A data driven heuristic for rapid convergence of general Scheduled Relaxation Jacobi (SRJ) schemes

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Abstract

The Scheduled Relaxation Jacobi (SRJ) method is a viable candidate as a high performance linear solver for elliptic PDEs. The method greatly improves the convergence of standard Jacobi iteration by applying a sequence of $M$ overrelaxation and underrelaxation steps in each cycle of the algorithm. In previous work, the relaxation factors associated with each of the $M$ steps (which characterize an SRJ scheme) were derived to be specific to the problem of interest and its discretization. In this work we develop a class of SRJ schemes which could be applied to solve any linear system as long as the original Jacobi iterative method would converge. Furthermore, we use data to train an algorithm to select which scheme to use at each cycle of the SRJ method for rapid convergence. Specifically, the algorithm is trained using convergence data obtained from randomly applying SRJ schemes to the 1D Poisson problem. The automatic selection heuristic that is developed based on this limited data is found to provide good convergence for a wide range of problems.

Keywords: Linear Solvers, Jacobi Iteration, Partial differential equations (PDEs), Iterative Methods

1 Introduction

The solution of large linear systems of equations is an important problem in computational science and engineering, and is of great practical interest to scientists and engineers who are modeling physical phenomena such as fluid flow [1] or electromagnetics [2]. These phenomena are usually modelled by partial differential equations (PDEs) which may not be amenable to analytic solution but can usually be solved numerically. The numerical solution of PDEs by a numerical method leads to a large sparse linear system of equations which must be solved efficiently.

A host of methods have been developed in order to solve these linear systems, usually classified into direct and iterative methods [3]. Direct methods solve linear systems exactly but may become intractable as the number of degrees of freedom grows. Iterative methods have become popular in recent years as computing capability has continued to improve due to advances in hardware. Stationary iterative methods such as Jacobi iteration [4] and Gauss-Seidel were the first iterative methods used for solving large linear systems, and utilize relaxation steps to remove components of the residual vector in order to converge towards the exact solution [5]. However, the number of iterations required for convergence grows rapidly with the size of the system [6]. Krylov subspace methods such as conjugate gradient [7] and GMRES [8] achieve

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faster convergence compared to stationary iterative methods and are therefore the most prominent iterative methods for solving sparse linear systems of equations. Despite this, Jacobi iteration is exceptionally well suited to implementation on the latest high performance computers and can achieve good performance due to its highly parallel nature and remarkable simplicity. Furthermore, Jacobi iteration is commonly applied as a smoother in multigrid solvers which exhibit fast convergence [9]. Therefore, theoretical improvements to the convergence of Jacobi iteration can augment its usability on high performance systems, and potentially make it a more viable method for solving large linear systems compared to the Krylov subspace methods, whose performance may be inhibited on large hierarchical high performance computing systems due to the reduction operations (e.g. dot products) that are required at every step of these algorithms.

There has been recent work to improve the convergence of Jacobi iteration. The Scheduled Relaxation Jacobi (SRJ) method developed by Yang and Mittal accelerates the convergence of the standard Jacobi iteration by applying prescribed relaxation factors in a cyclic fashion [10]. In each cycle of the algorithm, a fixed number of relaxed Jacobi iterations $M$ are performed with $P$ distinct predetermined factors which depend on the SRJ scheme one chooses to use. Each scheme is characterized by the number of distinct relaxation values used in the cycle (denoted by $P$), the specific relaxation factors used (listed in the vector $\vec{\Omega} = [\omega_1, \omega_2, ..., \omega_P]$ where $\omega_1 > \omega_2 > ... > \omega_P$), and the frequency with which each factor $\omega_i$ is applied (denoted by $q_i$ and stored in the vector $\vec{Q} = [q_1, q_2, ..., q_P]$). For a given $P$, one can derive a scheme characterized by the distinct relaxation factors $\vec{\Omega}$ and their frequency of use $\vec{Q}$ which results in optimal convergence. This is done by solving a min-max optimization problem in which the maximum possible amplification factor associated with the scheme is minimized. Yang and Mittal derive a variety of schemes for $P = 2, 3, 4, 5$ and derive parameters for different grid sizes $N$. Typical schemes involve a few overrelaxation steps followed by many underrelaxation steps so that the overall effect of the iterations attenuates certain modes. For a certain $P = 7$ scheme, they observe a 190 times speedup in convergence for the 2D Laplace and Poisson equations relative to standard Jacobi iteration. While schemes corresponding to larger $P$ would likely provide even faster convergence, deriving such schemes is difficult as the system of equations for the scheme parameters grows stiffer as $P$ and $N$ are increased. Adsuara et al. proposed a number of algebraic simplifications in order to make it easier to derive more complicated schemes for $P$ up to 15 and $N = 2^{15}$. They report even higher speedups than Yang and Mittal, nearly to a factor of 1000 for large $P$ and problem size $N$ [11]. In [12], Adsuara et al. propose SRJ schemes in which each relaxation factor is only used once per cycle. They reason that although a scheme with sufficiently large $P$ may greatly reduce the solution residual, the overall number of iterations associated with the cycle $M$ may be extremely large if each distinct relaxation factor is used many times. In this case, the SRJ scheme may not necessarily outperform Jacobi iteration. They introduce the Chebyshev Jacobi method (CJM) and find that Yang’s original min-max optimization problem for deriving an optimal SRJ scheme becomes a simpler problem of solving for the roots of a scaled Chebyshev polynomial, the reciprocal of which are the desired relaxation parameters. A CJM scheme can be derived for a given problem size based on the minimum and maximum wavenumbers. For a fixed number of iterations, their schemes with distinct relaxation factors converge faster relative to the original schemes by Yang and Mittal where relaxation parameters are repeatedly used. Specifically, SRJ schemes where $P = M$ are most effective for fast convergence.

