Computational Methods (practice) - Lecture 3

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- Krylov methods and approximate matrix inversion
- GMRES
- Conjugate Gradients
- Preconditioning
- Red black preconditioning
- Checkerboarded implementation
- Multigrid preconditioning
- Eigensolvers and Deflation

Krylov methods and approximate matrix inversion

- Algorithms minimise a residual $|r|^2$, where

$$r = M\psi - b$$

  - $r = 0 \Leftrightarrow \psi = M^{-1}b$ so minimise r under some norm
- *Krylov space* is the span of all polynomials of M and of O(N) $\mathrm{sp}b, Mb, \ldots M^N b$
- *Krylov solvers* iteratively apply a (sparse) matrix to build up this space
- Unlike Chebyshev approximation these algorithms require no prior knowledge of the spectral range of M
- Different algorithms invoke different rules for selecting these coefficients...
  ...and have different storage requirements

GMRES

https://github.com/paboyle/Grid/blob/develop/Grid/algorithms/iterative/GeneralisedMinimalResidual.h

- Consider $\psi = (c_n M^n) b$ in the Krylov space
- GMRES minimises the Euclidean norm $|r|^2$ with respect to the coefficients c_n
- Matrix elements are $c_m^* c_n \langle M^{m+1} b | M^{n+1} b \rangle$
- This requires all N vectors to be retained, and coefficients selected after dense matrix algebra to determine c_m
- GMRES(k) runs for k iterations and then *restarts* to limit storage
- Often used in a preconditioner/smoother

https://en.wikipedia.org/wiki/Generalized_minimal_residual_method

Lanczos orthogonal sequence

http://people.inf.ethz.ch/arbenz/ewp/Lnotes/chapter10.pdf
The Lanczos and conjugate gradient algorithms, Meurant

- Krylov space $K_n(b) = \{b, Ab, \ldots, A^n b\}$
- Seek orthonormal basis: normalise components perpendicular to all prior vectors
- $\beta_{j+1}|v_{j+1}\rangle = (1 - \sum_{i=1}^{j} |v_i\rangle\langle v_i|)|Av_j\rangle$
- Rewrite as:

$$|Av_j\rangle = \sum_{i=1}^{j+1} |v_i\rangle H_{ij}$$

  Where $H_{ij} = \langle v_i|A|v_j\rangle$ and is zero for $i > j + 1$ by virtue of our sequential orthogonalisation.
- The "Householder matrix" H is tridiagonal when A has Hermitian symmetry and an orthonormal basis for the Krylov space is mapped out with a three term recurrence relation.
- **Removes large storage requirements**
- Can use this basis to build solutions $\Rightarrow$ Conjugate Gradients

Conjugate Gradients

https://en.wikipedia.org/wiki/Conjugate_gradient_method

- Generate A-orthogonal sequence of search directions based on Lanczos sequence
- Residuals are parallel to the Lanczos basis, mutually orthogonal set
- Krylov solution to $Ax = b$ has $x = \sum_k \alpha_k p_k$:

$$p_j^\dagger A x = p_j^\dagger b = \sum_k \alpha_k p_j^\dagger A p_k = \alpha_j p_j^\dagger A p_j \Rightarrow \alpha_j = \frac{p_j^\dagger b}{p_j^\dagger A p_j}$$

