HPC – Algorithms and Applications

Dwarf # 2 – Sparse Linear Algebra

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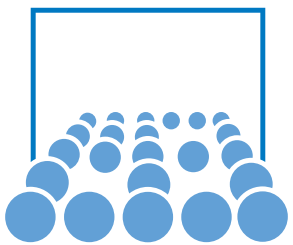

The Seven Dwarfs of HPC – Dwarf # 2

1. dense linear algebra
2. **sparse linear algebra**
3. spectral methods
4. N-body methods
5. structured grids
6. unstructured grids
7. Monte Carlo

Part I

Application Example: Page Rank

Ranking Problem for Websites

- given: n websites connected by hyperlinks
- wanted: rank websites according to "'importance"'
- idea: rank depends on links to a website

Quantitative approach – count the links:

- Graph model:
  websites $\rightarrow$ nodes, links $\rightarrow$ edges
- represented as *adjacency matrix*:
  $A_{ij} = 1$ if an edge exists from i to j, (else $A_{ij} = 0$)
- ranking depends on number of edges to j

$$r(j) := \sum_{i \neq j} A_{ij} \qquad \text{(column sum)}$$

PageRank

Qualitative approach:

- Goal: links from "'important"' website have higher impact
- Step 1: add weights (rank) instead of number of links
- Example: page 3 and 4 link to page 2
  $\Rightarrow$ impact x_2 of page 2 is $x_2 = x_3 + x_4$

Modelled by adjacency matrix:

- leads to system of equations:

$$x_j = \sum_{i \neq j} A_{ij} x_i = \sum_{i \neq j} (A^T)_{ji} x_i$$

- in matrix-vector notation: $x = A^T x$
  (search eigenvector for eigenvalue 1)

PageRank (2)

- Goal: reduce influence of pages with many links
- Step 2: weights divided by number of outgoing links (each website has a ”‘total impact”’/sum of weights of 1)
- Example: page 3 (three outgoing links) and 4 (two links) link to page 2
  $\Rightarrow$ impact x_2 of page 2 is $x_2 = \frac{1}{3}x_3 + \frac{1}{2}x_4$

Modelled by adjacency matrix:

- n_i: number of outgoing links of page i; $n_i = \sum_j A_{ij}$
- Resulting system of equations:

$$x_j = \sum_{i \neq j} \frac{1}{n_i} A_{ij} x_i = \sum_{i \neq j} \left(\frac{1}{n_i} (A^T)_{ji} \right) x_i$$

Page-Rank Matrix

- set $B_{ji} := \frac{1}{n_i}(A^T)_{ji} \rightarrow$ leads to system of equations:

$$x_j = \sum_{i \neq j} \frac{1}{n_i} A_{ij} x_i = \sum_{i \neq j} B_{ji} x_i$$

- search eigenvector for eigenvalue 1: $x = Bx$

Properties of the page-rank matrix:

- all column sums are 1
- all $B_{ji} \geq 0$, diagonal elements $B_{jj} = 0$
  (linking to your own page is not counted)
- B is a so-called (left) **stochastic matrix**

Stochastic Matrices – Properties

B a stochastic matrix, then:

1. B has 1 as eigenvalue;
   all elements of the corresp. eigenvectors $b^{(1)} \geq 0$
   $\rightarrow$ normalise $b^{(1)}$, such that $\sum b_j^{(1)} = 1$
2. element sum of $y = Bx$ is equal to the element sum of x;
   if $x \geq 0$ (element-wise), then also $y \geq 0$
3. v an eigenvector of B with eigenvalue $\neq 1$,
   $\Rightarrow$ element sum of v equal to 0
4. λ eigenvalue of B, then $|\lambda| \leq 1$

(without proofs $\rightarrow$ see a resp. textbook)

Vector Iteration with Stochastic Matrices

- examine iteration $x^{(m)} = Bx^{(m-1)}$,
  start vector $x^{(0)} \geq 0$ has element sum 1
- use eigenvector decomposition of $x^{(0)}$:

$$x^{(0)} = \sum_j \gamma_j b^{(j)}$$

- then: $x^{(m)} = B^m x^{(0)} = \sum_j \gamma_j \lambda_j^m b^{(j)}$
- if $\lambda_1 = 1$ and all other $0 < \lambda_j < 1$, then:

$$x^{(m)} = \sum_j \gamma_j \lambda_j^m b^{(j)} \to \gamma_1 b^{(1)} \qquad \text{for } m \to \infty$$