Both the SRJ and CJM schemes (which hereafter are also considered SRJ schemes where $P = M$) are specific to a problem size $N$. This presents two advantages; namely that the convergence rate of each individual SRJ scheme with $M$ relaxation parameters can be estimated based on the wavenumbers of the problem of interest for which the scheme was derived, and that the schemes will converge quickly as they are tailored to the specific problem. However, this second advantage is also a drawback. Constructing a new scheme for each problem can be a tedious process if one is interested in exploring a variety of problems, or even a single problem under a variety of discretizations. In this work, we consider a sequence of SRJ schemes that can be applied to all linear systems which would originally converge via Jacobi iteration. These schemes are equivalent to a non-stationary Richardson iteration which uses $P = M$ relaxation factors and assumes the matrix eigenvalues are bounded within $(-1, 1)$ [13]. For our sequence of schemes, estimating the convergence rate for a given problem is difficult. A good scheme for convergence is not known a-priori and must be found through experimentation for each linear system under consideration. Furthermore, the
convergence rate of each scheme is not necessarily static and may change throughout the solution process (a scheme that exhibits a fast convergence rate in one cycle may not do so in the next). As an alternative approach, we develop a data driven heuristic to determine which scheme to use at a given step of the solution process so that we can obtain rapid convergence for a variety of problems.

The remainder of this paper is organized as follows. Section 2 illustrates an approach for developing a class of general SRJ schemes. These schemes are not restricted to specific problem sizes as those in [10] and [11] so they may be used to solve a variety of linear systems (the only requirement is that the original systems could be solved by the standard Jacobi iterative method). Section 3 presents the data driven approach used to inform the automatic selection process for selecting which scheme to use in a given SRJ cycle. A simple heuristic is developed to select a scheme for the next cycle. Section 4 shows the performance of the SRJ schemes with this data based automatic selection heuristic for both in-sample matrices from which we collected data, as well as out-of-sample test matrices which are progressively more and more distinct from the in-sample matrices. Section 5 provides concluding remarks and a vision for SRJ on high performance computers. Our hope is that practitioners can derive their own SRJ schemes and apply our scheme selection heuristic to solve their problems of interest.

2 Derivation of General SRJ schemes

We present an approach to derive a set of relaxation factors (an SRJ scheme) which will improve convergence of Jacobi iteration when applied to a linear system of equations $Ax = b$, $A \in \mathbb{R}^{n \times n}$, $x \in \mathbb{R}^n$, $b \in \mathbb{R}^n$. We begin by defining the original Jacobi iterative method. This involves a matrix splitting of $A$ into the following form

$$A = D + L + U$$

(1)

where $D$ is a diagonal matrix containing the diagonal entries of $A$, and $L$ and $U$ are matrices containing the lower and upper portions of $A$ below and above the diagonal. The linear system can be written as the following fixed point update from step $n$ to step $n + 1$

$$x^{(n+1)} = -D^{-1}(L + U)x^{(n)} + D^{-1}b$$

(2)

Equation (2) represents the Jacobi iterative update for solving a linear system of equations where $B_J = -D^{-1}(L + U)$ is the iteration matrix associated with the Jacobi update. The rate of convergence of the iteration depends on the spectral radius of the iteration matrix $B_J$, which must be less than 1 for Jacobi iteration to converge [14]. We now consider the weighted Jacobi iteration which is given by the following update equation

$$x^{(n+1)} = \omega \left[ B_J x^{(n)} + D^{-1}b \right] + (1 - \omega)x^{(n)}$$

(3)

and involves weighting the original update equation (2) by some relaxation factor $\omega$. Setting $\omega < 1$ is known as underrelaxation while setting $\omega > 1$ is referred to as overrelaxation (applying overrelaxation alone is known to cause Jacobi iteration to diverge). The update equation (3) can also be written as

$$x^{(n+1)} = [(1 - \omega)I + \omega B_J] x^{(n)} + \omega D^{-1}b$$

(4)

We define the error vector at step $n$ as $e^{(n)} \equiv x^{(n)} - x$ where $x$ is the exact solution to the linear system. The exact solution satisfies the update equation exactly

$$x = [(1 - \omega)I + \omega B_J] x + \omega D^{-1}b$$

(5)

Subtracting Equation (5) from (4) yields an equation for the evolution of the error vector from one step to the next.

$$e^{(n+1)} = \left[ (1 - \omega)I + \omega B_J \right] e^{(n)}$$

(6)
The accumulation of error is based on the amplification matrix $B_\omega$. Convergence of weighted Jacobi is guaranteed if the matrix $B_\omega$ has a spectral radius less than 1.

We now consider an iteration scheme where $M$ iterations of the relaxed Jacobi method with distinct $\omega$ are performed. Let these iterations comprise one cycle of the SRJ algorithm, and denote the overall amplification matrix associated with these $M$ iterations by $B_{\omega,\text{cycle}}$. Also denote the amplification matrix associated with each individual iteration by $B_\omega$. If $e^{(n+1)}$ and $e^{(n)}$ represent the error prior to and after a cycle of $M$ iterations, then the error accumulates as follows

$$e^{(n+1)} = B_{\omega,\text{cycle}} e^{(n)} = \prod_{i=1}^{M} B_\omega e^{(n)} = \prod_{i=1}^{M} \left[(1 - \omega_i) I + \omega_i B_\omega\right] e^{(n)} \quad (7)$$

The amplification of the error at each cycle is related to the eigenvalues of the matrix $B_{\omega,\text{cycle}}$. It can be shown that the eigenvalues of $B_{\omega,\text{cycle}}$ are related to the eigenvalues of $B_\omega$ as follows

$$\lambda(B_{\omega,\text{cycle}}) = G_M(\lambda(B_\omega)) \quad \text{where} \quad G_M(\lambda) := \prod_{i=1}^{M} (1 - \omega_i) + \omega_i \lambda \quad (8)$$

