Iterative methods for linear systems

Chris H. Rycroft*

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Introduction

For many elliptic PDE problems, finite-difference and finite-element methods are the techniques of choice. In a finite-difference approach, a solution u_k on a set of discrete gridpoints $1, \ldots, k$ is searched for. The discretized partial differential equation and boundary conditions create linear relationships between the different values of u_k . In the finite-element method, the solution is expressed as a linear combination u_k of basis functions λ_k on the domain, and the corresponding finite-element variational problem again gives linear relationships between the different values of u_k .

Regardless of the precise details, all of these approaches ultimately end up with having to find the u_k that satisfy all the linear relationships prescribed by the PDE. This can be written as a matrix equation of the form

$$Au = b \tag{1}$$

where one aims to find a solution u, given that A is a matrix capturing the differentiation operator, and b corresponds to any source or boundary terms. Theoretically, this problem could be solved on a computer by any of the standard methods for dealing with matrices. However, the real challenge for PDEs is that frequently the dimensionality of the problem can be enormous. For example, for a two-dimensional PDE problem, a 100×100 grid would be a perfectly reasonable size to consider. Thus u would be a vector with 10^4 elements, and A would be a matrix with 10^8 elements. Even allocating memory for such a large matrix may be problematic. Direct approaches, such as the explicit construction of A^{-1} , are impractical.

The key to making progress is to note that in general the matrix A is extremely sparse, since the linear relationships usually only relate nearby gridpoints together. It is therefore natural to seek methods that do not require ever explicitly specifying all the elements of A, but exploit its special structure directly. Many of these methods are *iterative*—starting with

^{*}Electronic address: chr@seas.harvard.edu.

a guess u_k , a process is applied that yields a closer solution u_{k+1} . Typically, these iterative methods are based on a *splitting* of A. This is a decomposition A = M - K where M is non-singular. Any splitting creates a possible iterative process. Equation 1 can be rewritten as

$$(M - K)u = b, (2)$$

$$Mu = Ku + b, (3)$$

$$u = M^{-1}Ku + M^{-1}b, (4)$$

and hence a possible iteration is

$$u_{k+1} = M^{-1}Ku_k + M^{-1}b. (5)$$

Of course, there is no guarantee that an arbitrary splitting will result in an iterative method that converges. To study convergence, one must look at the properties of the matrix $R = M^{-1}K$. For convergence analysis, it is helpful to introduce the *spectral radius*

$$\rho(R) = \max_{j} \{|\lambda_{j}|\},\tag{6}$$

where the λ_j are the eigenvalues of R. It can be shown [2] that an iterative scheme converges if and only if $\rho(R) < 1$. The size of the spectral radius determines the convergence rate, and ideally one would like to find splittings that result in as small a $\rho(R)$ as possible.

An example: a two-dimensional Poisson problem

In the convergence analysis later, we will consider a two-dimensional Poisson problem on the square $-1 \le x \le 1, -1 \le y \le 1$, given by the equation

$$-\nabla^2 u = f, (7)$$

subject to the Dirichlet conditions that u(x,y) vanishes on the boundary. We use a source function of the form

$$f(x,y) = \begin{cases} 1 & \text{if } |x| < 0.5 \text{ and } |y| < 0.5 \\ 0 & \text{otherwise.} \end{cases}$$
 (8)

This is plotted on a 33 \times 33 grid in figure 1. For convergence properties, the eigenfunctions and eigenvalues of this function are very important, and to determine these, it is helpful to consider an associated one-dimensional Poisson problem on the interval $-1 \le x \le 1$,

$$-\frac{d^2u}{dx^2} = f(x),\tag{9}$$

subject to Dirichlet boundary conditions u(-1) = u(1) = 0. We consider a discretization into N+2 gridpoints such that $x_j = -1 + 2j/(N+1)$ for j = 0, ..., N+1. When constructing the corresponding matrix problem, u_0 and u_{N+1} need not be considered, since their values are always fixed to zero. By discretizing the second derivative according to

$$\left. \frac{d^2u}{dx^2} \right|_{x=x_j} = \frac{u_{j-1} + u_{j+1} - 2u_j}{h^2} \tag{10}$$

where h = 2/(N+1), the corresponding linear system is

$$T_{N} \begin{pmatrix} u_{1} \\ u_{2} \\ \vdots \\ u_{N} \end{pmatrix} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 & \ddots \\ 0 & -1 & \ddots & -1 & 0 \\ & \ddots & -1 & 2 & -1 \\ & & 0 & -1 & 2 \end{pmatrix} \begin{pmatrix} u_{0} \\ u_{1} \\ \vdots \\ u_{N} \end{pmatrix} = h^{2} \begin{pmatrix} f_{0} \\ f_{1} \\ \vdots \\ f_{N} \end{pmatrix}. \tag{11}$$

