Unifying relations between iterative linear equation solvers and explicit Euler approximations for associated parabolic regularized equations

R. Sala[1], A. Schlüter, C. Sator, R. Müller

Department of Mechanical and Process engineering, Technische Universität Kaiserslautern, 67633 Kaiserslautern, Germany

Abstract

Iterative methods to solve linear equation systems are widely used in computational physics, engineering and many areas of applied mathematics. In recent works, performance improvements have been achieved based on modifications of several classes of iterative algorithms by various research communities driven by different perspectives and applications. This note presents a brief analysis of conventional and unifying perspectives by highlighting relations between several well-known iterative methods to solve linear equation systems and explicit Euler approximations of the associated parabolic regularized equations. Special cases of equivalence and general relations between different iterative methods such as Jacobi iterations, Richardson iterations, Steepest Descent and Quasi-Newton methods are shown and discussed. The results and discussion extend the conventional perspectives on these iterative methods and give way to intuitive physical interpretations and analogies. The accessibly presented relations give complementary educational insights and aim to inspire transdisciplinary developments of new iterative methods, solvers and preconditioners.

Keywords: `Iterative methods, Sparse Linear Equations, Preconditioners, Parabolic Regularization`

1. Introduction and motivation

Efficient iterative solvers for linear equation systems are important in many areas of computing. This led to research and progress and algorithm performance improvements from various research communities with heterogeneous perspectives. In recent years several modifications of classical iterative methods such as Jacobi iterations, Richardson iterations, Steepest Descent and Quasi-Newton methods have been presented in various contexts.

The Jacobi method [1, 2] is a well known iterative procedure for the solution of linear equation systems. Although other iterative methods, such as the Krylov subspace-based Conjugate Gradient (CG) method are often preferred due to better convergence rates, Jacobi iterations and recently developed Jacobi-like iterations are still commonly used as preconditioners or smoothers as part of other iterative approaches such as multigrid methods [3]. Jacobi-like iterations are well suited for parallelization [4, 5, 6, 7, 8] and are therefore still a topic of active research and development [9, 10, 11, 12]. Investigations on a class of recently developed Jacobi-like methods (Anderson-Richardson methods) indicated that for particular problem types, these methods can show superior scaling performance compared to established Krylov subspace-based methods such as CG [4, 7]. Some of the relations between the Scheduled Relaxation Jacobi method and Richardson's non-stationary method were discussed in [10].

Other recent advances in gradient-based methods for linear equation systems showed advantages over Krylov subspace methods in particular situations [13]. In other contexts novel gradient descent-based approaches for linear equations in the setting for missing data [14], distributed linear regression [15] and quantum computing [16] were presented. Recently also quasi-Newton based approaches were developed and used in the context of linear equation systems and preconditioning [17, 18]. Besides non-stationary preconditioning, also preconditioner "switching" showed promising results for linear systems arising from interior point methods for linear programming problems [19].

The explicit Euler method [20, 21] is an iterative numerical method to approximate solutions of differential equations. In this context the method is well known due to its simplicity and educational value, but because of its rather limited stability and accuracy properties, other methods with higher-order accuracy are often more efficient. Because the previously mentioned classes of iterative methods for linear equations are generally targeted at different problem types they seem rather unrelated to the Explicit Euler method. This note, however, considers interesting relations between all of the previously mentioned classes of iterative methods for the solution of equation systems, and the use of the explicit Euler method for the solution of the associated parabolic regularization of the elliptic equations. Parabolic regularization techniques have been used in the context of element-by-element based solution approaches for discretized elliptic problems [22, 23], for which

[1] sala@rhrk.uni-kl.de

physically meaningful associated parabolic problems exist. These regularization concepts described in [22, 23, 24], can be considered as a generalization of the Dynamic Relaxation approach [25], which was developed in the scope of quasi-static problems in structural mechanics.

There exist only few works (e.g., [26] and [27]) in the literature that address the relations between the concept of parabolic regularization of elliptic problems combined with (pseudo) time integration, and other iterative equation solution techniques such as the Jacobi method, Richardson iterations and Quasi Newton methods. For the restricted setting of cellular neural network simulation, a relation between Jacobi iterations and Euler iterations for a particular choice of parameters was shown in an earlier work [27]. Some aspects related to the interpretation of time discretized differential equations as dynamical systems as a means to solve linear systems of equations were discussed in [26].