In other words, the eigenvalues of $B_{\omega,\text{cycle}}$ is an $M$-degree polynomial of the eigenvalues of $B_\omega$, which need to be in $(-1, 1)$ for Jacobi iteration to converge. We call this $M$-degree polynomial the amplification polynomial associated with the SRJ scheme, and denote it by $G_M$. In order to design an SRJ scheme with $M$ relaxation parameters, we only need to design a $M$-order polynomial $G_M$ and ensure it has $M$ real roots. The value of $G_M(\lambda)$ should lie in $(-1, 1)$ when $\lambda \in (-1, 1)$, in order for $B_{\omega,\text{cycle}}$ to have a spectral radius less than 1 when the Jacobi iteration matrix $B_\omega$ has a spectral radius less than 1. In fact, one can deliberately construct the amplification polynomial so that it converges more rapidly than Jacobi for ranges of $\lambda(B_\omega)$.

We construct a sequence of amplification polynomials of increasing order $M$. The resulting SRJ scheme has convergence properties suitable for matrices of different stiffness. Our amplification polynomials are shown in Figure 1 for $M = 1, 2, 3, 5, 7$. These polynomials are constructed such that they are bounded for the widest range possible in $(-1, 1)$ by some bounding value. For $M = 1$, the polynomial is a straight line and attenuates all modes associated with eigenvalues between $(-1, 0)$ by at least a factor of $\frac{3}{4}$. This bounding value corresponds to a Jacobi relaxation scheme with relaxation factor $\frac{2}{3}$, which is a popular choice as a smoother for multigrid methods because it decays the higher order modes of the error by a factor of $\frac{3}{4}$ each iteration [9]. As the degree of the polynomial $M$ grows, the range of eigenvalues over which the amplification is bounded also grows. Within this range, the amplification polynomial is actually a scaled version of a Chebyshev polynomial. These polynomials have the property that all extrema have the same absolute value, so they are useful as polynomials which are bounded in some interval. In this paper, we denote the $M$th Chebyshev polynomial by $T_M$.

Our amplification polynomials are scaled versions of the Chebyshev polynomials. One can derive the relationship between the amplification polynomials and the Chebyshev polynomials (done in Appendix A), which is

$$G_M(\lambda) = \frac{T_M(f(\lambda))}{3} \quad \text{where} \quad f(\lambda) := \frac{(\lambda^* + 1)\lambda + (\lambda^* - 1)}{2} \quad (9)$$

where $\lambda^*$ satisfies $T_M(\lambda^*) = 3$. Table 1 shows the amplification polynomials for $M = 1, 2, 3, 5$ (plotted in Figure 1) as well as the corresponding Chebyshev polynomials. The maximum eigenvalue $\lambda_{\text{max}}$ for which the amplification polynomial is bounded by $\frac{1}{2}$ is also shown (and grows with polynomial order $M$). The amplification polynomial is always bounded at the minimum eigenvalue of $\lambda_{\text{min}} = -1$ for all $M$.

The SRJ scheme with $M$ relaxation factors can be derived given the $M$-degree amplification polynomial. Given the $j$th root of $G_M(\lambda)$ which we denote by $\tilde{\lambda}_j$, it is true that

$$G_M(\tilde{\lambda}_j) = 0 \rightarrow \prod_{i=1}^{M} \left[(1 - \omega_i) + \omega_i \tilde{\lambda}_j\right] = 0 \rightarrow (1 - \omega_j) + \omega_j \tilde{\lambda}_j = 0 \quad (10)$$
Figure 1: Amplification polynomials $G_M(\lambda)$ for $M = 1, 2, 3, 5, 7$. The polynomials are bounded by $\frac{1}{3}$ for some region within $\lambda \in (-1, 1)$ which grows as $M$ increases. Applying the SRJ schemes corresponding to these amplification polynomials results in many of the solution error eigenmodes being attenuated by at least a factor of $\frac{1}{3}$.

Table 1: The amplification polynomials $G_M$ and the maximum $\lambda$ for which the polynomials are bounded by $\frac{1}{3}$, for $M = 1, 2, 3, 5$. The corresponding Chebyshev polynomials $T_M(\lambda)$ are also shown.

| $M$ | $T_M(\lambda)$                  | $G_M(\lambda)$                                         | $\lambda_{\text{max}}$ |
|-----|---------------------------------|--------------------------------------------------------|------------------------|
| 1   | $\lambda$                      | $\frac{2}{3}\lambda + \frac{1}{3}$                   | 0.0                    |
| 2   | $2\lambda^2 - 1$               | $\frac{2}{3}(1.2071\lambda + 0.2071)^2 - \frac{4}{3}$ | 0.6569                 |
| 3   | $4\lambda^3 - 3\lambda$       | $\frac{4}{3}(1.0888\lambda + 0.0888)^3 - (1.0888\lambda + 0.0888)$ | 0.8368                 |
| 5   | $16\lambda^5 - 20\lambda^4 + 5\lambda$ | $\frac{16}{3}(1.0314\lambda + 0.0314)^5 - \frac{\lambda}{3}(1.0314\lambda + 0.0314) + \frac{5}{3}(1.0314\lambda + 0.0314)$ | 0.9391                 |
The $j$th relaxation factor in the SRJ scheme is related to the $j$th root of the polynomial by Equation (11)

$$\omega_j = \frac{1}{1 - \bar{\lambda}_j}, \forall j \in 1 : M$$

We tabulate the relaxation factors associated with the SRJ schemes for size $M = 1, 2, 3, 5, 7$ in Table 2. Applying $M$ relaxation factors given in Equation (11) in an SRJ cycle results in the solution error eigenmodes being amplified by $G_M(\lambda)$. Each scheme results in a different amplification of the eigenmodes. Larger schemes attenuate modes corresponding a larger range of eigenvalues but are more computationally intensive to execute as they involve more iterations.