We expect that the eigenvectors of T_N may be based on sine functions. A reasonable guess for the jth eigenfunction is

$$z_j(k) = \sqrt{\frac{2}{N+1}} \sin \frac{\pi k j}{N+1}.$$
 (12)

To verify this is an eigenfunction, and find its eigenvalue, we apply T_N to obtain

$$(T_N z_j)(k) = \sqrt{\frac{2}{N+1}} \left(2\sin\frac{\pi kj}{N+1} - \sin\frac{\pi(k+1)j}{N+1} - \sin\frac{\pi(k-1)j}{N+1} \right). \tag{13}$$

Note that this expression will always be valid for the range k = 1, 2, ..., N, and the boundary values will automatically work out. The last two sine functions can be rewritten using a trigonometric identity to give

$$(T_N z_j)(k) = \sqrt{\frac{2}{N+1}} \left(2\sin\frac{\pi k j}{N+1} - 2\sin\frac{\pi k j}{N+1}\cos\frac{\pi j}{N+1} \right)$$

$$= \sqrt{\frac{2}{N+1}} 2\left(1 - \cos\frac{\pi j}{N+1} \right) \sin\frac{\pi k j}{N+1}$$

$$= 2\left(1 - \cos\frac{\pi j}{N+1} \right) z_j(k)$$

$$(14)$$

and hence z_j is an eigenvector with eigenvalue $\lambda_j = 2(1 - \cos \pi j/(N+1))$. The smallest eigenvalue is $\lambda_1 = 2(1 - \cos \pi/(N+1))$ and the largest is $\lambda_N = 2(1 - \cos N\pi/(N+1))$.

Returning to the two-dimensional problem, the corresponding derivative matrix $T_{N\times N}$ can be written as the tensor product of two one-dimensional problems T_N . Its eigenvectors are the tensor products of the one-dimensional eigenvectors, namely

$$z_{i,j}(k,l) = z_i(k)z_j(l), \tag{15}$$

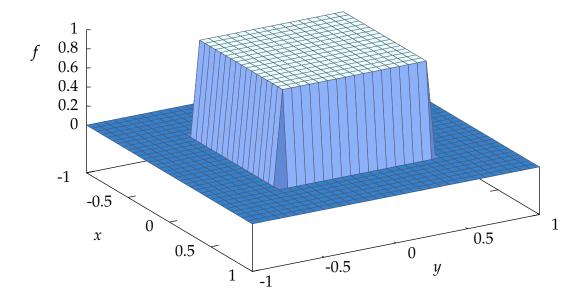


Figure 1: A sample source function f(x, y) on a 33 × 33 grid.

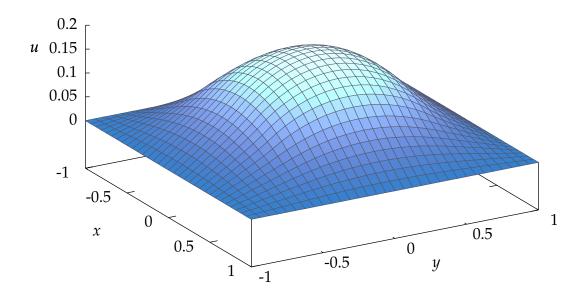


Figure 2: The exact solution to the 2D Poisson problem $-\nabla^2 u = f$, with zero boundary conditions and a source term given in figure 1.

