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Lattice Practices
Solvers I – Basics

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The purpose of this excercise it to familiarize you with some of the methods discussed in the lecture, namely, `Jacobi`, `Gauss-Seidel`, `CG`, `GMRES` and `BiCGstab`. There is an `octave`-demo (in the directories `task0/` and `task1-2-3/`; within `task1-2-3/` there are the scripts `taskX.m`, $X \in 1, 2, 3$) for each task, showing typical behaviour of these methods. To view the demo fire up Octave, switch to the octave folder and type in:

```
octave:xx>  taskX
```

for the `task1-2-3/` directory. For `task0/`, run `J_GS_for_discrete_Laplacian.m` or `J_GS_for_gauge_Laplacian.m` in there.

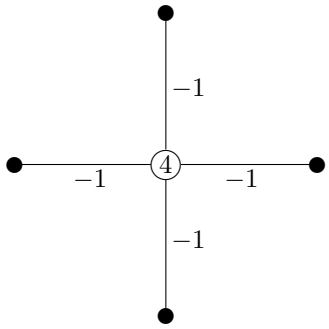
The questions given on this sheet are meant to be discussed with your fellow lattice practicioners while inspecting the demo. For some tasks there is an *advanced* question marked by a $\star$ which provides deeper understanding of the methods[1].

Task 0 *Basic Iterative Schemes*
We consider the linear system

$$Ax = b,$$

where A stems from the finite difference discretization of the Poisson equation $-\Delta u = f$ with Dirichlet boundary conditions on the unit-square $[0, 1] \times [0, 1]$ (*discrete Laplacian*). Each equation couples a central grid point with its 4 neighbors, as given by the "5-point stencil"

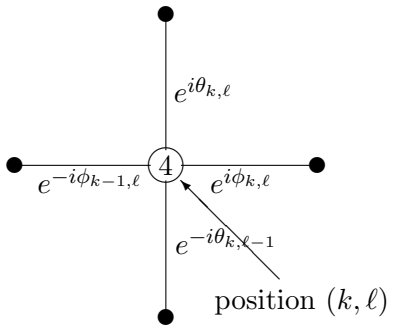
[1] It's probably best to think about these tasks in-between sessions.



1. Take a look at the convergence of the Jacobi method and the Gauss-Seidel method for the discretization on an $N \times N$ grid, $N = 4$, 8, 16, 32, 64, 128.

   - How does the number of iterations required for a given accuracy scale with N?
   - Which method performs better? How much?
   - Anything remarkable concerning the error?

We now consider the system of the *gauge Laplacian*, where on the links we have complex numbers with a randomly chosen phase, depending on the grid point.



2. Take a look at the convergence of the Jacobi method and the Gauss-Seidel method for the discretization on an $N \times N$ grid, $N = 4$, 8, 16, 32, 64, 128.

   - How does the number of iterations required for a given accuracy scale with N?
   - Which method performs better? How much?
   - What differences do you observe compared to the discrete Laplacian?

Task 1 *Conjugate Gradients*
We now use the conjugate gradients method on the discrete Laplacian.

1. Take a look at the convergence of the method for the discretization on a 64×64 grid.

   - Why is $\|r\|_2$ not monotone?
   - How do you explain the difference between $\|r\|_2$ and $\|e\|_2$?

2. Recall that the conjugate gradients method with $x^{(0)} = 0$ can be described by

$$\begin{aligned} r^{(k)} &= p_k(A)b \\ e^{(k)} &= p_k(A)e^{(0)} \\ p_k(t) &= 1 - tq_{k-1}(t) \\ x^{(k)} &= q_{k-1}(A)b \in \mathcal{K}_k(A, b), \end{aligned}$$

   where the polynomial p_k is the minimizer of

$$\min_{p_k \in \bar{\Pi}_k} \|p_k(\lambda)b\|_A$$

   The demo shows you both the roots and the corresponding polynomial.

   - Can you interpret the action of $p_k(A)$ on eigenmodes?
   - Why do small eigenvalues hamper the performance of Krylov subspace methods?
   - *Speculate&Try**: Does the polynomial change if you change the right-hand side b?

3. In most applications based on partial differential equations the condition number grows when increasing the accuracy of the discretization, i.e., mesh-size $a \to 0$.

   - What can you say about the solutions on different resolutions? (this will be explored further in the session Solvers II)

4. The convergence of Krylov subspace methods may depend on the right-hand side. Can you attach the correct right-hand side to the plot and explain your choice? In here v_i denotes an eigenmode of A, i.e., $Av_i = \lambda_i v_i$

   - $b = \texttt{random}_{N(0,1)}$, random normal distributed
   - $b = v_1$, the smallest eigenmode
   - $b = e_i$, a point source
   - $b = A\mathbf{1}$, right-hand side to the solution $\mathbf{1}$

- $b = v_1 + v_2$, the sum of two eigenmodes

5. **Bonus***: Consider the Arnoldi relation

$$AV_m = V_{m+1}H_{m+1,m}.$$

   - What can you say about the structure of $H_{m+1,m}$ in the case that A is hermitian positive definite?
   - Write down the simplified Arnoldi algorithm for hermitian positive definite A based on the observations made about the structure of $H_{m+1,m}$. (This algorithm is also known as *Lanczos algorithm*)

Task 2 *GMRES*
In order to show properties of the GMRES iteration we consider an example from Lattice QCD. The system matrix A is given by the Wilson discretization of the Dirac equation on a 4^4 lattice at $\beta = 6$ with an additive mass shift. The system matrix is non-hermitian with its eigenvalues in the right half-plane.

1. First consider the convergence of plain GMRES for this problem.
   - Does the monotonicity of $\|r\|_2$ surprise you?
2. Similarly to the observations made for CG, we can take a look at the polynomial associated with the GMRES iteration.
   - Do you see similar behaviour as in Task 1.2?
3. **Bonus*** It can be shown that inverses of the zeros Θ of the GMRES polynomials all lie in the field of values of A^{-1}, i.e.

$$\Theta^{-1} \in \mathcal{F}(A^{-1}) := \{x^\dagger A^{-1} x : x^\dagger x = 1, x \in \mathbb{C}^n\}.$$

   Argue why GMRES and restarted GMRES converge if $\mathcal{F}(A)$ is contained in the right half plane.
4. Restarted GMRES has been introduced to deal with the potentially large costs in storage and computational ressources due to large iteration count.
   - How can one explain why GMRES(m) converges much slower than GMRES?

Task 3 *BiCGstab*
To conclude we demonstrate the typical convergence behaviour of BiCGstab, applied again to the 4^4 Lattice Dirac Wilson operator and compare it to the GMRES and GMRES(m) method. Finally, we also consider CG applied to the normal equations

$$A^\dagger A x = A^\dagger b$$

to solve this problem.

- Why is it possible to apply CG to the normal equations?
- What is the severe drawback of doing so? (in terms of the condition number κ)
- Which method would you recommend for the lattice Dirac-Wilson system?