This communication highlights more general relations and similarities between several widely used numerical methods of which some are usually considered rather separately, and thereby complements the conventional perspectives on relations between iterative methods for linear equations [28, 29]. The resulting perspective provides additional insight and gives way to intuitive physical analogies, and aims to be of educational value as well as to inspire the development of new and alternative iterative methods of use in numerical computation. Although most of the iterative methods discussed are relatively straight forward and well-known, they are presented comprehensively in the Appendix to emphasize the spirit of the original references with the intention to illustrate how a variety of famous iterative methods developed from different views are deeply related in the view of a unifying perspective.

2. Parabolic regularization

In various settings of computational physics and engineering discrete elliptic problems of the following type occur:

$$\boldsymbol{K}\boldsymbol{u} = \boldsymbol{b} \tag{1}$$

where $\boldsymbol{K}$ is a real square positive definite matrix[2], $\boldsymbol{b}$ represents the vector of the discretized source term and $\boldsymbol{u}$ is a vector of unknown variables. The concept of Parabolic Regularization (PR) is to replace the discrete elliptic problem, by an associated parabolic problem with a transient vector of variables $\boldsymbol{v}$ for which the asymptotic solution coincides with the solution of the original problem [23]. For the stationary discrete elliptic problem (1) an associated non-stationary semi-discrete parabolic problem is:

$$\boldsymbol{C}\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}\tau} + \boldsymbol{K}\boldsymbol{v}(\tau) = H(\tau)\boldsymbol{b} \tag{2}$$

[2] In this context a real matrix $\boldsymbol{K}$ is said to be positive definite ($\boldsymbol{K} \succ 0$) if $\forall \boldsymbol{u} \in \mathbb{R}^n$, $\boldsymbol{u} \neq 0 \implies \boldsymbol{u}^T\boldsymbol{K}\boldsymbol{u} > 0$.

with Heaviside step function

$$H(\tau) = \begin{cases} 0 & \tau \leq 0 \\ 1 & \tau > 0, \end{cases}$$

pseudo time τ, and initial conditions $\boldsymbol{v}(0) = \vec{0}$. If $\boldsymbol{C}$ is chosen as a positive-definite matrix ($\boldsymbol{C} \succ 0$), the asymptotic solution of equation (2) approximates the solution of equation (1)

$$\lim_{\tau\to\infty} \boldsymbol{v}(\tau) = \boldsymbol{u}.$$

3. The explicit Euler method

In 1768 Euler described a method to approximate the solutions of ordinary differential equations with given initial values ([20, 21] part 1, section 2, ch. 7). The method is applicable to problems of the form:

$$\frac{\mathrm{d}w}{\mathrm{d}s} = f(s, w), \text{ with } w(s_0) = w_0.$$

The key idea was to iteratively attribute new values for w_{k+1} based on small changes of s by using the following approximation:

$$\frac{w_{k+1} - w_k}{\Delta s} \approx f(s_k, w_k), \quad k = 0, 1, 2, ..., n.$$

Where Δs is a small positive perturbation or explicit step to the next iteration $s_k + \Delta s = s_{k+1}$.

4. The explicit Euler method for parabolically regularized elliptic equations

If for a discrete stationary elliptic problem as given in equation (1), the explicit Euler method is applied to approximate an associated parabolic regularization as given in equation (2), one obtains:

$$\boldsymbol{C}\frac{\boldsymbol{v}_{k+1} - \boldsymbol{v}_k}{\Delta\tau} = (\boldsymbol{b} - \boldsymbol{K}\boldsymbol{v}_k), \text{ with } \boldsymbol{v}_0 = \vec{0}.$$

This can be rewritten as the following iterative scheme, with w.r.t pseudo time steps $\Delta\tau$:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \Delta\tau\boldsymbol{C}^{-1}(\boldsymbol{K}\boldsymbol{v}_k - \boldsymbol{b}). \tag{3}$$

