Sparse Matrices and Optimized Parallel Implementations

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Topics

Projection in Scientific Computing

(lecture 1)

Sparse matrices, parallel implementations

(lecture 3, 03/21/07)

PDEs, Numerical solution, Tools, etc.

(lecture 2, 02/28/07)

Iterative Methods

(lectures 4 and 5, 04/11 and 04/18/07)
Outline

• Part I
  – Review: projection and homework #5

• Part II
  – Sparse matrix computations

• Part III
  – Reordering algorithms and parallelization
Part I

Review: Projection
Projection in $\mathbb{R}^n / \mathbb{C}^n$

- $P$: Orthogonal projection of $u$ into $\text{span}\{e_1, \ldots, e_m\}$, $m \leq n$.

Let $e_i$, $i = 1 \ldots m$ is orthonormal basis, i.e.

\[
(e_i, e_j) = 0 \quad \text{for } i \neq j \quad \text{and} \quad (e_i, e_j) = 1 \quad \text{for } i = j
\]

\[
P u = (u, e_1) e_1 + \ldots + (u, e_m) e_m
\]

Orthogonal projection of $u$ on $e_1$
What if the basis is not orthonormal?

- We can orthonormalize it. **How?**
  
  Can get one from every subspace by **Gram-Schmidt** orthogonalization:

  **Input** : m linearly independent vectors $x_1, \ldots, x_m$
  
  **Output** : m orthonormal vectors $x_1, \ldots, x_m$

**CGS**

1. $x_1 = x_1 / \| x_1 \|$
2. do $i = 2, m$
3. $x_i = x_i - (x_i, x_1) x_1 - \ldots - (x_i, x_{i-1}) x_{i-1}$
4. $x_i = x_i / \| x_i \|$
5. enddo

**MGS**

3'. do $j = 1, i-1$

4. $x_i = x_i - (x_i, x_j) x_j$

5. enddo
What if the basis is not orthonormal?

- If we do not want to orthonormalize:
  \[ u \approx Pu = c_1 x_1 + c_2 x_2 + \ldots + c_m x_m \]
  \[ (u, x_1) = c_1 (x_1, x_1) + c_2 (x_2, x_1) + \ldots + c_m (x_m, x_1) \]
  \[ \ldots \]
  \[ (u, x_m) = c_1 (x_1, x_m) + c_2 (x_2, x_m) + \ldots + c_m (x_m, x_m) \]

- These are the so-called Petrov-Galerkin conditions

- We saw examples of their use in
  * optimization (problem 1 and 4, Homework 5), and
  * PDE discretization, e.g. FEM
Homework #5, Problem 3

- Is the following a QR factorization for $A$?
  1. $G = A^T A$
  2. $G = L L^T$ (Cholesky factorization)
  3. $Q = A (L^T)^{-1}$

- From (3), assuming the operations used make sense, we have
  $A = Q L^T$ here $L^T$ is upper triangular, so all is left is
  check if $Q$ is orthogonal, i.e. is $Q^T Q = I$?

  $Q^T Q = (A (L^T)^{-1})^T (A (L^T)^{-1}) = (L^{-1} A^T) (A L^{-T}) = L^{-1} L = L^T L^T = I$

Use (1) and (2) to replace it by $L L^T$
Homework #5, Problem 4

• Find the projection of \( f(x) = \sin(x) \) in \( V_1 = \text{span}\{x, x^3, x^5\} \) on interval \([-1, 1]\) using inner-product 

\[
(f, g) = \int_{-1}^{1} f(x) g(x) \, dx \quad \text{and norm} \quad \| f \| = (f,f)^{1/2}
\]

**Approach I**

* construct orthonormal basis, e.g. CGS

\[
y_1 = x / \| x \| \\
y_2 = x^3 - (x^3, y_1) y_1, \quad y_2 = y_2 / \| y_2 \| \\
y_3 = x^5 - (x^5, y_1) y_1 - (x^5, y_2) y_2, \quad y_3 = y_3 / \| y_3 \|
\]

\[
P f(x) = (\sin(x), y_1) y_1 + (\sin(x), y_2) y_2 + (\sin(x), y_3) y_3
\]

**Approach II**

* directly

\begin{align*}
(1) \quad \sin(x) & \approx Pf = c_1 x + c_2 x^3 + c_3 x^5 \quad / \text{mult. by } x,x^3,x^5 \\
(\sin(x),x) &= c_1 (x,x) + c_2 (x^3,x) + c_3 (x^5,x) \\
(\sin(x),x^3) &= c_1 (x,x^3) + c_2 (x^3,x^3) + c_3 (x^5,x^3) \\
(\sin(x),x^5) &= c_1 (x,x^5) + c_2 (x^3,x^5) + c_3 (x^5,x^5)
\end{align*}

solve this 3x3 system and plug \( c_1, c_2, c_3 \) back in (1)
Homework #5, Problem 4