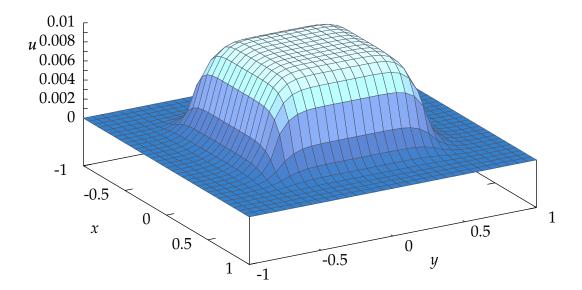


Figure 3: The solution to the example 2D Poisson problem after ten iterations of the Jacobi method.

and the corresponding eigenvalues are

$$\lambda_{i,j} = \lambda_i + \lambda_j. \tag{16}$$

The Jacobi Method

The Jacobi method is one of the simplest iterations to implement. While its convergence properties make it too slow for use in many problems, it is worthwhile to consider since it forms the basis of other methods. Starting with an initial guess u_0 , one successively applies an iteration of the form

for
$$j=1$$
 to N **do** $u_{m+1,j}=\frac{1}{a_{jj}}\left(b_j-\sum_{k\neq j}a_{jk}u_{m,k}\right)$ **end for**

In other words, the jth component of u is set so that it exactly satisfies equation j of the linear system. For the two-dimensional Poisson problem considered above, this corresponds to an iteration of the form

for
$$i = 1$$
 to N do for $j = 1$ to N do

$$u_{m+1,i,j} = \left(h^2 f_j + u_{m,i,j+1} + u_{m,i,j-1} + u_{m,i+1,j} + u_{m,i-1,j}\right)/4$$
 end for end for

To find the corresponding matrix form, write A = D - L - U where D is diagonal, L is lower-triangular, and U is upper-triangular. Then the above iteration is

$$u_{m+1} = D^{-1}(L+U)u_m + D^{-1}b. (17)$$

The Jacobi method has the advantage that for each m, the order in which the components of u_{m+1} are computed has no effect—this may be a favorable property to have in some parallel implementations. However, it can also be seen that u_m must be retained until after u_{m+1} is constructed, meaning we must store u_{m+1} in a different part of the memory. The listing given in Appendix A.1 carries out the Jacobi iteration on the Poisson test function. It makes use of two arrays for the storage of u, computing the odd u_k in one and the even u_k in the other. Figure 3 shows a the progress of the Jacobi method after ten iterations.

The Gauss-Seidel Method

The Gauss–Seidel method improves on the Jacobi algorithm, by noting that when updating a particular point $u_{m+1,j}$, one might as well reference the already updated values $u_{m+1,1}, \ldots, u_{m+1,j-1}$ in the calculation, rather than using the original values $u_{m,1}, \ldots, u_{m,j-1}$. The iteration can be written as

for
$$j = 1$$
 to N **do** $u_{m+1,j} = \frac{1}{a_{jj}} \left(b_j - \sum_{k=1}^{j-1} a_{jk} u_{m+1,k} - \sum_{k=j+1}^{N} u_{m,k} \right)$ **end for**

The Gauss–Seidel algorithm has the advantage that in a computer implementation, it is not necessary to allocate two arrays for u_{m+1} and u_m . Instead, a single array for u_m can be used and all updates can be carried out $in \ situ$. However, the Gauss–Seidel implementation introduces an additional complication that the order in which the updates are applied affects the values of u_m . For a two-dimensional problem, two particular orderings are worth special attention:

• Natural ordering – this is the typical ordering that would result in a **for** loop. We first loop successively through all elements of the first row $(1,1),\ldots,(1,n)$ before moving onto the second row, and so on. Since this frequently corresponds to the order that the grid is stored within the computer memory, this order can lead to performance improvements due to good cache efficiency.

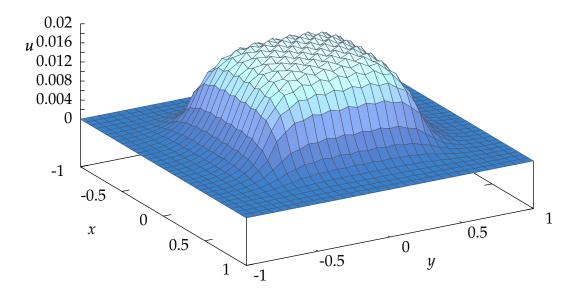


Figure 4: The Gauss–Seidel solution to the example 2D Poisson problem after ten iterations. The crinkles in the solution are due to the Red–Black update procedure.