5. Relations between several iterative schemes and physical analogies

In Table 1 the iterative scheme of the explicit Euler method for parabolically regularized equations is compared with various well known iterative schemes for linear equation systems, such as the Jacobi method, Richardson iterations and some of their variants which are often used as preconditioners or smoothing iterations as part of other iterative solution approaches. Although less conventional, also Gradient Descent and Quasi-Newton based methods have been developed in the context of iterative

linear equation solvers [15, 14, 17, 18] and are included in the overview. In order to highlight the similarities among the various methods, some iterative schemes are slightly rearranged, w.r.t. the common formulations. For details and derivations of the formulations for the iterative schemes, we refer to the previous sections and to the extensive Appendix. While in the previous sections we considered an equation system where the involved matrix ($\boldsymbol{K}$) is positive definite, this is in the following sections considered as a special case of the more general equation system $\boldsymbol{A}\boldsymbol{v} = \boldsymbol{b}$ with the less restrictive condition that matrix $\boldsymbol{A}$ must be non-singular. All of the iterative schemes in Table 1, can be considered special cases of the following (non-stationary) standard iteration scheme:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \boldsymbol{P}_k^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}), \tag{4}$$

to solve the general equation $\boldsymbol{A}\boldsymbol{v} = \boldsymbol{b}$, where $\boldsymbol{v}_k$ and $\boldsymbol{b}$ are arbitrary vectors, and where the Matrices $\boldsymbol{A}$ and $\boldsymbol{P}_k$ must be non-singular. In practice, knowledge of $\boldsymbol{P}_k^{-1}$ is not necessarily required, but instead the equation system

$$\boldsymbol{P}_k \Delta\boldsymbol{v}_{k+1} = \boldsymbol{r}_k \tag{5}$$

can be solved for $\Delta\boldsymbol{v}_{k+1}$, where $\boldsymbol{r}_k = \boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}$. With $\boldsymbol{v}_{k+1} = \boldsymbol{v}_k + \Delta\boldsymbol{v}_{k+1}$, and error $\boldsymbol{e}_k = \boldsymbol{v} - \boldsymbol{v}_k$, the resulting error from an iteration according to eq. 4 can be written as:

$$\boldsymbol{e}_{k+1} = (\boldsymbol{I} - \boldsymbol{P}_k^{-1}\boldsymbol{A})\boldsymbol{e}_k. \tag{6}$$

Therefore, if the following restriction on the spectral radius

$$\rho(\boldsymbol{I} - \boldsymbol{P}_k^{-1}\boldsymbol{A}) < 1 \tag{7}$$

holds, a decrease of the norm of the error ($\|\boldsymbol{e}_{k+1}\| < \|\boldsymbol{e}_k\|$) will be achieved in iteration k. To have benefit from the above iterative schemes, $\boldsymbol{P}_k^{-1}$ or $\boldsymbol{P}_k$ should be chosen in such a way that the operations for iterations of equation (4) or (5) require significantly less computational resources than the solution of the original equation system: $\boldsymbol{A}\boldsymbol{v} = \boldsymbol{b}$. This could be achieved by choosing $\boldsymbol{P}_k$ for example: diagonal, tridiagonal, lower triangular , or by directly estimating a $\boldsymbol{P}_k^{-1}$ such that (7) is satisfied, with a preferably small spectral radius.

By comparing the iterative schemes in the Table 1, a relation between the Jacobi method (see also equation (A.1) in the Appendix) and that of the explicit Euler method applied to the parabolically regularized equation in (3) can be identified. For the special but common case that in the initial equation system $\bar{\boldsymbol{A}}\boldsymbol{v} = \boldsymbol{b}$, the matrix is positive definite ($\bar{\boldsymbol{A}} \succ 0$), it follows that its diagonal matrix is also positive definite ($\mathrm{diag}(\bar{\boldsymbol{A}}) \succ 0$). If parabolic regularization is applied combined with the explicit Euler method, and if the regularization matrix $\boldsymbol{C}$ and the step size $\Delta\tau$ are chosen such that $\Delta\tau\boldsymbol{C}^{-1} = \boldsymbol{D}^{-1} = \mathrm{diag}(\bar{\boldsymbol{A}})^{-1}$, an iteration scheme equivalent to that of the Jacobi method can be obtained. The similarity or equivalence between the methods, thus depends on the parameterization of the parabolic regularization matrix $\boldsymbol{C}$, and the step size $\Delta\tau$. The 'weighted' Jacobi method also includes a scaling factor ω for the diagonal matrix $\boldsymbol{D}^{-1}$. It should be noted however that in the respective conventional settings the step size for the explicit Euler method is selected as a compromise between computational cost and accuracy, since the full transient solution is often of interest. While for a 'weighted' Jacobi method the weighing factor for the diagonal is typically chosen to increase convergence speed, since only the final (or 'steady-state') solution is of interest.

