lanczos method from the orthogonality relations; cf. [52, Section 6.7].

We consider the iteration (2.14), (2.15): First consider (2.14): Assume that p_n has been computed, and denote by r_n the residual $\mathcal{A}x_n - \mathrm{y}$. Then

$$x_n = x_{n-1} + \xi_n p_n \Rightarrow r_n = r_{n-1} + \xi_n \mathcal{A}p_n.$$

According to (2.19), we require that r_n is orthogonal to p_n, hence

$$\xi_n = -\frac{\langle r_{n-1}, p_n \rangle}{\langle \mathcal{A}p_n, p_n \rangle}. \tag{3.1}$$

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Next we focus on the iterations for p_n. Rewriting it without usage of the q_i is not so difficult for a Krylov step: Let $n = 2k+1$, and consider (2.15). It follows from (2.20) (after multiplying with Q) that $r_{n-1} \sim q_n$. Thus, the recursion (2.15) for $n = 2k+1$ can be replaced by

$$p_n = \sigma_n p_{n-1} + \eta_n p_{n-2} + \tau_n' r_{n-1},$$

where r_{n-1} is the residual of the previous step and τ_n' is some constant (possibly different from τ_n). To fix the constants, we observe from (3.1) that p_n may be rescaled by a multiplicative constant without changing the method. Thus we set $\tau_n' = 1$. The other constants are obtained by forcing the orthogonality relations $\langle \mathcal{A}p_i, p_j \rangle \sim \delta_{ij}$ to hold. This yields the iteration for a Krylov step, i.e., $n = 2k+1$:

$$p_n = -\frac{\langle r_{n-1}, \mathcal{A}p_{n-1}\rangle}{\langle \mathcal{A}p_{n-1}, p_{n-1}\rangle} p_{n-1} - \frac{\langle r_{n-1}, \mathcal{A}p_{n-2}\rangle}{\langle \mathcal{A}p_{n-2}, p_{n-2}\rangle} p_{n-2} + r_{n-1}. \tag{3.2}$$

The recursion for a rational step $n = 2k$ is more involved. Considering (2.15), $n = 2k$, the problem is that q_n does not have a simple expression in terms of residuals. However, by (2.21), (2.20), it may be written as a linear combination of r_n and r_{n-1}. From (2.14) it follows that $r_n = r_{n-1} - \xi_n \mathcal{A}p_n$. Thus p_n can be written as linear combination of p_{n-1}, r_{n-1}, and an implicit term $\mathcal{A}p_n$. Keeping in mind (2.7) and that p_n should represent an element in $\mathcal{KR}^n$ leads to idea that the factor in front of $\mathcal{A}p_n$ should be an $-\alpha_k^{-1}$. Thus, the form of the rational step should be (again using one rescaling degree of freedom for the factor in front of r_{n-1})

$$p_n = (\mathcal{A} + \alpha_k I)^{-1} \left[\rho_n p_{n-1} + r_{n-1}\right].$$

It remains to fix the factor ρ_n, which is obtained through the orthogonality relations as before. Putting the operator $(\mathcal{A} + \alpha_k I)$ on the right-hand side yields

$$\langle (\mathcal{A} + \alpha_k I) p_n, p_{n-1}\rangle = \rho_n \langle p_{n-1}, p_{n-1}\rangle + \langle r_{n-1}, p_{n-1}\rangle. \tag{3.3}$$

Thus, requiring $\langle \mathcal{A}p_n, p_{n-1}\rangle = 0$ and $\langle r_{n-1}, p_{n-1}\rangle = 0$ leads to

$$\rho_n = \frac{\alpha_k \langle p_n, p_{n-1}\rangle}{\langle p_{n-1}, p_{n-1}\rangle} = \frac{\alpha_k \langle (\mathcal{A} + \alpha_k I)^{-1}[\rho_n p_{n-1} + r_{n-1}], p_{n-1}\rangle}{\langle p_{n-1}, p_{n-1}\rangle},$$

which gives

$$\begin{aligned} \rho_n &= \frac{\alpha_k \langle (\mathcal{A} + \alpha_k I)^{-1} p_{n-1}, r_{n-1}\rangle}{\langle p_{n-1}, p_{n-1}\rangle - \alpha_k \langle (\mathcal{A} + \alpha_k I)^{-1} p_{n-1}, p_{n-1}\rangle} \\ &= \frac{\alpha_k \langle (\mathcal{A} + \alpha_k I)^{-1} p_{n-1}, r_{n-1}\rangle}{\langle \mathcal{A}p_{n-1}, (\mathcal{A} + \alpha_k I)^{-1} p_{n-1}\rangle}. \end{aligned} \tag{3.4}$$