• Red– $Black\ ordering$ – this is the ordering that results by coloring the gridpoints red and black in a checkerboard pattern. Specifically, a gridpoint (i,j) is colored red if i+j is even and colored black if i+j is odd. During the Gauss–Seidel update, all red points are updated before the black points. For the two-dimensional Poisson problem, updating a red grid point only requires information from the black gridpoints, and vice versa. Hence the order in which points in each set are updated does not matter. The whole Gauss–Seidel update is divided into a red gridpoint update and black gridpoint update, and this can be helpful in the convergence analysis.

From the algorithm above, the corresponding matrix splitting for the Gauss–Seidel method is

$$(D-L)u_{m+1} = Uu_m + b, (18)$$

$$u_{m+1} = (D-L)^{-1}Uu_m + (D-L)^{-1}b.$$
 (19)

Appendix A.2 contains a C++ code to carry out a Gauss–Seidel method on the example problem, and the result after ten iterations is shown in figure 4.

Successive Over-Relaxation

Successive Over-Relaxation (SOR) is a refinement to the Gauss–Seidel algorithm. At each stage in the Gauss–Seidel algorithm, a value $u_{m,j}$ is updated to a new one $u_{m+1,j}$, which is

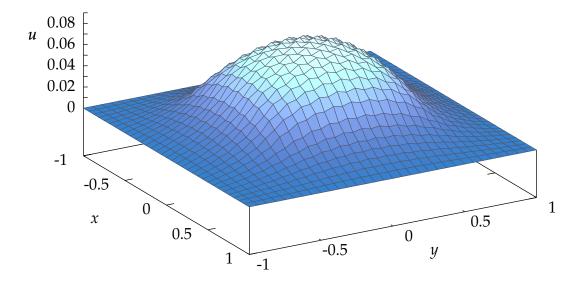


Figure 5: The SOR solution (using the theoretically optimal ω) to the example 2D Poisson problem after ten iterations. The solution is closer to the answer than the Jacobi or Gauss–Seidel methods.

equivalent to displacing $u_{m,j}$ by an amount $\Delta u = u_{m+1,j} - u_{m,j}$. The SOR algorithm works by displacing the values by an amount $\omega \Delta u$, where typically $\omega > 1$, in the hope that if Δu is a good direction to move in, one might as well move further in that direction. The iteration is

for
$$j = 1$$
 to N do $u_{m+1,j} = (1 - \omega)u_{m,j} + \frac{\omega}{a_{jj}} \left(b_j - \sum_{k=1}^{j-1} a_{jk} u_{m+1,k} - \sum_{k=j+1}^{N} u_{m,k} \right)$ end for

The corresponding matrix form is

$$(D + \omega L)u_{m+1} = [(1 - \omega)D - U\omega]u_m + \omega b, \tag{20}$$

$$u_{m+1} = (D + \omega L)^{-1} [(1 - \omega)D - U\omega] u_m + (D + \omega L)^{-1} \omega b.$$
 (21)

Appendix A.3 contains a C++ code to carry out the SOR iteration on the example problem, and the result is shown in figure 5. In the SOR algorithm, the value of ω can be chosen freely, and the best choices can be determined by considering the eigenfunctions of the associated problem. This is discussed in more detail below.

Convergence analysis and complexity

To examine the convergence properties of the different methods, we need to look at the associated spectral radii. For the Jacobi method, the matrix of interest is $R_J = D^{-1}(L+U)$. For the 2D Poisson problem, D=4I and hence

$$R_J = (4I)^{-1} (4I - T_{N \times N}) = I - \frac{T_{N \times N}}{4}.$$
 (22)

The largest eigenvalue of R_I corresponds to the smallest of $T_{N\times N}$, namely

$$\lambda_{1,1} = 4 - 2\cos\left(\frac{\pi}{N+1}\right) - 2\cos\left(\frac{\pi}{N+1}\right)$$

$$= 4 - 4\cos\left(\frac{\pi}{N+1}\right). \tag{23}$$

Hence

$$\rho(R_J) = \cos\left(\frac{\pi}{N+1}\right). \tag{24}$$

Expanding the cosine as a Taylor series shows that $\rho(R_J) \approx 1 - \frac{\pi^2}{2(N+1)^2}$. The time to gain an extra digit of accuracy is approximately

$$\frac{1}{\log_{10}\rho(R_I)} \propto N^2,\tag{25}$$

so the algorithm must be run for $O(N^2)$ iterations to attain a specific level of accuracy. Since there are $O(N^2)$ gridpoints for the 2D problem, the total running time is $O(N^4)$. For detailed proofs of the convergence properties of the other methods, the reader should consult the book by Demmel [2]. It can be shown that

