1 Introduction

As a continuation of last week's work on exercise 11, the conjugate gradient method was implemented to also solve the discretized Poisson equation in two dimensions for point charges in a grounded box. This time around, the time to solution was compared to a high performance library Cholesky solver as well as to the library Conjugate Gradient solver.

2 Algorithm Description

Repeating last week's description:
For all cases, the two-dimensional Poisson equation(equation 1) on Ω is discretized using second-order central finite differences in both the x- and the y-direction (equation 2). Both axes share a common grid spacing of $\Delta x = \frac{1}{N+1}$ where N is the number of interior points per axis direction on the grid. Following the established finite difference method procedure to employ natural ordering, the left-hand side of equation 2 then can be written in form of an $N*N \times N*N$ matrix $\mathbf{A}$ while the values of ϕ on the grid get unrolled into a vector $\mathbf{b}$ of size $N*N$ on the right-hand side (equation 3).
The resulting matrix A is both sparse and block tridiagonal.

$$\Delta\Phi = -\phi \quad \text{on } \Omega = (0,1) \times (0,1) \tag{1}$$

$$4x_{i,j} - x_{i-1,j} - x_{x+1,j} - x_{i,j-1} - x_{i,j+1} = -(\Delta x)^2 \cdot \rho(x_{i,j}) \tag{2}$$

$$Ax = b \tag{3}$$

2.1 Conjugate gradient method

The conjugate gradient method is the most well known member of the family of Krylov subspace methods [1]. Given the system of equations $\mathbf{Ax} = \mathbf{b}$ with $\mathbf{A}$ a symmetric positive definite (SPD) matrix, the method iteratively constructs a solution $\mathbf{x}^{(t)} \in \mathcal{K}_t(\mathbf{A}, \mathbf{r}^{(0)})$ using a starting solution $\mathbf{x}^{(0)} = (0, 0, \ldots, 0)^T$, the residual $\mathbf{r}^{(0)} = \mathbf{b} - \mathbf{Ax}^{(0)}$ and the associated Krylov subspace $\mathcal{K}_t(\mathbf{A}, \mathbf{r}^{(0)}) = \text{span}\{\mathbf{x}, \mathbf{Ax}, \mathbf{A}^2\mathbf{x}, \ldots, \mathbf{A}^{t-1}\mathbf{x}\}$. In this implementation, we use the simple Richardson iteration with $\mathbf{x}^{(t)} = \mathbf{x}^{(t-1)} + \alpha_{t-1}\mathbf{x}^{(t-1)}$ where α is a scalar factor calculated as shown in the outline below. $\mathbf{M}^{-1} = \frac{\delta_{ij}}{\mathbf{A}_{ii}}$ is the Jacobi preconditioner matrix. Setting $\mathbf{M} = \mathbf{M}^{-1} = \mathcal{I}$ instead trivially falls back to using no preconditioner:

- $\mathbf{r}^{(0)} \leftarrow \mathbf{b} - \mathbf{Ax}^{(0)}$
- $\mathbf{z}^{(0)} \leftarrow \mathbf{M}^{-1}\mathbf{r}^{(0)}$
- $\mathbf{p} \leftarrow \mathbf{z}^{(0)}$
- Iterate until convergence and/or iteration limit:
  - $\alpha \leftarrow \frac{(\mathbf{r}^{(t)})^T\mathbf{z}^{(t)}}{(\mathbf{p})^T\mathbf{Ap}}$
  - $\mathbf{x} \leftarrow \mathbf{x} + \alpha\mathbf{p}$
  - $\mathbf{r}^{(t)} \leftarrow \mathbf{r}^{(t-1)} - \alpha\mathbf{Ap}$
  - check preconditioned residual $\left\|\mathbf{r}^{(t)}\right\|_2$ for convergence; stop if reached
  - $\mathbf{z}^{(t)} \leftarrow \mathbf{M}^{-1}\mathbf{r}^{(t-1)}$

- $\beta \leftarrow \frac{(\mathbf{z}^{(t)})^T \mathbf{r}^{(t)}}{(\mathbf{z}^{(t-1)})^T \mathbf{r}^{(t-1)}}$
- $\mathbf{p} \leftarrow \mathbf{z}^{(t)} = \beta \mathbf{p}$
- $\mathbf{r}^{(t-1)} \leftarrow \mathbf{r}^{(t)}$
- $\mathbf{z}^{(t-1)} \leftarrow \mathbf{z}^{(t)}$

- return $\mathbf{x}$

3 Results

The program was implemented as described above and submitted with this report.
The conjugate gradient method was iterated until the residual's norm went below the set treshold: $\|\mathbf{r}\|_2 \leq 10^{-4}$. The conjugate gradient method took only $t = 82$ iterations and $\sim$ 1ms which compares very favourably with the Jacobi relaxation method ($t = 3478$ iterations in $\sim$ 45ms) and the Gauss-Seidel method ($t = 1922$ iterations in $\sim$ 6400ms examined in exercise 11. For comparison, Eigen's optimized library Cholesky method solver obtained the reference solution in $\sim$ 10ms while Eigen's own conjugate gradient method set to use a complete matrix took $\sim$ 3ms.
The conjugate gradient method with the set residual treshold reached a very minor deviation from the reference Cholesky solution:
$\left\| \mathbf{x}^*_{\text{Conjugate gradient}} - \mathbf{x}^*_{\text{Cholesky}} \right\|_2 \approxeq 0.0002.$
The heat map for the conjugate gradient solver is shown in figure 1.