In a straight forward way, the explicit Euler step size and the parabolic regularization matrix $\boldsymbol{C}$ can also be chosen such that the iterative scheme in equation (3) is equivalent to Richardson iterations, or Gradient Descent iterations. The combination of parabolic regularization with the explicit Euler method contains many of the so-called 'standard' iteration methods [29] for linear equation systems, as particular cases. Likewise, for non-stationary choices of the explicit Euler step size $\Delta\tau_k$ also schemes equivalent to non-stationary Richardson Iterations, or Scheduled Relaxation Jacobi (SRJ) iterations can be obtained. Also quasi-Newton methods with updating schemes that preserve positive definiteness of the inverse Hessian estimate $\boldsymbol{B}_k^{-1}$, correspond to a subset of non-stationary choices for the PR matrix $\boldsymbol{C}$.

For the particular case when matrix $\boldsymbol{A}$ is positive definite, interesting physical interpretations for a Jacobi-like iterations can be obtained. One example is the analogy of a Jacobi iteration with an Euler time step for a linear heat conduction problem, with a constant source term[3]. In the analogy, the heat conduction problem is described by equation (2), where $\boldsymbol{C}$ represents a diagonal positive definite capacity matrix, $\boldsymbol{K}$ represents a conductivity matrix, $\boldsymbol{v}$ represents a vector with the temperature distribution, and $\boldsymbol{b}$ represents the distribution of constant heat sources. If the capacity matrix $\boldsymbol{C}$ is chosen as the diagonal of the conductivity matrix $\boldsymbol{K}$, each explicit Euler time integration step to estimate the propagation of the spatial temperature distribution in a small time interval, corresponds to a Jacobi iteration and vice versa. When Jacobi iterations are used as 'smoothers' in multigrid methods, this analogy offers a physical interpretation behind the smoothing mechanism and the propagation of information during the iterations. Also for the other iterative schemes in Table 1 similar physical analogies can be found if $\boldsymbol{P}_k^{-1}$ and $\boldsymbol{A}$ are positive definite, such that they can be interpreted as "generalized" capacity and conductivity matrix respectively.

[3] Suitably this particular analogy is in content and spirit related to the work of Fourier who stated when speaking about mathematical analysis: "Its chief attribute is clearness ; it has no marks to express confused notations. It brings together phenomena the most diverse, and discovers the hidden analogies which unite them." [30] (p. 7,8).

Table 1: Overview of the iteration schemes

Method name	Iteration scheme	Parameter conditions
PR & explicit Euler	$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \Delta\tau \boldsymbol{C}^{-1}(\boldsymbol{K}\boldsymbol{v}_k - \boldsymbol{b})$	$\boldsymbol{C} \succ 0$, $\Delta\tau > 0$
Jacobi	$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \boldsymbol{D}^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b})$	
weighted Jacobi	$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \omega \boldsymbol{D}^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b})$	$\omega > 0$
SRJ	$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \omega_k \boldsymbol{D}^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b})$	$\omega_k > \omega_{k+1} > 0$
Richardson iterations	$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \bar{\omega}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b})$	$\bar{\omega} > 0$
Gradient Descent	$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \gamma_k(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b})$	$\gamma_k > 0$
Quasi-Newton	$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \gamma \boldsymbol{B}_k^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b})$	$\gamma > 0$

6. Discussion and outlook

While many of the previously mentioned iterative methods are well known, the relation between the iterative Jacobi-like methods and the concept of parabolic regularization combined with the explicit Euler method was previously not or rarely addressed in the literature. The application of the PR concept combined with (pseudo) time integration can be extended to error decreasing iterations in the solution of equation systems regardless of their physical origin, as long as $\boldsymbol{A}$ and $\boldsymbol{P}_k$ are positive-definite and equation (7) holds for each iteration. Compared to the conventional standard iterative methods, the preconditioner matrix $\boldsymbol{P}$, is composed of the PR matrix $\boldsymbol{C} \succ 0$, and a step length or scaling factor $\Delta\tau > 0$. From this perspective the scaling factor $\Delta\tau_k$ and the PR matrix $\boldsymbol{C}_k$ can also be chosen non-stationary.