Another equivalent formula for ρ_n is as follows:

$$\begin{aligned} \rho_n &= \frac{\langle [\mathcal{A} + \alpha_k - \mathcal{A}] p_{n-1}, (\mathcal{A} + \alpha_k I)^{-1} r_{n-1}\rangle}{\langle \mathcal{A}p_{n-1}, (\mathcal{A} + \alpha_k I)^{-1} p_{n-1}\rangle} \\ &= \frac{\langle p_{n-1}, r_{n-1}\rangle - \langle \mathcal{A}p_{n-1}, (\mathcal{A} + \alpha_k I)^{-1} r_{n-1}\rangle}{\langle \mathcal{A}p_{n-1}, (\mathcal{A} + \alpha_k I)^{-1} p_{n-1}\rangle} \\ &= -\frac{\langle \mathcal{A}p_{n-1}, (\mathcal{A} + \alpha_k I)^{-1} r_{n-1}\rangle}{\langle \mathcal{A}p_{n-1}, (\mathcal{A} + \alpha_k I)^{-1} p_{n-1}\rangle}, \end{aligned} \tag{3.5}$$

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exploiting the orthogonality $\langle p_{n-1}, r_{n-1}\rangle = 0$.

Thus, the formula for p_n can be computed from (3.4) by the steps

$$\begin{aligned} s_n &:= (\mathcal{A}+\alpha_k I)^{-1} p_{n-1}, \\ t_n &:= (\mathcal{A}+\alpha_k I)^{-1} r_{n-1}, \\ p_n &:= \frac{\alpha_k \langle s_n, r_{n-1}\rangle}{\langle \mathcal{A}p_{n-1}, s_n\rangle} s_n + t_n. \end{aligned}$$

REMARK 3.1. The computation of p_n in a rational step thus requires solving for s_n and t_n, i.e., two linear solves with the Tikhonov matrix $(\mathcal{A}+\alpha_k I)$, which is an overhead compared to the Lanczos method above that needs only one. Note, however, that the system matrix (Tikhonov matrix) is in both cases that same, only the right-hand sides differ. In Matlab, this can be computed by the statement

$$[s_n\ t_n] = (\mathcal{A}+\alpha_k I)\backslash[p_{n-1}\ r_{n-1}], \tag{3.6}$$

and we found that it does not require much more additional computation time. Observe that for a direct solver, the main work is in the matrix decomposition of the system matrix, which has to be performed only once per step. Using this for two right-hand sides is then negligible overhead work.

Interestingly, if one insists on using only one linear system solve with one right-hand side per step, then this can be achieved by a formula that uses complex variables. Indeed, ρ_n and the formula for p_n can be rewritten by (3.5)

$$\begin{aligned} p_n &= \frac{1}{\langle \mathcal{A}p_{n-1}, s_n\rangle}\Big[-\langle \mathcal{A}p_{n-1}, t_n\rangle s_n + \langle \mathcal{A}p_{n-1}, s_n\rangle t_n\Big] \\ &= \frac{1}{\langle \mathcal{A}p_{n-1}, s_n\rangle}\mathcal{I}\left[\langle \mathcal{A}p_{n-1}, \overline{s_n + it_n}\rangle (s_n + it_n)\right]. \end{aligned}$$

Here $\overline{s_n + it_n}$ denotes the complex conjugate, $\mathcal{I}$ is the imaginary part, and i the imaginary unit. In this formula, the common factor $\frac{1}{\langle \mathcal{A}p_{n-1}, s_n\rangle}$ can be ignored since a multiplicative factor of p_n does not change the iteration, hence the computational effort reduces to one linear solve with only one complex right-hand side. Yet, in the numerical calculations, we did not find much of a benefit of using this formula.

Finally, we are in the position to present the full rational CG algorithm. The only thing remaining open is the initial value for the p-variables, i.e., p_1. Setting $x_{-1} = 0$ and using (2.14) gives $p_1 = x$, noting the scaling freedom for the p-variables. Together, we obtain Algorithm 3 for solving the normal equations $\mathcal{A}x = \mathrm{y}$.

Let us comment about the well-definedness of the algorithm. As long as the failure criterion $\mathcal{A}p_n = 0$ is not satisfied, the fractions in the calculations are all well-defined: This is obvious for the terms $\langle \mathcal{A}p_n, p_n\rangle$, $\langle \mathcal{A}p_{\mathrm{old}}, p_{\mathrm{old}}\rangle$. The denominator $\langle \mathcal{A}p_n, s_n\rangle$ is well-defined under the non-failure condition since

$$\langle \mathcal{A}p, s_n\rangle = \langle \mathcal{A}(\mathcal{A}+\alpha_k I)s_n, s_n\rangle = \|\mathcal{A}s_n\|^2 + \alpha_k \langle \mathcal{A}s_n, s_n\rangle,$$

which is 0 if and only if $0 = \mathcal{A}s_n = (\mathcal{A}+\alpha_k I)^{-1}\mathcal{A}p$. Since $\mathcal{A}+\alpha_k I$ has no nontrivial nullspace, this can only happen if $\mathcal{A}p_n = 0$, which is excluded by the non-failure condition.

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Algorithm 3 RatCG method for $\mathcal{KR}$.