4 Discussion

The results are mostly are as expected, the exception being that the Jacobi preconditioner didn't make a difference for the system under consideration. Then again, neither is the Jacobi preconditioner sophisticated, nor does the given system setup (2D finite differences on a small system with $N = 50$) actually mandate using a preconditioner.

References

[1] Elman, H., Silvester, D., Wathen, A.
Finite Elements and Fast Iterative Solvers,
Oxford University Press,
2014.

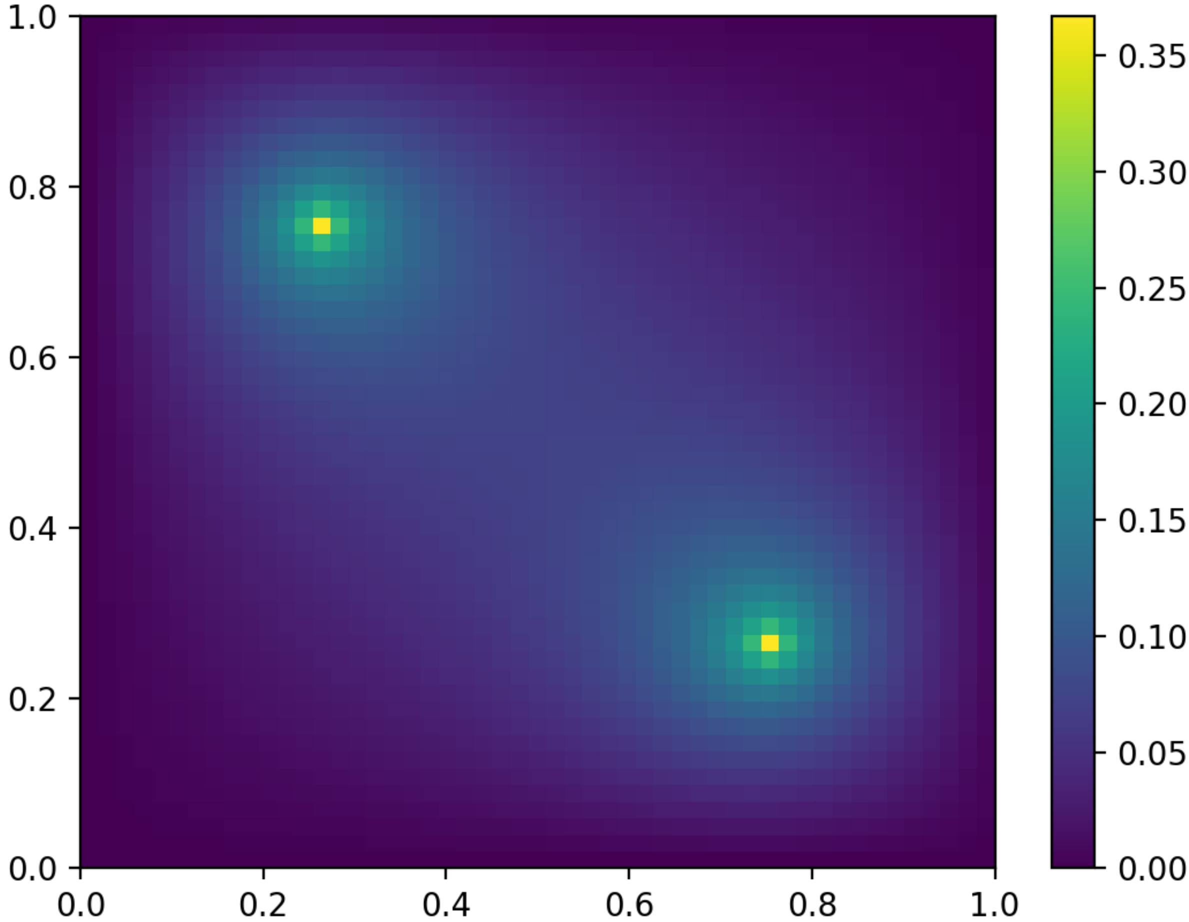

Figure 1: Conjugate gradient solver reference solution for Poisson equation with point charges at $(0.25, 0.75)$, $(0.75, 0.25)$; grid parameter $N = 50$.