| $M$ | SRJ scheme parameters |
|-----|-----------------------|
| 1   | 0.66666667            |
| 2   | 1.70710678, 0.56903559 |
| 3   | 3.49402108, 0.53277784, 0.92457411 |
| 5   | 9.23070105, 0.51215173, 0.97045899, 0.62486988, 2.1713295 |
| 7   | 17.84007924, 0.50624677, 0.9845549, 1.69891732, 0.56014439, 0.69311375 |

We can define a procedure to compute the $M$ order SRJ scheme for arbitrary $M$. The SRJ scheme is related to the roots of the $M$ order amplification polynomial, which is a scaled Chebyshev polynomial. Therefore, we can identify a relationship between the roots of the Chebyshev polynomial and those of the amplification polynomial. It is true that $G_M(\lambda) = \frac{T_M(f(\lambda))}{3}$ where $f(\lambda)$ is the transformation given in Equation (9), so it follows that $G_M(f^{-1}(\lambda)) = \frac{T_M(\lambda)}{3}$. Denote the transformation $f^{-1}$ as $g$. Given the roots $x_j$ of $T_M$, the roots of $G_M$ are $\bar{\lambda}_j$ where

$$\bar{\lambda}_j = g(x_j), \quad \text{where} \quad g(x) := \frac{2}{\lambda^* + 1}x + \frac{1 - \lambda^*}{1 + \lambda^*}$$

(12)

As before, $\lambda^*$ satisfies $T_M(\lambda^*) = 3$. This gives a relationship between the roots of the Chebyshev polynomial and those of the amplification polynomial.

The $M$ order SRJ scheme can be derived through the following three steps:

1. Find the roots of the $M$-degree Chebyshev polynomial $T_M$ denoted by $x_j$.
2. Given the roots $x_j$ of the Chebyshev polynomial $T_M$, the roots of the amplification polynomial $G_M$ are $\bar{\lambda}_j = g(x_j)$, where $g$ is the transformation defined in Equation (12).
3. Given the roots of the amplification polynomial $\bar{\lambda}_j$, solve for the corresponding relaxation factors $\omega_j$ using Equation (11).

The procedure outlined here provides a method to derive many SRJ schemes which can be used to solve linear systems that would converge using standard Jacobi iteration. The schemes here are equivalent to those which would be obtained from non-stationary Richardson iteration, if one prescribed $M$ relaxation factors and assumes that the matrix eigenvalues are bounded by $-1$ and $1$ in this procedure [13]. One difficulty that arises with the use of these SRJ schemes are issues of floating point error associated with the large range of relaxation factors. For example, applying all of the large relaxation parameters in a given SRJ scheme can potentially lead to overflow. To ameliorate these problems, we follow Yang’s suggestion in [10] of cycling through relaxation parameters and successively applying the parameters which will maximize the error reduction at each step for robust convergence in the presence of roundoff.
3 Developing a data-driven heuristic for selecting SRJ schemes

The Scheduled Relaxation Jacobi method provides an approach to accelerate Jacobi iteration by identifying sets of relaxation factors that can improve convergence. A number of schemes may be derived simply based on the number of distinct relaxation factors \( M \) desired in a cycle. Choosing an appropriate SRJ scheme which provides fast convergence for a given problem is not straightforward and requires experimentation. A scheme consisting of many distinct relaxation factors (corresponding to large \( M \)) may not necessarily provide better convergence than one which only utilizes a few relaxation factors (corresponding to small \( M \)). For example, linear systems with few degrees of freedom may converge in fewer iterations using a simpler scheme, whereas larger linear systems may require a scheme with more relaxation parameters. Furthermore, the convergence rate associated with applying a certain scheme may change from one cycle to the next upon repeated use, so selecting a single scheme to use for all cycles of SRJ may not always be optimal. Utilizing SRJ effectively in solving a linear system requires an informed choice of scheme in order to obtain fast convergence for the linear system of interest at each step of the solution process.

We utilize a data driven approach to determine which SRJ scheme to apply in a given cycle. This avoids the need for experimentation with SRJ schemes on different problems. The key idea of the approach is to develop a heuristic that is based on convergence data collected from randomly applying SRJ schemes. The heuristic can be used to decide the SRJ scheme at the next step which will provide the best overall convergence rate, based on current solution state parameters. To simplify the decision making process, we filter out select schemes corresponding to particular \( M \) and designate these as particular scheme levels we can select from (the values of \( M \) corresponding to a specific scheme level are shown in Appendix B). When selecting an SRJ scheme to use for the next cycle, the solver is restricted to three choices. Given the current scheme level, the solver can either choose to increase the level, keep the same level, or decrease the level and use the corresponding scheme at the next cycle. Our goal is to develop a heuristic that allows us to select the scheme that will provide the best convergence rate at the next cycle.