$$\rho(R_{GS}) = \cos^2\left(\frac{\pi}{N+1}\right),\tag{26}$$

so that one iteration of the Gauss–Seidel method is equivalent to two Jacobi iterations. Note however the complexity is the same: $O(N^2)$ iterations are still required to reach a desired level of accuracy. For the SOR algorithm, it can be shown that the optimal value of ω is

$$\frac{2}{1 + \sqrt{1 - \rho(R_J)^2}}. (27)$$

and that for this value

$$\rho(R_{SOR}) \approx 1 - 2\frac{2\pi}{N+1}.\tag{28}$$

Since there is a factor of N in the denominator as opposed to N^2 , the order of computation decreases to O(N) per gridpoint.

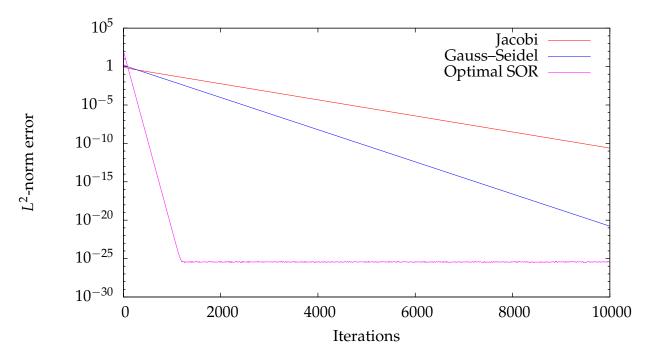


Figure 6: Errors versus the number of effective iterations for the Jacobi, Gauss–Seidel, and SOR methods, applied to the example 2D Poisson problem on a 65×65 grid. The plots are in line with the theoretical results of the text. The Gauss–Seidel method is faster than the Jacobi method, but has still not reached double numerical precision after 10000 iterations. The SOR method is significantly faster, but still requires 1200 iterations to reach double numerical precision.

Figure 6 shows a plot of mean square error against the number of iterations for the model problem with the Jacobi, Gauss–Seidel, and optimal SOR method. The lines agree with the above results. The SOR method reaches numerical precision within 1200 iterations, while the other two methods have not fully converged even after 10^4 iterations.

Multigrid

One of the major problems with the three methods considered so far is that they only apply locally. Information about different cell values only propagates by one or two gridpoints per iteration. However, for many elliptic problems, a point source may cause an effect over the entire domain. The above methods have a fundamental limitation that they will need to be applied for at least as many iterations as it takes for information to propagate across the grid. As such, we should not expect to ever do better than O(N) operations per point. This can also be seen by considering the eigenvalues. The maximal eigenvalue of R_J was set by the $\lambda_{1,1}$, corresponding to the lowest order mode. While the methods may effectively damp out high frequency oscillations, it takes a very long time to correctly capture the lowest modes with the largest wavelengths.

The multigrid method circumvents these limitations by introducing a hierarchy of

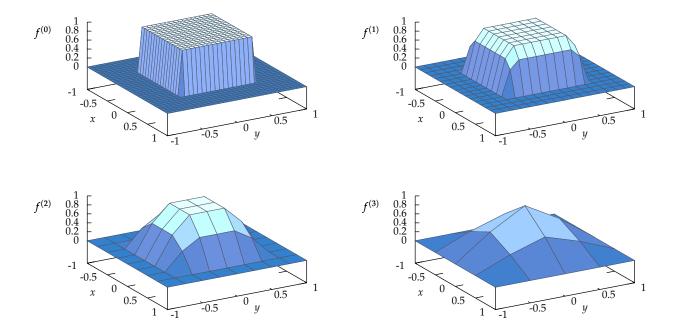


Figure 7: The restriction of the example source term f using the multigrid method with $v_{\text{down}} = 0$, $v_{\text{up}} = 2$. Top left: the initial grid, with 33 × 33 gridpoints. Top right: grid 1, with 17 × 17 gridpoints. Bottom left: grid 2, with 9 × 9 gridpoints. Bottom right: grid 3, with 5 × 5 gridpoints.

coarser and coarser grids. Typically, at each level, the number of gridpoints is reduced by a factor of two in each direction, with the coarsest grid having roughly ten to twenty points. To find a solution, we restrict the source term to the coarse grids, refine the solution on each, and interpolate up to the original grid. On the coarser grids, the lower frequency modes in the final solution can be dealt with much more effectively. Since the coarser grids have progressively fewer gridpoints, the time spent computing them is minimal. Because of this, the multigrid algorithm requires only O(1) computation per point, which is the best order of complexity that can be achieved.