PageRank in Practice

- use a start vector $x^{(0)}$ with element sum 1
  (then: $\gamma_1 = 1$)
- vector iteration $x^{(m)} = Bx^{(m-1)}$ converges to ranking vector
  $\gamma_1 b^{(1)} = b^{(1)}$ (with element sum 1)
- as every page has only few outgoing links
  $\rightarrow$ B a sparse matrix
- n pages with an average of k links per page:
  $\rightarrow$ kn mult/add operations per iteration
- convergence faster for smaller values of the largest eigenvalue (except $\lambda_1 = 1$)

Vector Iteration in Practice

Problem: two separate partitions

- consider the following page-rank matrix:

$$B = \begin{pmatrix} B_I & 0 \\ 0 & B_{II} \end{pmatrix}$$

  (web divided into two non-linked partitions)
- B_I and B_{II} are stochastic matrices, each with eigenvectors b_I and b_{II} for eigenvalue 1
- $(b_I\ b_{II})^T$, but also $(b_I\ 0)^T$ and $(0\ b_{II})^T$ are eigenvectors of B (for eigenvalue 1)
- consequences for convergence and ranking?

Vector Iteration in Practice (2)

Problem: slow convergence

- happens, if at least one $\lambda \approx 1$ (but $\neq \lambda_1 = 1$)
- modify page-rank matrix B:

$$\tilde{B} \rightsquigarrow \alpha B + (1-\alpha)\frac{1}{n}\begin{pmatrix} 1 & \cdots & 1 \\ \vdots & & \vdots \\ 1 & \cdots & 1 \end{pmatrix}$$

- new system of equations $x = \tilde{B}x$,
  or: $x = \alpha Bx + (1-\alpha)\frac{1}{n}ee^T x$, with $e = (1, \ldots, 1)^T$
- equivalent to: $x - \alpha Bx = (1-\alpha)\frac{1}{n}ee^T x$
- $\frac{1}{n}ee^T$ stochastic, therefore $\tilde{B}$ a stochastic matrix, as well

Vector Iteration in Practice (3)

Regularisation

- $x = \tilde{B}x$ iff $x - \alpha Bx = (1-\alpha)\frac{1}{n}ee^T x$
- as $e^T x = 1$ (element sum $= 1$):

$$(I - \alpha B)x = \frac{1}{n}(1-\alpha)e \qquad \text{where } 0 < \alpha < 1$$

- eigenvalues of αB are $\leq \alpha$
  $\Rightarrow (I - \alpha B)$ not singular (all eigenvalues $\geq 1 - \alpha$)
- leads to **unique solution**

Vector Iteration in Practice (4)

Convergence

- compute solution via vector iteration:

$$x^{(m)} = \alpha B x^{(m-1)} + (1-\alpha)\frac{1}{n}e$$

- corresponds to iteration for error vector $\epsilon(m) = x^{(m)} - x$:

$$\epsilon(m) = \alpha B \epsilon(m-1)$$

- now: all eigenvalues of αB are $\leq \alpha$
- therefore $\|\epsilon(m)\| \sim \alpha^m \|\epsilon(0)\|$
  (convergence faster for smaller α)

Vector Iteration in Practice (5)

Regularisation vs. Convergence:

- Vector iteration converges faster for smaller α
- solution is better, the closer α is to 1
  (then $\tilde{B} \approx B$)
- task: find an optimal α
  (common page-rank choice: $\alpha = 0.85$)
- regularisation parameter balances between exact solution and “well-behaved” problem
- regularisation therefore a frequent technique for ill-posed problems

PageRank as a Population Model: Random Surfer

- each website "populated" by x_i web surfers
- total population: $\sum x_i = 1$ (normalised)
- population corresponds to page rank: how many surfer are expected to be on each site?

PageRank: "'Random Surfer"'

- surfers randomly follow a link from the current page (and change to a different website)
- thus: $\frac{1}{n_i} A_{ij} x_i$ surfers change to website j
- regularisation: with probability $(1 - \alpha)$, a surfer will jump to another (random) page in the internet
- vector iteration $\rightarrow$ population evolves towards an equilibrium

Part II

Data Structures for Sparse Matrices

A matrix is called sparse, if it contains that many zero elements (i.e., that few non-zeros), such that it becomes worthwhile to change to special data structures and algorithms to store and process them.