$\mathcal{A} = A^*A$, $\mathrm{y} = A^*y$
$x = \frac{\langle \mathrm{y},\mathrm{y}\rangle}{\langle \mathcal{A}\mathrm{y},\mathrm{y}\rangle}\mathrm{y}$.
$r = \mathcal{A}x - \mathrm{y}$.
$p = x$. # x_1, p_1, r_1 are defined
for $n = 2 \ldots \mathrm{MAXIT}$ **do**
  if n is even **then**
    $k := \frac{n}{2}$
    $s := (\mathcal{A} + \alpha_k I)^{-1} p$
    $t := (\mathcal{A} + \alpha_k I)^{-1} r$ # Implementation as in (3.6)
    $\zeta := -\frac{\langle \mathcal{A}r, s\rangle}{\langle \mathcal{A}p, s\rangle}$
    $p_{\mathrm{old}} = p$ # $p_{\mathrm{old}} = p_{n-1}$
    $p := \zeta s + t$ # $p = p_n$ Even case
  else
    $p = -\frac{\langle r, \mathcal{A}p\rangle}{\langle \mathcal{A}p, p\rangle} p - \frac{\langle r, \mathcal{A}p_{\mathrm{old}}\rangle}{\langle \mathcal{A}p_{\mathrm{old}}, p_{\mathrm{old}}\rangle} p_{\mathrm{old}} + r$ # $p = p_n$ Odd case
  end if
  if $\mathcal{A}p = 0$ **then**
    Terminate algorithm # Failure by Breakdown
  else
    $\eta := \frac{\langle r, p\rangle}{\langle \mathcal{A}p, p\rangle}$
    $x = x - \eta p$ # Solution x_n at step n
    $r = r - \eta \mathcal{A}p$ # Step n completed
  end if
end for

Finally, we show that the rational CG method does what it is supposed to do.

THEOREM 3.2. *Denote by x_n, p_n, r_n the respective variables x, p, r at iteration n in Algorithm 3. Then, they satisfy the orthogonality conditions*

$$\langle \mathcal{A}p_n, p_j\rangle = 0, \quad j = 1, \ldots, n-1, \qquad \textit{and} \qquad \langle r_n, p_j\rangle = 0, \qquad j = 1, \ldots, n. \tag{3.7}$$

As a result, Algorithm 3 computes at iteration n the solution to the least-squares problem in the mixed Krylov space $\mathcal{KR}^n$ (2.5).

Proof. With the notation in the theorem, at the initialization, we obviously have that $x_1, p_1 \in \mathcal{KR}^1$ and $r_1 \in \mathcal{Q}_{\mathcal{KR}^1} \subset \mathcal{KR}^2$. Suppose that $x_{n-1}, p_{n-1} \in \mathcal{KR}^{n-1}$ and $r_{n-1} \in \mathcal{Q}_{\mathcal{KR}^{n-1}} \subset \mathcal{KR}^n$. In a Krylov step, it follows immediately that $p_n \in \mathcal{KR}^n$. In a rational step we have by (2.7) that $p_n \in \mathcal{KR}^n$. Thus, in any case $x_n \in \mathcal{KR}^n$ and $r_n \in \mathcal{Q}_{\mathcal{KR}^n} \subset \mathcal{KR}^{n+1}$. By induction we have proven that

$$x_n, p_n \in \mathcal{KR}^n \qquad r_n \in \mathcal{Q}_{\mathcal{KR}^n}.$$

Next, we verify the orthogonality conditions (3.7) by induction. Assume that (3.7) holds with n replaced by $n-1$.

In a Krylov step, $n = 2k+1$, it follows by construction of the coefficients (cf. (3.2)) that

$$\langle \mathcal{A}p_n, p_j\rangle = 0, \quad j = n-1, n-2.$$

For $j < n-2$ we find by the induction hypothesis that, with some coefficients b_1, b_2 from (3.2),

$$\langle \mathcal{A}p_n, p_j\rangle = \langle b_1 p_{n-1} + b_2 p_{n-1} + r_{n-1}, \mathcal{A}p_j\rangle = \langle r_{n-1}, \mathcal{A}p_j\rangle.$$

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However, $\mathcal{A}p_j \in \mathcal{KR}^{n-1}$, thus the right-hand side vanishes by the induction hypothesis. Thus $\langle \mathcal{A}p_n, p_j \rangle \sim \delta_{n,j}$ is shown. The orthogonality of the residuals and p_j in (3.7) follows by $r_n = r_{n-1} - \eta \mathcal{A}p_n$ and by construction: Taking the inner product with p_n leads to $\langle r_n, p_n \rangle = 0$ by the definition of η, while $\langle r_n, p_j \rangle = 0$, for $j = 1, \ldots, n-1$, by the induction hypothesis and the just proven orthogonality. This settles the Krylov step case.