To be more specific, let the original problem be on grid 0, and we then introduce a sequence of successively coarser grids $1, \ldots, g$. Write $u^{(i)}$ and $b^{(i)}$ to represent the solution and source terms on the ith grid. A multigrid algorithm requires the following:

- A solution operator $S(u^{(i)}, b^{(i)})$ that returns a better approximation $u^{(i)}$ to the solution on the ith level,
- An interpolation operator $T(u^{(i)})$ that returns an interpolation $u^{(i-1)}$ on the (i-1)th level,
- A restriction operator $R(b^{(i)})$ that returns a restriction $b^{(i+1)}$ on the (i+1)th level.

The interpolation and restriction operators can be thought of as rectangular matrices. As an example, consider a problem with nine equally-spaced gridpoints on the unit interval,

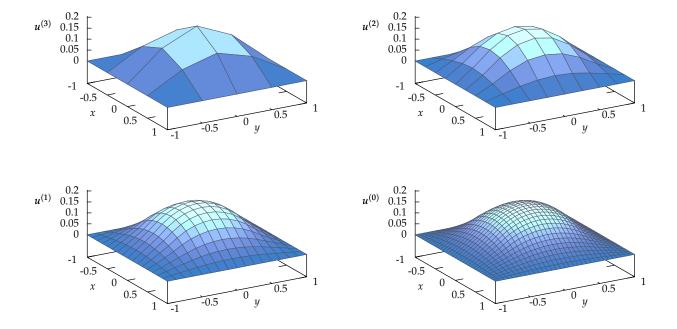


Figure 8: The solution of the v in the first multigrid V-cycle for the example 2D Poisson problem. Top left: the exact solution on grid 3 to the $f^{(3)}$ source term in figure 7. Top right: the interpolation and refinement on grid 2. Bottom left: the interpolation and refinement on grid 1. Bottom right: the interpolation and refinement on grid 0. Even after a single V-cycle, the solution is closer to the exact solution than the plots of 3, 4, and 5.

at $(0, \frac{1}{8}, \frac{2}{8}, \dots, 1)$. Let grid 1 have five points at $(0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1)$, and let grid 2 have three gridpoints at $(0, \frac{1}{2}, 1)$. Interpolation operators between the grids can be written as

$$T^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1/2 & 1/2 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \qquad T^{(2)} \begin{pmatrix} 1 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 1 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & 0 & 1 \end{pmatrix}$$
(29)

where the function values at gridpoints common between the two levels are kept, and the function values at midpoints are calculated using linear interpolation. Similarly, the restriction operators can be written as

$$R^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 1/2 & 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1/4 & 1/2 & 1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/4 & 1/2 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad R^{(1)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1/4 & 1/2 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$
(30)

Without the boundary points, $R^{(i)}$ is the proportional to the transpose of $T^{(i+1)}$, and this property is very useful in proving the convergence of the multigrid method. However, this property is not strictly necessary to create an efficient multigrid algorithm. Other methods of interpolating and restricting are also possible, and it should also be noted that while a grid of size $2^n + 1$ has a particularly convenient multigrid formulation, the multigrid method can be applied to grids of arbitrary size. Given a differential operator matrix $A = A^{(0)}$ on the top level, corresponding matrices on the lower levels can be calculated according to

$$A^{(i)} = R^{(i-1)}A^{(i-1)}T^{(i)}. (31)$$

With this definition, a solution operator $S(u^{(i)}, b^{(i)})$ can be constructed as a single red–black Gauss–Seidel sweep. The multigrid algorithm is then given by

```
function \operatorname{Multi}(u^{(i)},b^{(i)})

if i=g then

compute exact solution to A^{(i)}u^{(i)}=b^{(i)}

return u^{(i)}

else

for j=1 to v_{\operatorname{down}} do

u^{(i)}=S(u^{(i)},b^{(i)})

end for

r^{(i)}=b^{(i)}-A^{(i)}u^{(i)}

d^{(i)}=T(\operatorname{Multi}(0^{(i+1)},R(r^{(i)})))

u^{(i)}=u^{(i)}+d^{(i)}

for j=1 to v_{\operatorname{up}} do

u^{(i)}=S(u^{(i)},b^{(i)})

end for

end if
```