(graph from Daniel Lucio)

\[ f(x) = \sin(x) \]
Part II
Sparse matrix computations
Sparse matrices

• Sparse matrix: substantial part of the coefficients is zero
• Naturally arise from PDE discretizations
  – finite differences, FEM, etc; we saw examples in the

5-point finite difference operator

Row 6 will have 5 nonzero elements:
\[ A_{6,2}, A_{6,5}, A_{6,6}, A_{6,7}, \text{ and } A_{6,10} \]

1-D piece-wise linear FEM

Row 3, for example, will have 3 nonzeros
\[ A_{3,2}, A_{3,3}, A_{3,4} \]
**Sparse matrices**

- **In general:**
  
  * Degrees of freedom (DOF), associated for ex. with vertices (or edges, faces, etc.), are indexed
  
  * A basis function is associated with every DOF (unknown)
  
  * A **Petrov-Galerkin condition** (equation) is derived for every basis function, representing a row in the resulting system

  * Only 'a few' elements per row will be nonzero as the basis functions have local support
  
    - eg. row 10, using continuous piecewise linear FEM, will have 6 nonzeros:
      
      \[ A_{10,10}, A_{10,35}, A_{10,100}, A_{10,332}, A_{10,115}, A_{10,201} \]

  - physical intuition behind: PDEs describe changes in physical processes;
    describing/discretizing these changes numerically, based only on local/neighborhood information, results in sparse matrices

  eg. what happens at '10' is described by the physical state at '10' and the neighboring 35, 201, 115, 100, and 332.
Sparse matrices

• Can we take advantage of this sparse structure?
  – To solve for example very large problems
  – To solve them efficiently

• Yes! There are algorithms
  – Linear solvers and preconditioners (to cover some in the last 2 lectures)
  – Efficient data storage and implementation (next ...)
Sparse matrix formats

• It pays to avoid storing the zeros!

• Common sparse storage formats:
  – AIJ
  – Compressed row/column storage (CRS/CCS)
  – Compressed diagonal storage (CDS)
    * for more see the 'Templates' book
      http://www.netlib.org/linalg/html_templates/node90.html#SECTION00931000000000000000
  – Blocked versions (why?)
• Stored in 3 arrays
  – The same length
  – No order implied

\[
\begin{bmatrix}
1 & 2 & 0 & 0 & 0 \\
3 & 0 & 4 & 0 & 0 \\
0 & 5 & 0 & 6 & 0 \\
0 & 0 & 7 & 0 & 8 \\
\end{bmatrix}
\]

<table>
<thead>
<tr>
<th>I</th>
<th>J</th>
<th>AIJ</th>
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</thead>
<tbody>
<tr>
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<td>7</td>
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<tr>
<td>4</td>
<td>4</td>
<td>8</td>
</tr>
</tbody>
</table>
**CRS**

- Stored in 3 arrays
  - J and AIJ the same length
  - I (representing rows) is compressed

<table>
<thead>
<tr>
<th>I</th>
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<th>AIJ</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
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<td>1</td>
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<tr>
<td>3</td>
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<td>7</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>8</td>
</tr>
</tbody>
</table>

\[
\begin{bmatrix}
1 & 2 & 0 & 0 & 0 \\
3 & 0 & 4 & 0 & 0 \\
0 & 5 & 0 & 6 & 0 \\
0 & 0 & 7 & 0 & 8 \\
\end{bmatrix}
\]

array I: think of it as pointers to where next row starts

CCS: similar but J is compressed
CDS

• For matrices with nonzeros along subdiagonals

Subdiagonal index

| subdiagonals | | | | | |
| --- | --- | --- | --- | --- |
| -1 | 0 | 3 | 7 | 8 | 9 | 2 |
| 0 | 10 | 8 | 8 | 7 | 9 | -1 |
| 1 | -3 | 6 | 7 | 5 | 13 | 0 |

\[
A = \begin{pmatrix}
10 & -3 & 0 & 0 & 0 & 0 & 0 \\
3 & 8 & 6 & 0 & 0 & 0 & 0 \\
0 & 7 & 8 & 7 & 0 & 0 & 0 \\
0 & 0 & 8 & 7 & 5 & 0 & 0 \\
0 & 0 & 0 & 0 & 9 & 13 & 0 \\
0 & 0 & 0 & 0 & 2 & -1 & 0
\end{pmatrix}
\]
Performance (Mat-vec product)

- Notoriously bad for running at just a fraction of the performance peak!
- Why?
  