For a rational step $n = 2k$, it follows by construction, cf. (3.3), and the induction hypothesis for $n-1$ that

$$\langle \mathcal{A}p_n, p_{n-1} \rangle = 0.$$

Consider the equation for p_n

$$\mathcal{A}p_n + \alpha_k p_n = \rho_n p_{n-1} + r_{n-1}.$$

Taking the inner product with $\mathcal{A}p_j$, for any $1 \leq j \leq n-2$, leads to

$$\langle \mathcal{A}p_n, \mathcal{A}p_j \rangle + \alpha_k \langle p_n, \mathcal{A}p_j \rangle = 0. \tag{3.8}$$

Indeed, this follows since $\langle p_{n-1}, \mathcal{A}p_j \rangle = 0$ by the induction hypothesis, and, since we have $\mathcal{A}p_j \subset \mathcal{KR}^{n-1}$ by Theorem 2.8 and (2.9), we conclude that

$$\langle r_{n-1}, \mathcal{A}p_j \rangle = \langle r_{n-1}, \operatorname{span}\{p_1, \ldots, p_{n-1}\} \rangle = 0$$

again by the induction hypothesis. Thus, (3.8) holds.

Define the matrix/operator that maps coefficients from $\mathbb{R}^{n-1}$ to the associated linear combination of p_i, $i = 1, \ldots n-1$, which is an element in $\mathcal{KR}^{n-2}$. It can be represented by the matrix

$$P_{n-1} = [p_1 \cdots p_{n-1}],$$

It follows from (3.8) that for any coefficient vector $\vec{c} \in \mathbb{R}^{n-2}$

$$\langle \mathcal{A}p_{n-1}, \mathcal{A}P_{n-2}\vec{c} \rangle + \alpha_k \langle \mathcal{A}p_n, P_{n-2}\vec{c} \rangle = 0. \tag{3.9}$$

By Theorem 2.8 and (2.9) again it follows that $\mathcal{A}P_{n-2}\vec{c} \in \mathcal{KR}^{n-1}$, thus there exists a vector $\vec{g} \in \mathbb{R}^{n-2}$ and $g_{n-1} \in \mathbb{R}$ with

$$\mathcal{A}P_{n-2}\vec{c} = P_{n-2}\vec{g} + g_{n-1}p_{n-1} \tag{3.10}$$

since the p_i, $i = 1, \ldots, n-1$, span $\mathcal{KR}^{n-1}$. Hence, inserting this into (3.9) and noting $\langle \mathcal{A}p_n, p_{n-1} \rangle = 0$ gives

$$\langle \mathcal{A}p_n, P_{n-2}\vec{g} + \alpha_k P_{n-2}\vec{c} \rangle = 0. \tag{3.11}$$

Taking the inner product with $\mathcal{A}P_{n-2}$, we get from (3.10)

$$P_{n-2}^T \mathcal{A}\mathcal{A}P_{n-2}\vec{c} = P_{n-2}^T \mathcal{A}P_{n-2}\vec{g},$$

where we again used the induction hypothesis $\langle \mathcal{A}p_j, p_{n-1} \rangle = 0$ and where P_{n-2}^T denotes the transposed operator. The matrix on the right-hand side is invertible (in fact it is diagonal by the induction hypothesis) and nonsingular since $\mathcal{A}$ has no nontrivial nullspace on $\mathcal{KR}^{n-2}$. Thus, we can invert to find

$$\vec{g} = (P_{n-2}^T \mathcal{A}P_{n-2})^{-1} P_{n-2}^T \mathcal{A}\mathcal{A}P_{n-2}\vec{c},$$

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and inserting this into (3.11) gives

$$\langle \mathcal{A}p_n, [P_{n-2}(P_{n-2}^T\mathcal{A}P_{n-2})^{-1}P_{n-2}^T\mathcal{A}\mathcal{A}P_{n-2}\vec{c} + \alpha_k P_{n-2}\vec{c}]\rangle = 0. \tag{3.12}$$

Now for any $j \in \{1, \ldots, n-2\}$ we find a vector $\vec{c} \in \mathbb{R}^{n-2}$ such that

$$[(P_{n-2}^T\mathcal{A}P_{n-2})^{-1}P_{n-2}^T\mathcal{A}\mathcal{A}P_{n-2} + \alpha_k I]\vec{c} = e_j.$$

Indeed, this identity can be rewritten as

$$P_{n-2}^T\mathcal{A}\mathcal{A}P_{n-2} + \alpha_k(P_{n-2}^T\mathcal{A}P_{n-2})]\vec{c} = (P_{n-2}^T\mathcal{A}P_{n-2})e_j.$$

The matrix on the left-hand side is a sum of positive semidefinite and positive define matrices, hence invertible, and such a vector $\vec{c}$ exits. Inserting that into (3.12) yields

$$\langle \mathcal{A}p_n, P_{n-2}e_j\rangle = 0,$$

and thus $\langle \mathcal{A}p_n, p_j\rangle = 0$ by the definition of P_{n-2}. Hence the orthogonality for p_n is proven. The orthogonality for r_n in (3.7) follows by the induction hypothesis, the update formula for r_n, the definition of η, and the just proven orthogonality relation for p_n. Together, (3.7) is proven.