The challenge of finding effective matrices $\boldsymbol{P}_k$ can also be related to the various strategies to update the Hessian approximations in Quasi-Newton methods. Instead of the explicit Euler method, other higher order explicit (pseudo) time integration methods (e.g. Runge-Kutta methods) could be combined with parabolic regularized equations to achieve improved performance of iterative equation solvers by reusing information of previous iteration steps. In addition to the choice of the integration scheme parameters and the regularization matrix $\boldsymbol{C}$, also alternative (higher order) parabolic regularization formulations could be explored, to formulate alternative iterative methods. As an outlook or example, the concept of dynamic relaxation could be applied to the solution of general equation systems with positive definite matrices, by the construction of second-order parabolic regularizations with parameters that result in near critical damping of the unknown variables $\boldsymbol{v}_k$ w.r.t pseudo time τ.

7. Concluding remarks

This brief note highlighted that the concept of parabolic regularization of elliptic problems combined with explicit Euler (pseudo) time integration, has strong relations to many of the well known iterative methods to solve linear equation systems. It was shown that for particular choices of the parabolic regularization parameters and step size of the explicit Euler method, iterative schemes can be obtained which are equivalent to various types of Jacobi-like iterations. Previously these topics were regarded in rather disjoint contexts, perspectives and communities, and their relations were only scarcely scattered in the literature. The presented work aimed to give an accessible overview of conventional perspectives on iterative methods for linear equations in their original historical context and complemented these with unifying relations. This gave way to intuitive physical interpretations for some of these iterative methods. Besides the educational value, the presented perspectives, references and relations between these algorithms, could be of interest to cross inspire the development of novel efficient iterative schemes, solvers and preconditioners of use in Computational Rational Engineering [31], computational physics and in the general scope of applied mathematics.

Funding sources

This work was partially funded by the Deutsche Forschungsgemeinschaft (DFG) Project-ID 465355776.

References

[1] C. G. Jacobi, Ueber eine neue auflösungsart der bei der methode der kleinsten quadrate vorkommenden lineären gleichungen, Astronomische Nachrichten 22 (20) (1845) 297–306.

[2] C. G. Jacobi, G. J. Stewart, On a new way of solving the linear equations that arize in the method of least squares, IMA Prepring Series 951.

[3] X. Yang, R. Mittal, Efficient relaxed-jacobi smoothers for multigrid on parallel computers, Journal of Computational Physics 332 (2017) 135–142.

[4] P. P. Pratapa, P. Suryanarayana, J. E. Pask, Anderson acceleration of the jacobi iterative method: An efficient alternative to krylov methods for large, sparse linear systems, Journal of Computational Physics 306 (2016) 43–54.

[5] J. Hook, N. Dingle, Performance analysis of asynchronous parallel jacobi, Numerical Algorithms 77 (3) (2018) 831–866.

[6] A.-K. C. Ahamed, F. Magoulès, Efficient implementation of jacobi iterative method for large sparse linear systems on graphic processing units, The Journal of Supercomputing 73 (8) (2017) 3411–3432.

[7] P. Suryanarayana, P. P. Pratapa, J. E. Pask, Alternating anderson–richardson method: An efficient alternative to preconditioned krylov methods for large, sparse linear systems, Computer Physics Communications 234 (2019) 278–285.

[8] H. Anzt, J. Dongarra, G. Flegar, E. S. Quintana-Ortí, Variable-size batched gauss–jordan elimination for block-jacobi preconditioning on graphics processors, Parallel Computing 81 (2019) 131–146.