To develop a rule for selecting SRJ schemes, we collect convergence data from a specific matrix, namely, the tridiagonal linear system arising from discretization of the 1D Poisson equation. The 1D Poisson equation is a prototypical test PDE and is given in Equation (13)

\[
-\frac{d^2u}{dx^2} = f(x), \quad x \in [0,1]
\]

A finite difference discretization of the PDE leads to a symmetric and tridiagonal matrix with the following structure

\[
A = \frac{1}{\Delta x^2} \begin{pmatrix}
2 & -1 & & & \\
-1 & 2 & -1 & & \\
& -1 & \ddots & \ddots & \\
& & -1 & 2 & -1 \\
& & & -1 & 2
\end{pmatrix}
\]

where \( \Delta x = \frac{1}{N+1} \) and \( N \) is the number of degrees of freedom. We consider matrices of the following sizes: \( N = 2, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400 \). We perform a data collection process for each matrix. In each case, the initial solution is a vector of zeros while the right hand side is a vector of ones. We begin by applying the simplest SRJ scheme corresponding to \( M = 1 \) (scheme level 0) at the initial step. Applying a cycle of SRJ involves a series of \( M \) relaxed Jacobi updates given by Equation (3). Afterwards, the ratio of the residual before and after applying the scheme is recorded along with the scheme level that was used. All subsequent data collection steps involve the following procedure (depicted visually in Figure 2). The three choices for the SRJ scheme to use at the next cycle (corresponding to increasing the level, decreasing the level, or keeping the same level) are employed and the average rate of convergence of the iterations associated with using each scheme is computed. The average convergence rate of the iterations comprising an SRJ cycle is computed by Equation (14), where \( r_i \) is the initial residual at the beginning of the cycle, \( r_{i+1} \) is the final residual after performing the SRJ iterations in the cycle, and \( M \) is the number of
iterations performed, equal to the number of distinct relaxation parameters in the given SRJ scheme.

\[
\text{Average Convergence Rate} = \log \left( \frac{r_{i+1}}{r_i} \right) M
\]

(14)

The action taken to modify the scheme level (increase, decrease, same) and the associated convergence rate are recorded. The residual ratio observed at the last step and the current scheme level (before any modifications) are recorded as well. These are the same for the three actions and are considered our state variables. Given the previous residual ratio and current level, we now have the average convergence rate that will be achieved by taking each of the three possible actions at the next cycle. The best scheme to use at the next cycle given our state is now easy to determine - it is the one which provides the best convergence rate. To finish this data collection step, we randomly select one of the three schemes to use and record the residual ratio obtained from utilizing this scheme as well as the level associated with the scheme. This is the given data we store in preparation for the next data collection step, which follows the same procedure as before (determine the convergence rates associated with the three possible actions, record data, and randomly select an action and record the residual ratio and level). It is worth noting that at the first step, we will not be able to decrease the level (due to being at the lowest scheme level) so only two actions (increasing the level or keeping the scheme level) are available.

![Figure 2: Depiction of data collection procedure. Three data points are collected at each step corresponding to each of the three possible schemes we can select for the next cycle (resulting from increasing, decreasing or keeping the scheme level). Each data point contains four parameters - the action taken, the average convergence rate of SRJ using the new level, the current scheme level, and the residual ratio obtained at the previous cycle. Note that the average convergence rate associated with each action/scheme taken will differ.](image)

This illustrates one step of our data collection process, which is shown in Figure 2. In summary, we collect data regarding our current state (the residual ratio at the previous step and the current scheme level) and the convergence rate associated with each of the three possible schemes (each step provides three data points). Data is collected by performing many trials in which SRJ is used to reduce the residual of the solution below an \( L_2 \) norm of 1e-8. Each trial consists of many cycles of the SRJ algorithm applied using the data collection procedure described. We collected roughly 1 million data points for each size \( N \). Given the residual ratio achieved at the previous step and the current level, we can determine which action will result in the best convergence rate based on our data.

The collected data is postprocessed to develop a heuristic for selecting SRJ schemes. All of the convergence data obtained is organized according to the current scheme level state variable. All data points in each level are sorted in order of increasing previous residual ratio value and grouped into clusters of \( N \text{set} = 10000 \) data points. Within each cluster, the data points corresponding to increasing the level, decreasing the level and keeping the level are identified, and the mean of the average convergence rates associated with each of the actions is computed along with a 95% confidence interval to ensure we are confident about which action is the best within the cluster. The action corresponding to the highest average convergence rate is recorded after ensuring that the confidence interval associated with it does not overlap with the confidence intervals of the other two actions. The mean residual ratio of all data points in the cluster is also recorded. The best action for every cluster of points can be plotted as a single data point in the level and residual ratio space as shown in Figure 3.
Figure 3: Visualization of the best action to take within the level vs residual ratio space. We develop simple heuristics to determine which action to take based on the previous residual ratio. The current level does not appear to affect the best action.

The region of the level and residual ratio state space where a specific cluster lies appears to have a big influence on the best action to take at the next cycle. In general, when the residual ratio in the previous step is high, the best action for obtaining a good convergence rate at the next cycle is to increase the scheme level. If the residual ratio at the previous step is very low, it is best to continue using the same set of relaxation factors as before. In between these regions, it is best to decrease the level. We develop a simple rule to decide how to select between SRJ schemes. If the previous residual ratio is above 0.4, we should increase the scheme level. If the residual ratio is between 0.2 and 0.4, it is best to decrease the level. When the residual ratio is lower than 0.2, it is best to keep using the same SRJ scheme for continued good performance. The data suggests a general and simple heuristic that can be used to determine the best action to take at a given step for selecting SRJ schemes and obtaining robust convergence. The current scheme level being used does not appear to affect the best action to take at the next step, so our rule is independent of this parameter. Our heuristic is summarized in Algorithm 1, and can be used to automatically select SRJ schemes for each problem in order to solve linear systems with SRJ efficiently.