The statement that x_n is a least-squares solution in $\mathcal{KR}^n$ is a now a simple consequence of the facts that $x_n \in \mathcal{KR}^n$, that p_i span $\mathcal{KR}^n$, and the orthogonality relations for the residual, which together implies $\langle r_n, \mathcal{KR}^n\rangle = 0$. The latter is just the least-squares optimality condition in $\mathcal{KR}^n$. We also note that in case of a breakdown the same conclusion is valid as well, except that the sequence of optimal x_n saturates at the breakdown-index. If we extend the definition of the solution sequence x_n in Algorithm 3 as the last computed x_n before breakdown, then this still yields the least-squares solution even in this case. □

REMARK 3.3. Since the Lanczos iteration Algorithm 2 also computes a least-squares solution in $\mathcal{KR}^n$ and since by our assumptions the x_n are uniquely defined, it follows that the sequences x_n from Algorithm 2 and Algorithm 3 are identical in exact arithmetic. (The corresponding p_n might differ, though.)

Regularization and stopping rule. The derived Algorithms 2 and 3 and also the aggregation method above shares some conceptional similarities with the CGNE method as they are (generalized) Krylov-space methods. In particular, all are nonlinear methods in the data y. Note that the CGNE method without stopping rule is even discontinuous in y [17], and we expect the same to be true for the stated method (including the aggregation method). However, it has been shown by Nemirovskii [38, 39] that the CGNE method with the discrepancy principle is a regularization method in the classical sense [17, 28]. Thus, showing that the algorithms are regularization methods is most probably impossible without including a stopping criterion.

Therefore, by analogy, we include in the algorithms a discrepancy stopping rule and terminate the method for the first iteration index n for which

$$\|Ax_n - y\| \leq \tau\delta,$$

where δ is the known noise level and $\tau > 1$ is a tuning parameter, e.g., $\tau = 1.1$. This residual can be easily calculated after x_n is known, and the for-loop in the algorithms has to be terminated if the stopping criterion is satisfied. As mentioned above, a proof that this provides a regularization method is outside the scope of this work.

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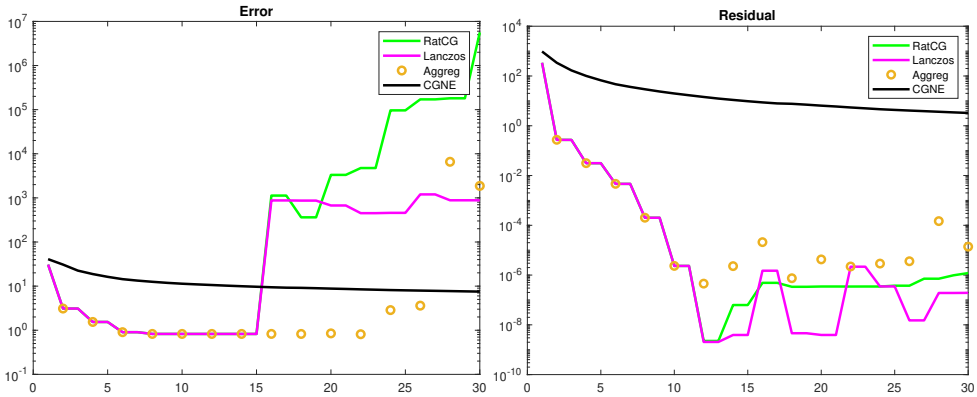

FIG. 4.1. *Logarithm of the error $\|x_n - x_{exact}\|$ and the residual $\|Ax_n - y\|$ versus the iteration number for the "tomo" problem employing the rational CG method (Alg. 3), the Lanczos method (Alg. 2), the aggregation method (2.4), and the conjugate gradient method for the normal equation (CGNE). The circles represent values for the aggregation method, plotted at the index $n = 2k$, where k is the dimension of the aggregation space (number of Tikhonov solutions). The noise level is* 0.

4. Numerical results. We test the rational CG algorithm, Algorithm 3, the rational Lanczos method, Algorithm 2, the aggregation method (2.4) (referred to as "rational methods") and compare them with the classical conjugate gradient method for the normal equation, CGNE, as given, e.g., in [17]. As simple test cases we use ten problems from the well-known Hansen's Regularization Toolbox [30]: baart(2000), blur(60), deriv2(1000), gravity(1000), heat(1000), phillips(1000), shaw(1000), spikes(1000), wing(1000), tomo(35), and their default exact solutions. In case of no noise we use the default data; in case of a nonzero noise level, we add standard normal distributed random noise to the data (by Matlab's randn command). In the latter case, all algorithms are stopped using a discrepancy principle with $\tau = 1.01$. All problems have matrices with sizes of the order of $10^3 \times 10^3$. The "blur" and "tomo" examples have sparse matrices.

Error performance. At first we test the performance for the noise-free case using the exact toolbox data. The sequence of regularization parameters α_i was for all problems set as exponentially decreasing:

$$\alpha_i = 10^{-i-1}. \tag{4.1}$$

Note that in all the examples, the operators are scaled such that $\|A\| = O(1)$. If this were not the case, one should multiply the parameter choice (4.1) by $\|A^*A\|$ to achieve a scaling-invariant method.

In Figure 4.1, we display the least-squares residual $\|Ax_n - y\|$ and the error $\|x_n - x_{exact}\|$ for the "tomo" problem and for the three proposed methods and the CGNE method. In the figure, the circles correspond to the values of the aggregation method with the same α_i, i.e., the results for the aggregation method with a number of k Tikhonov regularizations x_{α_i} are plotted at $n = 2k$, which is the index where the RatCG and the rational Lanczos method require the same number of Tikhonov solves as the aggregation method.