[9] X. I. Yang, R. Mittal, Acceleration of the jacobi iterative method by factors exceeding 100 using scheduled relaxation, Journal of Computational Physics 274 (2014) 695–708.
[10] J. E. Adsuara, I. Cordero-Carrión, P. Cerdá-Durán, V. Mewes, M. A. Aloy, On the equivalence between the scheduled relaxation jacobi method and richardson's non-stationary method, Journal of Computational Physics 332 (2017) 446–460.
[11] G. J. Kimmel, A. Glatz, Extensions and analysis of worst-case parameter in weighted jacobi's method for solving second order implicit pdes, Results in Applied Mathematics 1 (2019) 100003.
[12] A. Maity, K. M. Singh, Scheduled relaxation jacobi method as preconditioner of krylov subspace techniques for large-scale poisson problems, Numerical Heat Transfer, Part B: Fundamentals 77 (2) (2020) 152–179.
[13] Q. Zou, F. Magoulès, Fast gradient methods with alignment for symmetric linear systems without using cauchy step, Journal of Computational and Applied Mathematics (2021) 113033.
[14] A. Ma, D. Needell, A gradient descent approach for incomplete linear systems, in: 2018 52nd Asilomar Conference on Signals, Systems, and Computers, IEEE, 2018, pp. 764–768.
[15] K. Chakrabarti, N. Gupta, N. Chopra, Robustness of iteratively pre-conditioned gradient-descent method: The case of distributed linear regression problem, IEEE Control Systems Letters.
[16] I. Kerenidis, A. Prakash, Quantum gradient descent for linear systems and least squares, Physical Review A 101 (2) (2020) 022316.
[17] R. M. Gower, P. Richtárik, Randomized quasi-newton updates are linearly convergent matrix inversion algorithms, SIAM Journal on Matrix Analysis and Applications 38 (4) (2017) 1380–1409.
[18] L. Bergamaschi, J. Marín, Á. Martínez, Compact quasi-newton preconditioners for symmetric positive definite linear systems, Numerical Linear Algebra with Applications 27 (6) (2020) e2322.
[19] P. M. Bartmeyer, S. Bocanegra, A. R. L. Oliveira, Switching preconditioners using a hybrid approach for linear systems arising from interior point methods for linear programming, Numerical Algorithms (2020) 1–28.
[20] L. Euler, Institutiones calculi integralis, Vol. 1. XI, Lipsiae et Berolini B.G. Teubneri, 1768.
[21] I. Bruce, Euler's Institutionum calculi integralis Translated and annotated by Ian Bruce, http://www.17centurymaths.com, 2010.
[22] T. J. Hughes, I. Levit, J. Winget, Element-by-element implicit algorithms for heat conduction, Journal of Engineering Mechanics 109 (2) (1983) 576–585.
[23] T. J. Hughes, I. Levit, J. Winget, An element-by-element solution algorithm for problems of structural and solid mechanics, Computer Methods in Applied Mechanics and Engineering 36 (2) (1983) 241–254.
[24] R. Sala, C. Kuhn, C. Sator, R. Müller, Topology optimization combined with element-by-element solution techniques, PAMM 19 (1) (2019) e201900173.
[25] A. Day, An introduction to dynamic relaxation, The engineer 219 (1965) 218–221.
[26] J.-P. Chehab, J. Laminie, Differential equations and solution of linear systems, Numerical Algorithms 40 (2) (2005) 103–124.
[27] V. Tavsanoglu, Jacobi's iterative method for solving linear equations and the simulation of linear cnn, in: 2006 10th International Workshop on Cellular Neural Networks and Their Applications, IEEE, 2006, pp. 1–5.
[28] Y. Saad, Iterative methods for sparse linear systems, Vol. 82, siam, 2003.
[29] G. H. Golub, C. F. Van Loan, Matrix computations, JHU press, 2012.
[30] J. Fourier, The Analytical Theory of Heat. Translated, with notes, by Alexander Freeman, Cambridge University Press., 1878.
[31] R. Sala, Computational rational engineering and development: Synergies and opportunities, in: Intelligent Systems and Applications. IntelliSys 2021, Springer, 2021, pp. 744–763.
[32] L. F. Richardson, Ix. the approximate arithmetical solution by finite differences of physical problems involving differential equations, with an application to the stresses in a masonry dam, Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character 210 (459-470) (1911) 307–357.
[33] A. Cauchy, Méthode générale pour la résolution des systemes d'équations simultanées, Comp. Rend. Sci. Paris 25 (1847) (1847) 536–538.
[34] Y.-x. Yuan, Step-sizes for the gradient method, AMS IP Studies in Advanced Mathematics 42 (2) (2008) 785.
[35] T. J. Ypma, Historical development of the newton–raphson method, SIAM review 37 (4) (1995) 531–551.
[36] R. H. Byrd, J. Nocedal, R. B. Schnabel, Representations of quasi-newton matrices and their use in limited memory methods, Mathematical Programming 63 (1-3) (1994) 129–156.