Here, $0^{(i+1)}$ represents a zero vector on grid level i+1. The multigrid function is applied recursively, and at each stage, the remainder of the problem on the level above is sent to the lower level. The algorithm starts on level 0, descends to level g, and then ascends to level 0 again, following the shape of a V. It is therefore referred to as the *multigrid V-cycle*. Other more elaborate methods of moving between grids are possible, although the V-cycle is very efficient in many situations. In the algorithm, we are free to choose the number of

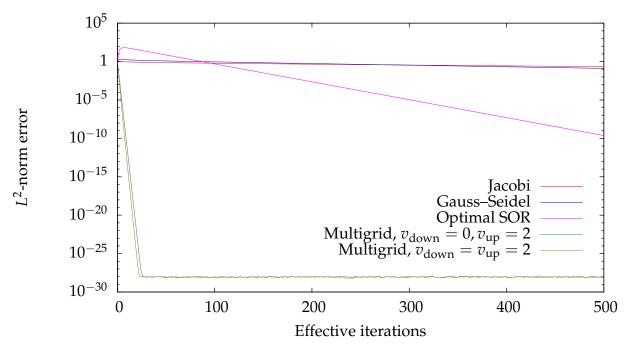


Figure 9: Errors versus the number of effective iterations for the several different iteration techniques. Here, to allow a direct comparison, "effective iterations" for the multigrid methods is defined by the number of Gauss–Seidel iterations that are applied on the top grid level, since the Gauss–Seidel iterations on the coarser grids are small in comparison. For the $v_{\rm down}=0$, $v_{\rm up}=2$ method, the effective number of iterations is twice the number of V-cycles. For the $v_{\rm down}=v_{\rm up}=2$ method, the algorithm was slightly modified, so that only two Gauss–Seidel iterations were applied at the top level each time, instead of the expected four. Thus the effective number of iterations is also twice the number of V-cycles. The speed of the multigrid methods is startling when compared to any of the other three iterations.

times the solution operator is applied on the way down and on the way up, and typical good values to try may be $v_{\rm down} = v_{\rm up} = 2$, or even $v_{\rm down} = 0$, $v_{\rm up} = 2$. It may also be worthwhile to carry out more iterations on the coarser grids, since the computation is much cheaper there.

Figure 7 shows the restriction of the source term in the test problem on the coarser grids. Figure 8 shows the solution being successively refined on the grids. Even after a single V-cycle, the solution is close to the exact answer. Figure 9 shows the computation times for two different multigrid algorithms, compared with the previous three methods considered. The multigrid algorithms reach numerical precision extremely quickly, much faster even than SOR. Only twenty Gauss–Seidel iterations are applied at the top level before double numerical precision has been reached.

A Code listings

The following codes were used to generate the Jacobi, Gauss–Seidel, and SOR diagrams in these notes. They are written in C++ and were compiled using the GNU C++ compiler.

Each of the first three routines calls a common code listed in appendix A.4 for setting up useful constants and defining common routines. This common code also contains a function for outputting the 2D matrices in a matrix binary format that is readable by the plotting program *Gnuplot* [1]. This output routine could be replaced in order to save to different plotting programs.