The observation that seems to be true throughout is that the results for the rational CG method and the rational Lanczos method are in general identical (as predicted by the theory) as long as the α_i are not too small, but the methods differ when we are in the realm of ill-conditioning (for α too small). Note that the theory assumes exact arithmetic, which is no longer true when rounding errors play a significant role. However, the difference of the two methods usually occurs beyond a reasonable stopping rule. We also note that for all tested

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TABLE 4.1
Error $\|x_n - x_{exact}\|$, computation time (Time (s)), and number of iterations for various problems from the Regularization Toolbox for the aggregation method (2.4), the Lanczos method (Alg. 2), the rational CG method (Alg. 3), and the CGNE method. 5000 is n_{max} for CGNE. α_k is chosen by (4.1).

Problem		Aggreg.	Lanczos	RatCG	CGNE
baart	Error	5.85E-02	6.58E-02	6.06E-02	2.47E-02
	Time	2.57	0.33	0.86	0.47
	Iter.	1	6	15	125
blur	Error	3.13E-07	2.81E-12	2.88E-12	1.15E-13
	Time	4.84	2.49	2.32	0.11
	Iter.	1	13	13	575
deriv2	Error	7.41E-04	6.97E-04	9.17E-05	8.43E-03
	Time	0.71	0.50	0.27	1.24
	Iter.	1	77	34	5000
gravity	Error	7.50E-03	4.48E-03	5.33E-03	3.70E-05
	Time	0.29	0.11	0.15	1.13
	Iter.	1	18	18	5000
heat	Error	1.41E-02	1.18E-02	1.20E-02	1.40E-02
	Time	0.46	0.14	0.18	1.11
	Iter.	1	25	25	5000
phillips	Error	1.89E-04	4.61E-05	5.71E-05	2.40E-05
	Time	0.28	0.11	0.13	1.12
	Iter.	1	17	16	5000
shaw	Error	2.33E-01	2.31E-01	2.22E-01	2.86E-03
	Time	0.36	0.07	0.16	1.11
	Iter.	1	13	21	5000
spikes	Error	2.60E+01	2.60E+01	2.60E+01	2.59E+01
	Time	0.24	0.10	0.14	1.01
	Iter.	1	17	17	5000
wing	Error	1.90E-01	2.57E-01	1.90E-01	1.80E-01
	Time	0.32	0.04	0.06	0.03
	Iter.	1	5	7	83
tomo	Error	8.39E-01	8.39E-01	8.39E-01	1.18E+00
	Time	0.63	0.22	0.29	0.74
	Iter.	1	13	12	5000

examples, the residual is smaller than that of the CGNE method as long as we are not in the ill-conditioning region. In many cases the errors for the rational CG/Lanczos method agree with the corresponding ones of the aggregation method in the "reasonable" region. Note that the decay of the residual for the CGNE method is much slower, but of course one has to take into account that each iteration of the method is of different complexity.

Computational performance. In Table 4.1, we present the value of the error $\|x_n - x_{exact}\|$, the computation time in seconds, and the number of iteration for the various methods and for the noise-free case. In order to find an appropriate n in this case we first run the problem each up to a given maximal number of iteration and then choose that index n where the error is the smallest (a kind of "oracle" stopping rule). The results are given in Table 4.1 together with the total running time (using Matlab's tic/toc command). The value of 5000 for the CGNE method is the maximal number of used iteration.

We observe that the RatCG and the Lanczos method perform roughly the same and outperform the aggregation method both in terms of error and time. The CGNE method has a smaller error in 7 cases but requires less time in only 3 cases.

The next experiments concerns the case of nonzero noise level. The results for two noise levels $\delta = 1\%, 0.1\%$ (using the discrepancy stopping rule) are given in Table 4.2. It can be seen that the Lanczos and rational CG method are about similar in behaviour. The running

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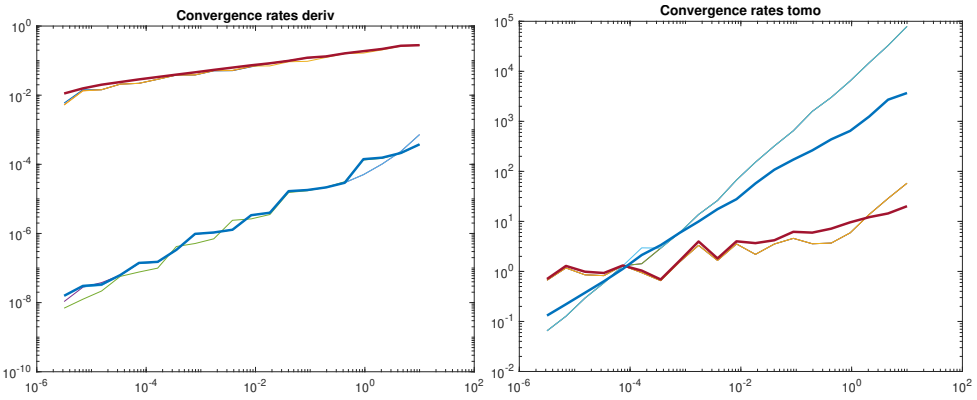