Algorithm 1 Select SRJ Schemes using data driven heuristic

| Given Previous Residual Ratio and Current Scheme Level |
|-------------------------------------------------------|
| if Residual Ratio > 0.4 then |
|  Level = Level + 1 |
| else if Residual Ratio < 0.4 and Residual Ratio > 0.2 then |
|  Level = Level - 1 |
| else |
|  Level = Level |
| end if |
4 Results

To understand how effective SRJ with our scheme selection heuristic is for achieving fast convergence, we perform convergence tests on a variety of linear systems. We begin by testing on linear systems involving the training matrices from which we initially collected data (specifically, those arising from discretization of the 1D Poisson equation). Afterwards, we test matrices which are progressively more different from our in-sample matrices. In particular, these test matrices are:

- Tridiagonal matrices corresponding to the 1D Poisson equation (of different sizes from those in the training set)
- Random tridiagonal matrices which are symmetric and diagonally dominant
- Pentadiagonal matrices corresponding to the 2D Poisson equation
- Random pentadiagonal matrices which are symmetric and diagonally dominant

4.1 In-sample testing

As a first test of our data based heuristic, we solve the in-sample training linear systems we initially collected data from. The matrices comprising these linear systems are the tridiagonal matrices of size \( N = 2, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400 \) corresponding to discretization of the 1D Poisson equation using finite differences on a uniform grid with Dirichlet boundary conditions. For each system, the right hand side is set to a vector of ones of size \( N \) and the initial solution vector is the zero vector of the same size. The performance of the SRJ method using our heuristic to choose a scheme for the next cycle is compared to unrelaxed Jacobi iteration as well as an SRJ method with an approach which always increases the scheme level at each subsequent cycle. This approach can be thought of as a simple brute force heuristic one could use to select schemes without the need to experiment with each scheme, and provides a benchmark approach that our heuristic should outperform. Convergence is assumed when the \( L_2 \) norm of the residual \( ||b - Ax|| \) falls below a tolerance value of 1e-7. Figure 4 illustrates a convergence plot for the case of \( N = 100 \). In this case, SRJ with the heuristic outperforms the other approaches. Our heuristic approach begins at a scheme level of 0, and increases the scheme level until reaching scheme level 11, and which point it alternates between using the SRJ schemes corresponding to scheme level 10 (\( M = 47 \)) and 11 (\( M = 63 \)). This approach requires approximately 1000 iterations for convergence. Meanwhile, SRJ with a purely increasing rule requires over 3000 iterations for convergence. The standard Jacobi method without relaxation would require many more iterations.

This comparison is performed for all of the training matrix sizes. In each case, the number of iterations required for each method to converge is recorded. The results are shown in Figure 5. For all cases, SRJ with our heuristic outperforms a brute force SRJ approach with a purely level increasing rule, and generally requires at most half the number of iterations as the increasing approach. The Jacobi method works well for small \( N \) but the number of iterations increases rapidly as \( N \) grows larger. For \( N > 100 \), Jacobi iteration does not converge in a reasonable number of iterations so we do not record this data in Figure 5. Overall, the heuristic performs well on the training matrices and does not require the user to explore the effect of each individual SRJ scheme on each matrix system to achieve fast convergence.

4.2 Out of sample testing

Generalizeability is an important aspect of any tool based on data. While the heuristic works well for in-sample matrices, it is important that it generalizes well to arbitrary matrices and provides good convergence to those which are out of sample. 1D Poisson matrices of sizes differing from our training matrices are the most similar to those in our training set which are out of sample, providing a good initial test of our rule on unseen matrices. We test our approach on 1D Poisson matrices of size \( N = 15, 25, 35, 45, 55, 65, 75, 85, 95, 150, 250, 350 \) which can be regarded as interpolated samples of our in-sample
Figure 4: Convergence of SRJ and standard Jacobi approaches for the 1D Poisson matrix of size $N = 100$. The SRJ solver with our heuristic gives the best convergence compared to SRJ with an increasing level approach or a standard unrelaxed Jacobi iteration.

Figure 5: Convergence of 1D Poisson Training Matrices. SRJ with the data based rule achieves convergence in the fewest number of iterations for all in-sample matrices.
matrices. Additionally, we test extrapolated samples corresponding to sizes \( N = 500, 600, 700 \) (which are larger than the maximum size of our training matrices). As before, the three approaches (standard Jacobi, SRJ with increasing rule, and SRJ with our data driven heuristic) are used. Figure 6 shows the number of overall iterations required for the three methods to converge for all of the test \( N \). For the interpolated cases, we find that SRJ with our data based heuristic achieves convergence in the fewest number of iterations. For the extrapolated cases (shown with a dotted line), standard Jacobi iteration and SRJ with a level increasing rule do not converge in a reasonable number of iterations. SRJ with the data driven rule outperforms these methods in this case as well. These results illustrate that the data based heuristic does not overfit to the training matrices but can work well on matrices outside of the training set.

![Test Matrix Convergence for 1D Poisson](image)

Figure 6: Convergence of Out of sample 1D Poisson Matrices. SRJ with the data based rule performs well for both the interpolated and extrapolated matrices, suggesting that it does not overfit to the training matrices.

As a more general test of the efficacy of our rule, we test our SRJ approach on random symmetric tridiagonal systems which are diagonally dominant. We constructed random symmetric tridiagonal systems of various sizes, ensuring that they are diagonally dominant so that Jacobi iteration would converge. This was done by creating a random array for the diagonal components as well as a random array for the subdiagonal and superdiagonal (set to the same array to enforce symmetry). For each row that was not diagonally dominant, the diagonal was modified so that its absolute value was equivalent to the sum of the absolute value of the off diagonal entries of that row. The first and last diagonal entries were set to twice the value of the superdiagonal and subdiagonal entry of that row respectively, to resemble the structure of the 1D Poisson equation and to make the linear system easier for Jacobi iteration to solve. Matrices of the following sizes were considered: \( N = 2, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500, 600, 700, 800, 900, 1000 \). For each \( N \), 20 different tridiagonal matrices which satisfy the symmetric diagonally dominant requirements are constructed and the number of iterations required for standard Jacobi iteration, SRJ with an increasing scheme, and SRJ with our heuristic to converge are recorded. The mean number of iterations required for each approach is plotted as a function of matrix size \( N \) in Figure 7. For very small \( N \) the Jacobi method outperforms the increasing SRJ approach. However, for large \( N \) Jacobi iteration generally requires an order of magnitude more iterations than the SRJ approaches. The SRJ approach with the heuristic outperforms the increasing SRJ approaches in all cases. For the larger \( N \), SRJ with the data based heuristic takes approximately half the number of iterations as SRJ with the increasing level rule. Despite being developed
on limited convergence data from the 1D Poisson matrices, the heuristic can be used to obtain relatively good convergence for general symmetric tridiagonal matrices which could be solved by the standard Jacobi iteration.