(following a definition by Wilkinson)

Coordinate Scheme (aka Triple Scheme)

- store a triple (a_{ij}, i, j) for each non-zero a_{ij} (not necessarily sorted)
- implementation as "array of struct":

```
struct sparseElement {
    int i; int j; int value
};
typedef struct sparseElement[] sparseMatrix;
```

- implementation as $3 \times K$ matrix (K non-zeros):

a_{ij}	2.	–1.	–1.	2.	–1	–1.	2.	–1.	–1.	2.
i	1	1	2	2	2	3	3	3	4	4
j	1	2	1	2	3	2	3	4	3	4

- used, for example, in Matlab, or as input format

Compressed Row Storage (CRS)

- two arrays of size K with a_{ij} and j:

a[k]	2.	–1.	–1.	2.	–1	–1.	2.	–1.	–1.	2.
j[k]	1	2	1	2	3	2	3	4	3	4

(sorted by increasing row)

- third array points to start of a row in a[k]:

start[i]	0	2	5	8	10

- implementation of sparse-matrix-vector mult. (SpMV):

```
for(i=0; i<n; i++) {
    for(k=start[i]; k<start[i+1]; k++)
        y[i] += a[k] * x[ j[k] ];
};
```

Variants of CRS

Compressed Column Storage (CCS)

- same as CRS, but with rows and columns exchanged
- used in Harwell-Boeing / Rutherford Boeing collection

Gustavson: Combine CRS and CCS

- compressed row storage format plus:
- column starts (start[j]) and row indices i[k] as in CCS
- improves column-wise access to sparse matrices

Block CRS

- store small matrix blocks (e.g.: 2×2, 4×4) instead of single elements
- improves exploitation of SIMD capabilities of CPUs

Incremental CRS

- use $\tilde{j} = (i-1) \cdot n + (j-1)$ as element index
- store increments of $\tilde{j}$ in array inc[k]

a[k]	2.	–1.	–1.	2.	–1	–1.	2.	–1.	–1.	2.
inc[k]	0	1	3	1	1	3	1	1	3	1
$\tilde{j}$[k]	0	1	4	5	6	9	10	11	14	15

- implementation of sparse-matrix-vector mult. (SpMV):

```
for(k=0,i=0, jj =inc [0];  i<n; i  += j/n)
    for( j  = j%n; j<n; j+=inc[k], k++ )
        y[ i ]  += a[k]  * x[ j ];
```

- C impl. of SpMV found to be faster than for CRS (Bisseling)
- avoids array start[i] (esp. attractive, if $K < n$)

ELLPACK Format – Rectangular Storage

- scenario: at most $k_{\max}$ non-zeros per row
- store values in $n \times k_{\max}$ matrix/array a_{ik}
- store column indices in $n \times k_{\max}$ matrix/array j_{ik}

$$a_{ik}: \begin{pmatrix} 2. & -1. & 0 \\ -1. & 2. & -1 \\ -1. & 2. & -1. \\ -1. & 2. & 0 \end{pmatrix} \qquad j_{ik}: \begin{pmatrix} 1 & 2 & * \\ 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & * \end{pmatrix}$$

- very regular data structure
- supports vectorisation

ELLPACK Format – SpMV Implementation

- row-oriented implementation:

```
for( i=0; i<n; i++)
    for(k=0; k<kmax; k++ )
        y[ i ] += a[i ][ k] * x[ j[ i ][ k] ];
```

- column-oriented implementation:

```
for(k=0; k<kmax; k++ )
    for( i=0; i<n; i++)
        y[ i ] += a[i ][ k] * x[ j[ i ][ k] ];
```

$\rightarrow$ second for-loop leads to vector access to y, a and j

Jagged Diagonal Storage (JDS)

- sort rows according to number of non-zeros
- consider matrices a_{ik} and j_{ik} as in ELLPACK
- store a_{ik} and j_{ik} sequentially and in column-major order
- but do not store a_{ik}, j_{ik} for zero elements
  $\Rightarrow$ requires additional array start[k] (start of k-th column)
- SpMV implementation (column-oriented):

```
for(k=0; k<kmax; k++ )
    for( i=0;  i< (start[k+1]−start[k]);  i++)
        y[i]  += a[start[k]+i] ∗ x[  j[start[k]+i]  ];
```

Reference/Literature (Sparse Linear Algebra)

Rob H. Bisseling:
Parallel Scientific Computing –
A structured approach using BSP and MPI.
Oxford University Press, 2004.