FIG. 4.2. *Convergence rates for the the aggregation method (2.4), the Lanczos method (Alg. 2), the rational CG method (Alg. 3), and the CGNE method for the "deriv2" (left) and the "tomo" (right) problems (overlayed plots). Displayed is the error $\|x_n - x_{exact}\|$ vs. the noise level in a log-log plot for two smoothness cases for each problem. (The steeper slopes correspond to the case of a smoother solution.) The error for CGNE is plotted by a thicker line as reference.*

time of the CGNE method cannot be beaten by any of the rational methods. The rational method need about 10 times more running time than CGNE. However, compared to the CGNE method, we observe that in a majority of cases (17 out of 20) the error of the proposed RatCG methods is smaller or equal to that of the CGNE method. One reason for this is that the latter does not allow for fine-tuning of the regularization parameter (which is the iteration index in this case). An optimal stopping index for the CGNE method would be "in between" two iterations.

Convergence rates. The next figures concern the convergence rates of the discussed rational methods, i.e., aggregation, rational Lanczos, and the rational CG method, which are compared with the rates of the classical CGNE method. In Figure 4.2 we display the error $\|x_n - x^\dagger\|$ against various noise levels δ on a log-log plot for all methods for four cases: First for the problem "deriv2" with the default true solution x_{exact} and then again with a smoother solution, which is simply calculated by $x_{smooth} = A^*Ax_{exact}$. This automatically implies a higher convergence rates for the latter case because a higher source condition is satisfied. We do the same for the problem "tomo", i.e., default solution and smooth solution. The noise is generated again by samples from a standard normal random distribution.

The results for the two test cases for "deriv2" are displayed together in the left plot and that for "tomo" on the right. (The steeper slope corresponds to the smoother solution). The reason for using smoother solutions is to investigate whether the methods show a saturation [17] in the convergence rates, which is known to happen for Tikhonov regularization. For the "deriv2" problem, all methods perform equally well; for the tomo problem this is true except for the CGNE method for the smooth solution, which has a slightly smaller slope (and thus a worse convergence rate). These figures should illustrate that all proposed methods show a similar (or even slightly better) rate than the CGNE method, which is known to achieve the theoretically optimal-order rates. We observe that no saturation seems to happen, and we conjecture from the results that the rational methods are optimal-order method for all classical smoothness classes [17].

Parameter robustness. Finally, we test the performance of the methods with respect to the choice of the sequence of regularization parameters. That is, we choose a geometrically decaying sequence of the form $\alpha_k = 0.1q^{s-k}$, for various $q \in 2, 4, 6, 8, 10$, and various starting values $s = -12, -10, \ldots, 8, 10$. Thus, in the extreme cases, we start with a very large

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TABLE 4.2

Error $\|x_n - x_{exact}\|$, computation time (Time (s)), and number of iterations for various problems from the Regularization Toolbox for the aggregation method (2.4), the Lanczos method (Alg. 2), the rational CG method (Alg. 3), and the CGNE method and for two noise levels $\delta = 1\%$ and 0.1%. Stopping rule by the discrepancy principle with $\tau = 1.01$.