$\mathbf{r}_0 := \mathbf{b} - \mathbf{A}\mathbf{x}_0$
if $\mathbf{r}_0$ is sufficiently small, then return $\mathbf{x}_0$ as the result
$\mathbf{p}_0 := \mathbf{r}_0$
$k := 0$
repeat
  $\alpha_k := \dfrac{\mathbf{r}_k^\mathsf{T}\mathbf{r}_k}{\mathbf{p}_k^\mathsf{T}\mathbf{A}\mathbf{p}_k}$
  $\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k\mathbf{p}_k$
  $\mathbf{r}_{k+1} := \mathbf{r}_k - \alpha_k\mathbf{A}\mathbf{p}_k$
  if $\mathbf{r}_{k+1}$ is sufficiently small, then exit loop
  $\beta_k := \dfrac{\mathbf{r}_{k+1}^\mathsf{T}\mathbf{r}_{k+1}}{\mathbf{r}_k^\mathsf{T}\mathbf{r}_k}$
  $\mathbf{p}_{k+1} := \mathbf{r}_{k+1} + \beta_k\mathbf{p}_k$
  $k := k + 1$
end repeat
return $\mathbf{x}_{k+1}$ as the result

```
void operator()(LinearOperatorBase<Field> &Linop, const Field &src, Field &psi)
{
  RealD cp, c, a, d, b, ssq, qq;

  Field p(src), mmp(src), r(src);

  Linop.HermOpAndNorm(psi, mmp, d, b);

  r = src - mmp;
  p = r;

  a = norm2(p);
  cp = a;
  ssq = norm2(src);

  RealD rsq = Tolerance * Tolerance * ssq;

  for (int k = 1; k <= MaxIterations; k++) {
    c = cp;

    Linop.HermOp(p, mmp);

    ComplexD dc  = innerProduct(p,mmp);
    d = dc.real();
    a = c / d;

    cp = axpy_norm(r, -a, mmp, r);
    b = cp / c;

    psi = psi + a* p ;
    p   = r   + b* p ;

    if (cp <= rsq) {
      return;
    }
  }
  assert(0);
}
```

BiCGstab

For Wilson Fermions, BICGstab is the fastest conventional Krylov solver It is suited to solving the non-Hermitian system

$$D_w \psi = b$$

https://github.com/paboyle/Grid/blob/develop/Grid/algorithms/iterative/BiCGSTAB.h
https://en.wikipedia.org/wiki/Biconjugate_gradient_stabilized_method

Convergence rate, critical slowing down, and preconditioning

- The uniformity of the Chebyshev polynomial oscillations can be used to bound convergence rate via a maximum error over the spectral range
  - Krylov solvers can do better than this worst case bound as polynomial coefficients are selected based on the actual spectrum
  - QCD often (index theorem) has a detached number of low modes (topological nature)
- Condition numer

$$\kappa = \frac{\lambda_{\max}}{\lambda_{\min}}$$

- Theoretical convergence factor per iteration (c.f. R-number in epidemiology!)

$$\sigma = \frac{\sqrt{k} - 1}{\sqrt{k} + 1}$$

- In infinite volume limit spectrum is dense and the worst case is the guaranteed case
- Empirically, the theoretical σ governs the long tail convergence of CG in practice
- (left) Preconditioning: changing κ by solving a related system

$$PM\psi = Pb$$

- If the condition number of PM is substantially reduced, preconditioned system converges faster

Convergence rate, critical slowing down, and preconditioning

- If the condition number of PM is substantially reduced, preconditioned system converges faster
- Ideally P is a cheap-to-apply *approximate inverse* of M
- Left preconditioning
$$PM\psi = Pb$$
- Right preconditioning
$$MP\psi' = b; \psi = P\psi'$$
- Approximating M^{-1} can be focussed regions of spectrum
- Lower $\lambda_{\max}$
  - Polynomial preconditioner (e.g. Chebyshev $1/x$ over high end of spectrum); reduce rate of inner-products / reductions
  - Domain decomposed smoother such Schwarz Alternating procedure : works for high end of spectrum; reduces communication and rate of inner-products / reductions
- Raise $\lambda_{\min}$
  - Deflation of low modes $P = (1 - \sum |i\rangle\langle i|) + \sum_i \frac{|i\rangle\langle i|}{\lambda_i}$
  - Up to rounding, deflation can be applied infrequently in CG due to orthogonal search sequence

Schur decomposition

https://github.com/paboyle/Grid/blob/develop/Grid/algorithms/iterative/SchurRedBlack.h
A matrix can be LDU factorised as follows. Each of A, B, C or D can themselves be sub-matrices

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ CA^{-1} & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{pmatrix} \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix}, \tag{1}$$

where the Schur complement,

$$S = D - CA^{-1}B.$$

Red-Black preconditioning

We can write the Dirac operator in terms of even and odd lattice sites and perform an LDU decomposition:

$$M = \begin{pmatrix} M_{ee} & M_{eo} \\ M_{oe} & M_{oo} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ M_{oe}M_{ee}^{-1} & 1 \end{pmatrix} \begin{pmatrix} M_{ee} & 0 \\ 0 & M_{oo} - M_{oe}M_{ee}^{-1}M_{eo} \end{pmatrix} \begin{pmatrix} 1 & M_{ee}^{-1}M_{eo} \\ 0 & 1 \end{pmatrix}, \tag{2}$$

where the Schur complement, is written as $M_{pc} = M_{oo} - M_{oe}M_{ee}^{-1}M_{eo}$.

