The Fréchet derivative of rational approximations to the matrix exponential and its application on inverse parabolic problems

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We consider an inverse problem, where a high dimensional parameter $\mathbf{c}$ has to be identified from measurements of some components of the solution of the parametric initial value problem

$$\mathbf{u}'(t) = A(\mathbf{c})\mathbf{u}(t), \quad \mathbf{u}(0) = \mathbf{b}$$

at some given time points. Here $A(\mathbf{c})$ is a large sparse symmetric negative definite matrix. Applying Gauß-Newton's method it is important to have information about the sensitivity of the forward solution with respect to the parameter $\mathbf{c}$. But due to the size of the problem, it is unfeasible to compute the dense and large Jacobian J directly. Therefore we will solve the linearized least square problems iteratively (e. g. by LSQR) which requires algorithms to compute products of the form $J\mathbf{v}$ and $J^T\mathbf{w}$

We present a new approach, where the forward solution is approximated using the rational best approximation of the exponential function. We will focus on the Fréchet derivatives of the corresponding rational matrix functions, their numerical evaluation and approximation errors with respect to the Fréchet derivative of the matrix exponential. We show how products with the Jacobian and its transpose can be implemented in an economic way, and present numerical examples.