Appendix A. Appendix

Appendix A.1. The Jacobi method for systems of linear equations

In 1845, Jacobi proposed an iterative method for the solution of linear equation systems occurring in the method of least squares in [1] (an English translation is available in [2]). In [1] it was also recognized that the method is suitable to obtain solutions for the more general class of equation systems with diagonally dominant matrices. The method is now commonly known as the Jacobi method for systems of linear equations.

The iterative solution scheme described in [1] can be summarized as follows: For a system of equations $\boldsymbol{A}\boldsymbol{v} = \boldsymbol{b}$, with a full rank matrix $\boldsymbol{A}$ with nonzero diagonal elements and a known vector $\boldsymbol{b}$, a first estimate $\boldsymbol{v}_1$ for the unknown solution $\boldsymbol{v}$ is given by

$$\boldsymbol{v}_1 = \boldsymbol{D}^{-1}\boldsymbol{b}$$

where $\boldsymbol{D}$ is a diagonal matrix with the diagonal components of $\boldsymbol{A}$. The non-zero off-diagonal terms cause an error for which the first correction $\boldsymbol{\delta}_1$ is given by

$$\boldsymbol{\delta}_1 = -\boldsymbol{D}^{-1}(\boldsymbol{A} - \boldsymbol{D})\boldsymbol{v}_1.$$

Note that $\boldsymbol{D}^{-1}$ is constant throughout the iterations, and easy to compute because $\boldsymbol{D}$ is diagonal. A sequence of decreasing corrections is given by

$$\boldsymbol{\delta}_{i+1} = -\boldsymbol{D}^{-1}(\boldsymbol{A} - \boldsymbol{D})\boldsymbol{\delta}_i.$$

The estimate for $\boldsymbol{v}$ after k corrections is given by the first estimate and the sum of the available corrections:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_1 + \sum_{i=1}^{k} \boldsymbol{\delta}_i.$$

Alternatively, using initial values $\boldsymbol{v}_0 = \vec{0}$, this iterative scheme can be written as:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \boldsymbol{D}^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}), \quad k = 0, 1, 2, ..., n. \quad \text{(A.1)}$$

The iterations for the modified or weighted Jacobi method are given by:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \omega \boldsymbol{D}^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}). \tag{A.2}$$

where ω is a non negative scaling factor $\omega \in (0, 1]$. A sufficient condition for convergence is strict diagonal dominance of matrix $\boldsymbol{A}$. A relatively recent extension of the Jacobi method; The Scheduled Relaxation Jacobi (SRJ) method [9] can be expressed as:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \omega_k \boldsymbol{D}^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}), \tag{A.3}$$

where ω_k are different relaxation factors ordered such that $\omega_k > \omega_{k+1}$. For the details regarding the choices for ω_k, convergence and further information on this method we refer to [9] and [10].

Appendix A.2. Richardson iterations

In 1911, Richardson proposed an iteration scheme for the solution of linear equation systems [32]. The Richardson iteration scheme for a equation system $\boldsymbol{A}\boldsymbol{v} = \boldsymbol{b}$ is given by:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \bar{\omega}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}). \tag{A.4}$$

where $\bar{\omega}$ is a positive scalar. The method converges when the spectral radius satisfies:

$$\rho(\boldsymbol{I} - \bar{\omega}\boldsymbol{A}) < 1.$$

For a positive definite matrix $\boldsymbol{A}$ the optimal choice for a fixed $\bar{\omega}$ is

$$\bar{\omega}^* = \frac{2}{\lambda_{min} + \lambda_{max}}$$

where λ_{min} and λ_{max} are the smallest and largest eigenvalue of $\boldsymbol{A}$ respectively. These conditioning eigenvalues are however often not known, and their estimation requires considerable effort. Instead of fixed values of $\bar{\omega}$, also non-stationary values for $\bar{\omega}$ can be used. For details about the relation between non-stationary Richardson iterations and the Scheduled Relaxation Jacobi method is referred to [10] and [9]. Stationary Richardson iterations are also known to be equivalent with Gradient Descent iterations with a constant step size (see Appendix A.3).