Figures 5, 6, and 7 illustrate that the SRJ method with the data based heuristic provides good convergence for a variety of matrices including those that were not observed before. The matrices tested were arbitrary tridiagonal matrices which are symmetric and diagonally dominant, which tend to arise from discretization of one-dimensional problems. To test a more general class of matrices that exhibits behavior further from our in-sample training matrix set, we consider linear systems that arise from two-dimensional PDEs. We consider the 2D Poisson equation given by Equation (15)

$$- \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) = f(x,y), \ x, y \in [0, 1] \quad (15)$$

The linear system $Ax = b$ which arises from discretization of Equation (15) by the finite difference method on a uniform grid is the following pentadiagonal matrix

$$A = \begin{pmatrix} d & a & c & \cdots & \cdots \\ a & d & a & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ c & \cdots & \cdots & \cdots & a \\ \cdots & \cdots & \cdots & a & d \end{pmatrix}$$

where

$$a = -\frac{1}{(\Delta x)^2}, \ c = -\frac{1}{(\Delta y)^2}, \ d = \frac{2}{(\Delta x^2 + \Delta y^2)} \quad (16)$$
and $\Delta x = \frac{1}{N_x+1}$ and $\Delta y = \frac{1}{N_y+1}$ denote the grid spacing and $N_x$ and $N_y$ represent the number of degrees of freedom in the $x$ and $y$ directions, respectively.

We consider matrices corresponding to grid sizes $N_x = N_y = 2, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100$ which correspond to linear systems with $N_{\text{dofs}} = N_x N_y = 2^2, 5^2, 10^2, 20^2, 30^2, 40^2, 50^2, 60^2, 70^2, 80^2, 90^2, 100^2$ degrees of freedom. We record the number of iterations required for the three methods to converge for each case which is shown in Figure 8. Interestingly, the data driven heuristic is still a reliable metric for determining which scheme to use and gives good convergence compared to the other two approaches.

![2D Poisson Test Matrix Convergence](image)

Figure 8: Convergence of 2D Poisson Matrices of various sizes. The SRJ method with heuristic leads to convergence in fewest iterations.

As a final test, we consider random pentadiagonal matrices which are symmetric and diagonally dominant, and of the same size as the 2D Poisson matrices considered. This is an even more general class of matrices that the 2D Poisson matrix falls into. For each size, 20 different matrices which are pentadiagonal, symmetric and diagonally dominant are constructed and the number of iterations required for each approach to converge below the tolerance is measured. The procedure for constructing these matrices is similar to that for constructing the tridiagonal matrices except that an extra random array must be generated now that there is an extra nonzero subdiagonal and superdiagonal (which have the same values due to symmetry). Figure 9 shows the mean number of iterations required for each method as a function of matrix size $N$. As before, the SRJ method with our heuristic outperforms the other approaches. The disparity in the number of iterations required between the two SRJ approaches is not very large in this case. In particular, for large $N$ the increasing approach takes approximately only 1.5 times more iterations than SRJ with the data based approach. The heuristic possibly does not generalize as well to this new class of matrices compared to the tridiagonal matrices. Regardless, it provides good convergence even for general pentadiagonal systems which could arise from two dimensional PDEs, despite being developed based on data from a single matrix corresponding to a one-dimensional Poisson problem.

The data based rule for selecting SRJ schemes provides a mechanism to apply SRJ effectively to a variety of matrices without the need to specifically tailor schemes to the given matrix or problem size. Despite being developed from convergence data from a specific matrix, the rule generalizes well to matrices outside of the training set. Namely, SRJ with the data based heuristic provided fast convergence for arbitrary symmetric and diagonally dominant tridiagonal and pentadiagonal matrices. Such matrices arise from discretization
Figure 9: Convergence of Random Pentadiagonal Matrices of various sizes. The SRJ method with heuristic leads to convergence in fewest iterations, although the increasing approach takes only 1.5 more iterations for larger $N$ (suggesting that the disparity between the two approaches is lower compared to earlier cases).

of 1D and 2D PDEs, suggesting that SRJ with the heuristic can provide a good avenue for solving matrix problems arising from PDEs. Additionally, it is likely that the heuristic could be used to solve linear systems corresponding to 3D problems as well. One could develop alternative SRJ heuristics based on the type of matrix being studied. However, we found that our heuristic developed from convergence data from 1D Poisson matrices already provides a good rule for solving a large class of matrices.

To further improve the convergence associated with the heuristic, we found during our studies that starting from the lowest scheme level and increasing the scheme until the residual ratio achieved is below 20%, at which point the scheme should be kept the same, generally provides equal or faster convergence than our current heuristic. This is equivalent to removing the decrease action when the residual ratio is between 0.2 and 0.4 and simply replacing it with the increase action. Our current heuristic is robust to the initial starting scheme chosen and provides more flexibility in scheme selection for tougher problems. However, this alternative heuristic may improve convergence in some cases (including the cases explored here).

5 Conclusion

Scheduled Relaxation Jacobi improves upon the convergence of the classic unrelaxed Jacobi iteration by utilizing optimal relaxation parameters. Many different schemes can be derived based on the number of relaxed iteration steps one wants to employ in a given cycle. The best scheme for the optimal convergence for a given problem at a given point in the linear solution process can only be found after experimenting with many different schemes and analyzing which gives the best convergence. Using SRJ with our general schemes to solve a particular problem requires some experimentation before it can be employed to solve a problem effectively.