Problem			Aggreg.	Lanczos	RatCG	CG
baart	$\delta = 1\%$	Error	3.23E-01	3.20E-01	3.20E-01	2.09E-01
		Time	0.176	0.160	0.174	0.020
		Iter.	1	2	2	3
	$\delta = 0.1\%$	Error	2.06E-01	2.08E-01	2.08E-01	2.08E-01
		Time	0.353	0.165	0.181	0.020
		Iter.	1	3	3	3
blur	$\delta = 1\%$	Error	2.39E+00	4.63E+00	4.63E+00	5.23E+00
		Time	0.733	0.327	0.342	0.004
		Iter.	1	2	2	9
	$\delta = 0.1\%$	Error	1.16E+00	1.09E+00	1.09E+00	1.36E+00
		Time	0.745	0.713	0.785	0.010
		Iter.	1	4	4	36
deriv2	$\delta = 1\%$	Error	1.66E-01	1.88E-01	1.88E-01	1.88E-01
		Time	0.115	0.036	0.037	0.005
		Iter.	1	4	4	4
	$\delta = 0.1\%$	Error	1.22E-01	1.20E-01	1.20E-01	1.22E-01
		Time	0.187	0.070	0.076	0.007
		Iter.	1	8	8	9
gravity	$\delta = 1\%$	Error	7.19E-01	7.18E-01	7.18E-01	1.75E+00
		Time	0.037	0.030	0.031	0.003
		Iter.	1	2	2	4
	$\delta = 0.1\%$	Error	5.23E-01	5.22E-01	5.22E-01	8.06E-01
		Time	0.040	0.027	0.026	0.003
		Iter.	1	2	2	6
heat	$\delta = 1\%$	Error	1.11E+00	9.92E-01	9.92E-01	1.30E+00
		Time	0.075	0.059	0.056	0.005
		Iter.	1	6	6	9
	$\delta = 0.1\%$	Error	4.16E-01	4.02E-01	4.02E-01	5.02E-01
		Time	0.150	0.068	0.074	0.008
		Iter.	1	8	8	18
phillips	$\delta = 1\%$	Error	3.96E-02	3.94E-02	3.94E-02	7.98E-02
		Time	0.028	0.024	0.024	0.002
		Iter.	1	2	2	4
	$\delta = 0.1\%$	Error	3.77E-02	3.76E-02	3.76E-02	7.30E-02
		Time	0.027	0.025	0.024	0.002
		Iter.	1	2	2	4
shaw	$\delta = 1\%$	Error	4.16E+00	4.15E+00	4.15E+00	5.25E+00
		Time	0.038	0.024	0.024	0.002
		Iter.	1	2	2	4
	$\delta = 0.1\%$	Error	1.63E+00	1.89E+00	1.89E+00	1.67E+00
		Time	0.110	0.038	0.041	0.003
		Iter.	1	5	5	6
spikes	$\delta = 1\%$	Error	2.68E+01	2.68E+01	2.68E+01	2.67E+01
		Time	0.039	0.025	0.024	0.003
		Iter.	1	2	2	7
	$\delta = 0.1\%$	Error	2.62E+01	2.62E+01	2.62E+01	2.63E+01
		Time	0.047	0.025	0.025	0.004
		Iter.	1	2	2	13
wing	$\delta = 1\%$	Error	3.48E-01	3.48E-01	3.48E-01	3.48E-01
		Time	0.062	0.028	0.027	0.002
		Iter.	1	2	2	2
	$\delta = 0.1\%$	Error	3.48E-01	3.48E-01	3.48E-01	3.48E-01
		Time	0.056	0.024	0.024	0.001
		Iter.	1	2	2	2
tomo	$\delta = 1\%$	Error	6.31E+00	6.31E+00	6.31E+00	8.78E+00
		Time	0.105	0.078	0.083	0.006
		Iter.	1	2	2	16
	$\delta = 0.1\%$	Error	3.10E+00	3.10E+00	3.10E+00	5.03E+00
		Time	0.105	0.075	0.091	0.018
		Iter.	1	2	2	76

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α or a very small one, and the q controls the speed of the decay. We tested this for the "tomo" problem with 0.01% noise. Without details, we made the following observations:

- For most cases, the results were good, the speed of decay (choice of q) did not have much of an influence.
- The number of iterations is high (and the methods are slow) if we start with a very large α, i.e., far away from a reasonable good regularization parameter.
- Starting with a too-small α (much below an "optimal" value) yields comparably bad results (large error). In this case, the aggregation, the rational CG, and the Lanczos method become unstable. However, such a failure only happened for the extreme case $\alpha_k = 10^{-12-k}$.
- Starting with a too-large regularization parameter α leads to stability problems for the Lanczos method, for instance, when $\alpha_k = 10^{10-k}$. This can be explained by the fact that in such a case the Tikhonov inverse $(A^*A + \alpha I)^{-1}A^*y \sim \frac{1}{\alpha}A^*y + O(\frac{1}{\alpha^2})$ is almost a scaled multiple of the first element in the Krylov space, and thus the mixed Krylov space is close to breakdown. The rational CG method behaved more robust in that respect.
- As to be expected, if we start with an α that is already a good choice for classical Tikhonov regularization, then the methods terminate after 2 iteration (i.e., after the first rational step) with good results.

4.1. Summary and comments. In terms of error we have verified an excellent performance of the rational methods, sometimes even better than the CGNE method. The downside is, however, the additional computation time required. However, though we did not focus on it, there is plenty of room for generalizing the methods and further improvements:

- An obvious improvement can be made by the inclusion of preconditioning.
- The Tikhonov inversion can be simplified by a-priori matrix factorizations, for instance, using a bidiagonalization of the operator A ([17, Chpt. 9], [6, 15, 31]).
- A stimulating piece of research would be to investigate the effect of an incomplete computation of the Tikhonov solutions.
- The concept of rational and mixed rational Krylov spaces can be extended to the non-Hermitean case, which is of high interest in recent regularization theory; e.g., [20, 21, 46]. Whether an analogue of a RatCG can be derived in this situation is not clear.
- As stated above, a proof that the RatCG method with the discrepancy principle is a regularization method is challenging.
- Furthermore, an extension of the method to the nonlinear case is highly interesting, but the modality is not obvious.

5. Conclusion. We derived the rational CG (RatCG) method as well as the rational Lanczos method for iteratively minimizing linear least-squares problems over mixed rational Krylov spaces. The main novelty is the RatCG method, which is based on short recursions, with Tikhonov regularization in each second step, and which requires nearly no additional memory requirements. We illustrate that these methods and the associated aggregation method perform equally well or better than the conjugate gradient method for the normal equations in terms of the error, though not necessarily in terms of runtime. Numerical experiments suggest that the new methods can act as regularization when combined with a stopping rule with optimal-order convergence.

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