- For Wilson Fermions the M_{ee} is proportional to the identity.
- For DWF and Wilson Clover Fermions the terms are non-trivial.
- For the Wilson Clover term M_{ee} depends on the gauge fields.
- For DWF M_{ee} is independent of the gauge fields.

U and L have determinant 1 and are trivially invertible:

$$L^{-1} = \begin{pmatrix} 1 & 0 \\ -M_{oe}M_{ee}^{-1} & 1 \end{pmatrix} \quad ; \quad U^{-1} = \begin{pmatrix} 1 & -M_{ee}^{-1}M_{eo} \\ 0 & 1 \end{pmatrix}$$

For the odd checkerboard, $M\psi = \eta$ becomes

$$M_{pc}\psi_o = \eta'_o = (L^{-1}\eta)_o = \eta_o - M_{oe}M_{ee}^{-1}\eta_e$$

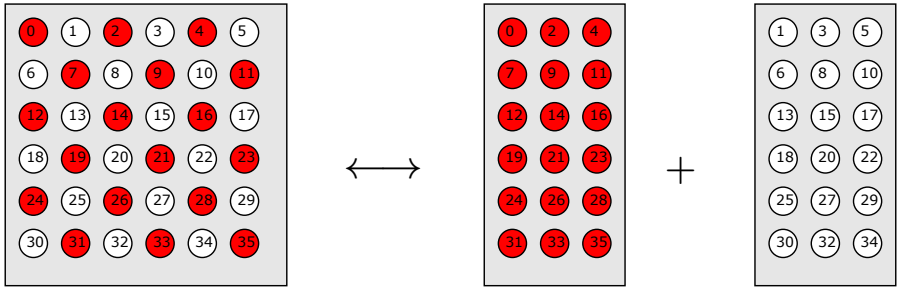
The even checkerboard solution can be inferred via

$$M_{ee}\psi_e + M_{eo}\psi_o = \eta_e \Rightarrow \psi_e = M_{ee}^{-1}(\eta_e - M_{eo}\psi_o)$$

M_{pc} (empirically) better conditioned than M: red black solvers converge O(3x) faster

Checkerboarding

- Lattice QCD makes use of red-black preconditioning in many algorithms
- Support for checkerboarded grids is required
  - e.g. a field that lives only on the white or black sites of a chessboard
  - Shifting a "black" field by one site produces a white field and vice versa
    Indexing and neighbour indexing is complicated by this
  - Stencil operators work with checkerboarded grids



- Checkerboarded Grid objects can have arbitrary subset of dimensions involved in checkerboarding
- Dimension "collapsed" can be selected (typically x-direction)
- Natural support for 4d and 5d checkerboarded chiral fermions
  - Neighbour indexing is integer heavy divide/modulo arithmetic
  - Precompute neighbour tables in high performance Stencil objects
  - Calculate dynamically for Cshift, looping over planes

Eigensolvers

- The Lanczos sequence can also be used to solve for eigenvectors, known as the Lanczos algorithm.
- Grid has a Chebyshev polynomial preconditioned Lanczos algorithm:

https://github.com/paboyle/Grid/blob/develop/Grid/algorithms/iterative/ImplicitlyRestartedLanczos.h

- We will not discuss Lanczos in detail: it is used to produce the lowest lying eigenvectors of the Dirac operator
- These can be handled exactly, and removed from the problem to eliminate critical slowing down

Exercise

- Write a conjugate gradients algorithm to invert the (massive) Laplacian
  - Introduce a small mass m^2 to the Laplacian example in Lecture 1.
  - Verify the results on the free field via Fourier methods
  - Check gauge covariance