In this work, we have developed a data based heuristic to determine which scheme a user should use each cycle when solving a linear system using SRJ. Although the rule was developed using only convergence data from a single problem (several matrices corresponding to the 1D Poisson problem), the rule outperforms an SRJ approach which uses a brute force level increasing rule and generalizes well to a large class of matrices.
including tridiagonal and pentadiagonal matrices which commonly arise from discretization of 1D and 2D PDEs. The data based heuristic provides an additional tool that allows practitioners to take advantage of the simplicity of SRJ and apply it very easily for solving a variety of problems without having to hand tailor a scheme for each problem.

The SRJ method provides a promising approach for solving large linear systems of equations. A wide variety of schemes can be easily developed based on the roots of the Chebyshev polynomials, and cycled through using our heuristic for efficient convergence. Furthermore, the method can provide good performance on the latest hardware architectures. Adsuara et al. have explored the performance of an SRJ implementation on GPUs [15]. Furthermore, implementation of SRJ schemes as smoothers within a larger multigrid framework can also provide additional convergence acceleration as shown by Yang and Mittal [16]. The SRJ algorithm may pave the way for a new class of high performance and parallel linear solvers for general PDE problems.
A Amplification polynomials as Chebyshev polynomials

In this appendix, we derive the relationship between the amplification polynomials corresponding to our SRJ scheme and the Chebyshev polynomials, shown in Figure 10 on the left and right respectively.

Figure 10: Amplification polynomials $G_M(\lambda)$ corresponding to SRJ schemes (left) and Chebyshev polynomials $T_M(\lambda)$ for $M = 1, 2, 3, 5, 7$

The original Chebyshev polynomials are bounded by ±1. However, the amplification polynomials we have derived are bounded by $\frac{1}{3}$, suggesting that a vertical scaling of $\frac{1}{3}$ is required to transform from the Chebyshev polynomials to our amplification polynomials. We can define an intermediate polynomial $\tilde{T}_M(\lambda) = \frac{1}{3}T_M(\lambda)$.

In addition to a vertical scaling, a horizontal scaling is required to map between the two polynomials. In particular, we may define an affine transformation $f(\lambda)$ such that $G_M(\lambda) = \tilde{T}_M(f(\lambda))$. The affine transformation must satisfy two requirements which are derived below:

1. By definition, $G(-1) = \tilde{T}_M(f(-1))$. Furthermore, it is true that $G(-1) = \tilde{T}_M(-1)$. Therefore it follows that $G(-1) = \tilde{T}_M(f(-1)) = \tilde{T}_M(-1)$ so the affine transformation obeys $f(-1) = -1$.

2. By definition, $G(1) = \tilde{T}_M(f(1))$. Define $\lambda^*$ as the argument which satisfies $T_M(\lambda^*) = 3$, so that $\tilde{T}_M(\lambda^*) = 1$. It is also true that $G_M(1) = 1$. Therefore, it follows that $G(1) = \tilde{T}_M(f(1)) = \tilde{T}_M(\lambda^*)$ so the affine transformation obeys $f(1) = \lambda^*$.

The first condition follows from enforcing that the vertically scaled Chebyshev polynomial and the amplification polynomial have the same value at $\lambda = -1$, and the second condition ensures that the transformation will result in an amplification polynomial with value 1 at $\lambda = 1$. Assume that the affine transformation has the following form

$$f(\lambda) = c_1 \lambda + c_0$$  \hspace{1cm} (17)

Substituting the two conditions $f(-1) = -1$ and $f(\lambda^*) = 1$ results in the following system of equations for the coefficients $c_0$ and $c_1$

$$- c_1 + c_0 = -1$$  \hspace{1cm} (18)

$$c_1 + c_0 = \lambda^*$$  \hspace{1cm} (19)

Solving for the constants $c_0$ and $c_1$ of the affine transformation yields

$$c_1 = \frac{\lambda^* + 1}{2}, \quad c_0 = \frac{\lambda^* - 1}{2}$$  \hspace{1cm} (20)
Therefore, the affine transformation is given by

\[ f(\lambda) = \frac{(\lambda^* + 1)\lambda + (\lambda^* - 1)}{2} \]  \hspace{1cm} (21)

Lastly, the overall transformation which transforms the original Chebyshev polynomials \( T_M(\lambda) \) to the amplification polynomials \( G_M(\lambda) \) is

\[ G_M(\lambda) = \frac{T_M(f(\lambda))}{3} \]  \hspace{1cm} (22)

where \( f(\lambda) \) is defined in Equation (21).
In this appendix, we show the relationship between the SRJ scheme level and $M$ (given in Table 3). We chose SRJ schemes corresponding to specific $M$ to be selectable in our implementation, in order to prevent the available schemes from being too similar. The results in this paper can be reproduced by utilizing the specific SRJ schemes below.

Table 3: Relationship between $M$ and scheme level used in this work

| Scheme Level | $M$ |
|--------------|-----|
| 0            | 1   |
| 1            | 2   |
| 2            | 3   |
| 3            | 5   |
| 4            | 7   |
| 5            | 10  |
| 6            | 14  |
| 7            | 19  |
| 8            | 26  |
| 9            | 35  |
| 10           | 47  |
| 11           | 63  |
| 12           | 84  |
| 13           | 111 |
| 14           | 147 |
| 15           | 194 |
| 16           | 256 |
| 17           | 338 |
| 18           | 446 |
| 19           | 589 |
| 20           | 778 |
| 21           | 1027|
| 22           | 1356|
| 23           | 1790|
| 24           | 2362|
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