Appendix A.3. Gradient descent

The gradient descent or steepest descent algorithm by Cauchy [33] is widely known due to its intuitive nature and educative value. During an iterative solution procedure, the equation $\boldsymbol{A}\boldsymbol{v}_k = \boldsymbol{b}$ is generally not satisfied, and a residual $\boldsymbol{r}_k$ for each iteration k can be defined as:

$$\boldsymbol{r}_k = \boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}$$

For a positive definite matrix $\boldsymbol{A}$ the solution of the equation $\boldsymbol{A}\boldsymbol{v} - \boldsymbol{b} = \vec{0}$ is equivalent to finding the solution to the optimization problem:

$$\underset{\boldsymbol{v}}{\text{minimize}}\, f(\boldsymbol{v}) \quad \text{with} \quad f(\boldsymbol{v}) := \frac{1}{2}\boldsymbol{v}^T\boldsymbol{A}\boldsymbol{v} - \boldsymbol{b}^T\boldsymbol{v} \tag{A.5}$$

The gradient of $f(\boldsymbol{v})$ for a given $\boldsymbol{v}_k$ is equal to the residual of the equation system

$$\nabla f(\boldsymbol{v}_k) = \boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}.$$

For an initial guess $\boldsymbol{v}_0$ and fixed step size γ in the negative gradient direction $\boldsymbol{r}_k$, a gradient Descent iteration can be written as:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \gamma(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b}). \tag{A.6}$$

If instead of an fixed step size γ an exact line search is performed, γ_k can be determined for iteration k by:

$$\gamma_k = \frac{\boldsymbol{r}_k^T\boldsymbol{r}_k}{\boldsymbol{r}_k^T\boldsymbol{A}\boldsymbol{r}_k}$$

An overview of alternative choices for the step size, in other settings can be found in [34] and [13].

Appendix A.4. Newton and Quasi-Newton methods

The analysis in [35] indicated that, what is commonly called Newton's method for equation systems, developed to its current form by contributions of many among which al-Khayyam, Vieta, Newton, Raphson and Simpson. The resulting procedure to solve a general nonlinear system of equations $\boldsymbol{f}(\boldsymbol{v}) = \vec{0}$ can be stated as follows:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - [\boldsymbol{J}_{\boldsymbol{f}}]^{-1}\boldsymbol{f}(\boldsymbol{v}_k) \tag{A.7}$$

where J_f is the left inverse of the Jacobian matrix with first order derivatives. In the context of unconstrained minimization problems

$$\underset{\boldsymbol{v}}{\text{minimize}}\, f(\boldsymbol{v})$$

the application of the iterative method (A.7) to find stationary points $\nabla f(\boldsymbol{v}) = \vec{0}$ results in:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - [\nabla^2 f(\boldsymbol{v}_k)]^{-1}\nabla f(\boldsymbol{v}_k)$$

where $\nabla^2 f(\boldsymbol{v}_k)$ is the Hessian matrix $\boldsymbol{H}(\boldsymbol{v}_k)$ with second order derivatives evaluated at $\boldsymbol{v}_k$. For functions $f(\boldsymbol{v})$ as defined in (A.5), it follows:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \boldsymbol{H}^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b})$$

For this special case $\boldsymbol{H}(\boldsymbol{v}_k) = \boldsymbol{A}$, and if $\boldsymbol{H}^{-1} = \boldsymbol{A}^{-1}$ was available the solution could be obtained in a single step. In the context of iterative methods for linear equations $\boldsymbol{A}^{-1}$ is generally not directly available. In quasi-Newton methods the Hessian matrix or more often its inverse is iteratively approximated using information from previous iterations [36]. Often also not full Newton steps are performed, but the step size is relaxed. The iterative scheme can then be written as:

$$\boldsymbol{v}_{k+1} = \boldsymbol{v}_k - \gamma\boldsymbol{B}_k^{-1}(\boldsymbol{A}\boldsymbol{v}_k - \boldsymbol{b})$$

where $\boldsymbol{B}_k^{-1}$ is an approximation of the inverse of the Hessian or $\boldsymbol{A}^{-1}$ at iteration k, and with step size $\gamma \in (0, 1]$. An overview of conventional estimation schemes for $\boldsymbol{B}_k^{-1}$ is given in [36]. For recent developments regarding Quasi-Newton methods in the scope of preconditioning for linear systems we refer to [17] and [18].