A.1 Jacobi method – jacobi.cc

```
// Load common routines and constants
#include "common.cc"
int main() {
  int i, j, ij, k;
  double error, u[m*n], v[m*n], z;
  double *a,*b;
  // Set initial guess to be identically zero
  for(ij=0;ij<m*n;ij++) u[ij]=v[ij]=0;</pre>
  output_and_error("jacobi_out",u,0);
  // Carry out Jacobi iterations
  for (k=1; k<=total_iters; k++) {</pre>
    // Alternately flip input and output matrices
    if (k%2==0) {a=u;b=v;} else {a=v;b=u;}
    // Compute Jacobi iteration
    for ( j=1; j<n-1; j++) {
      for (i=1; i<m-1; i++) {
        ij=i+m*j;
        a[ij] = (f(i, j) + dxxinv*(b[ij-1] + b[ij+1])
          +dyyinv*(b[ij-m]+b[ij+m]))*dcent;
    }
    // Save and compute error if necessary
    output_and_error("jacobi_out",a,k);
 }
     Gauss-Seidel – gsrb.cc
// Load common routines and constants
#include "common.cc"
int main() {
```

```
int i, j, ij, k;
double error, u[m*n], z;
// Set initial guess to be identically zero
for (ij=0;ij<m*n;ij++) u[ij]=0;</pre>
output_and_error("gsrb_out",u,0);
// Compute Red-Black Gauss-Seidel iteration
for (k=1; k<=total_iters; k++) {</pre>
  for(j=1; j<n-1; j++) {
    for (i=1+(j&1);i<m-1;i+=2) {
      ij=i+m*j;
      u[ij] = (f(i, j) + dxxinv*(u[ij-1]+u[ij+1])
        +dyyinv*(u[ij-m]+u[ij+m]))*dcent;
  }
  for (j=1; j<n-1; j++) {
    for (i=2-(j&1); i<m-1; i+=2) {
      ij=i+m*j;
      u[ij] = (f(i, j) + dxxinv*(u[ij-1] + u[ij+1])
         +dyyinv*(u[ij-m]+u[ij+m]))*dcent;
  }
  // Save the result and compute error if necessary
  output_and_error("gsrb_out",u,k);
}
```

A.3 Successive Over-Relaxation – sor.cc

A.4 Common routine for setup and output – common.cc

```
// Load standard libraries
#include <cstdio>
#include <cstdlib>
#include <iostream>
#include <fstream>
#include <cmath>
using namespace std;
// Set grid size and number of iterations
const int save_iters=20;
const int total_iters=200;
const int error_every=2;
const int m=33, n=33;
const double xmin=-1, xmax=1;
const double ymin=-1, ymax=1;
// Compute useful constants
const double pi=3.1415926535897932384626433832795;
const double omega=2/(1+sin(2*pi/n));
const double dx=(xmax-xmin)/(m-1);
const double dy=(ymax-ymin)/(n-1);
const double dxxinv=1/(dx*dx);
const double dyyinv=1/(dy*dy);
const double dcent=1/(2*(dxxinv+dyyinv));
```

```
// Input function
inline double f(int i,int j) {
  double x=xmin+i*dx,y=ymin+j*dy;
  return abs (x) > 0.5 || abs (y) > 0.5?0:1;
}
// Common output and error routine
void output_and_error(char* filename,double *a,const int sn) {
  // Computes the error if sn%error_every==0
  if(sn%error_every==0) {
    double z,error=0;int ij;
    for(int j=1; j<n-1; j++) {
      for(int i=1; i<m-1; i++) {
        ij=i+m*j;
        z=f(i,j)-a[ij]*(2*dxxinv+2*dyyinv)
          +dxxinv*(a[ij-1]+a[ij+1])
          +dyyinv*(a[ij-m]+a[ij+m]);
        error+=z*z;
    cout << sn << "" << error*dx*dy << endl;</pre>
  }
  // Saves the matrix if sn<=save_iters
  if(sn<=save_iters) {</pre>
    int i, j, ij=0, ds=sizeof(float);
    float x,y,data_float;const char *pfloat;
    pfloat=(const char*)&data_float;
    ofstream outfile;
    static char fname[256];
    sprintf(fname, "%s.%d", filename, sn);
    outfile.open(fname, fstream::out
                 fstream::trunc|fstream::binary);
    data_float=m; outfile.write(pfloat, ds);
    for(i=0;i<m;i++) {
      x=xmin+i*dx;
      data_float=x; outfile.write(pfloat, ds);
    for(j=0; j<n; j++) {
      y=ymin+j*dy;
      data_float=y;
```

```
outfile.write(pfloat,ds);
for(i=0;i<m;i++) {
    data_float=a[ij++];
    outfile.write(pfloat,ds);
    }
}
outfile.close();
}</pre>
```

References

- [1] http://gnuplot.info/.
- [2] J. W. Demmel, Applied numerical linear algebra, SIAM, 1997.
- [3] G. H. Golub and C. H. Van Loan, *Matrix computations*, Johns Hopkins University Publishers, 1996.