  Consider Mat-vec product for matrix in CRS:

  ```
  for i = 1, n
    for j = I[i], I[i+1]-1
      x[i] += AIJ[j] * x[J[j]]
  ```
Performance (Mat-vec product)

• **Notoriously bad** for running at just a fraction of the performance peak!

• Why?

Consider Mat-vec product for matrix in CRS:

```plaintext
for i = 1, n
    for j = I[i], I[i+1]-1
        x[i] += A[I][j] * x[J[j]]
```

* Irregular indirect memory access for x 
  - result in cache trashing
* performance often <10% peak
Performance (Mat-vec product)

* Performance of mat-vec products of various sizes on a 2.4 GHz Pentium 4

(a) Untuned SpMV performance
Performance (Mat-vec product)

• How to improve the performance?
  – A common technique
    (as illustrated in Lecture #9 and Homework #6)
    is **blocking** (register, cache: next ... )
  – **Index reordering** (in Part II)
  – Exploit special matrix structure (eg. symmetry, bands, other structures)
Block Compressed Row Storage (BCRS)

• Example of using 2x2 blocks

<table>
<thead>
<tr>
<th>BI</th>
<th>BJ</th>
<th>AIJ</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
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<tr>
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<td>2</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>0</td>
</tr>
</tbody>
</table>

* Reduced storage for indexes
* Drawback: add 0s
* What block size to choose?
* BCRS for register blocking
* Discussion?
BCRS

(a) Untuned SpMV performance

(b) Speedups obtained from tuning
Cache blocking

• Improve cache reuse for $x$ in $Ax$ by splitting $A$ into a set of sparse matrices, eg.

Sparse matrix and its splitting

For more info check:
Eun-Jin Im, K. Yelick, R. Vuduc
Part III
Reordering algorithms and Parallelization
Reorder to preserve locality

eg. Cuthill-McKee Ordering: start from arbitrary node, say '10' and reorder
* '10' becomes 0
* neighbors are ordered next to become 1, 2, 3, 4, 5, denote this as level 1
* neighbors to level 1 nodes are next consecutively reordered, and so on until end
Cuthill-McKee Ordering

- Reversing the ordering (RCM) results in ordering that is better for sparse LU
- Reduces matrix bandwidth (see example)
- Improves cache performance
- Can be used as partitioner (**parallelization**) but in general does not reduce edge cut
Self-Avoiding Walks (SAW)

- Enumeration of mesh elements through 'consecutive elements' (sharing face, edge, vertex, etc)

  * similar to space-filling curves but for unstructured meshes
  * improves cache reuse
  * can be used as partitioner with good load balance but in general does not reduce edge cut
Graph partitioning

- Refer back to Lecture #8, Part II
  Mesh Generation and Load Balancing
- Can be used for reordering
- Metis/ParMetis:
  - multilevel partitioning
  - Good load balance and minimize edge cut
Parallel Mat-Vec Product

- Easiest way:
  - 1D partitioning
  - May lead to load unbalance (why?)
  - May need a lot of communication for x
- Can use any of the just mentioned techniques
- Most promising seems to be spectral multilevel methods (as in Metis/ParMetis)
Possible optimizations

• Block communication
  – And send the min required from x
  – eg. pre-compute blocks of interfaces

• Load balance, minimize edge cut
  – eg. a good partitioner would do it

• Reordering

• Advantage of additional structure (symmetry, bands, etc)
Comparison

Distributed memory implementation
(by X. Li, L. Oliker, G. Heber, R. Biswas)

<table>
<thead>
<tr>
<th>P</th>
<th>ORIG</th>
<th>MeTiS</th>
<th>RCM</th>
<th>SAW</th>
<th>ORIG</th>
<th>MeTiS</th>
<th>RCM</th>
<th>SAW</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>3.684</td>
<td>3.034</td>
<td>3.749</td>
<td>2.004</td>
<td>3.228</td>
<td>0.011</td>
<td>0.031</td>
<td>0.049</td>
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<tr>
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<td>0.971</td>
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<tr>
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<td>0.030</td>
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<tr>
<td>64</td>
<td>0.601</td>
<td>0.358</td>
<td>0.515</td>
<td>0.290</td>
<td>0.828</td>
<td>0.008</td>
<td>0.032</td>
<td>0.023</td>
</tr>
</tbody>
</table>

- ORIG ordering has large edge cut (interprocessor comm) and poor locality (high number of cache misses)
- MeTiS minimizes edge cut, while SAW minimizes cache misses
Learning Goals

• Efficient sparse computations are challenging!

• Computational challenges and issues related to sparse matrices
  – Data formats
  – Optimization
    • Blocking
    • Reordering
    • Other

• Parallel sparse Mat-Vec product
  – Code optimization opportunities