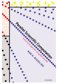
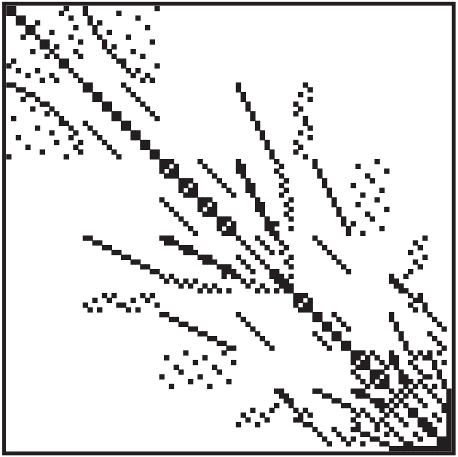
Sequential sparse matrix–vector multiplication (PSC §4.1)



Sparse and dense matrices

- Sparse matrices are sparsely populated by nonzero elements.
- Dense matrices have mostly nonzeros.
- Sparse matrix computations save time: operations with zeros can be skipped or simplified; only the nonzeros must be handled.
- Sparse matrix computations also save memory: only the nonzero elements need to be stored (together with their location).

Sparse matrix cage6



$n = 93$, $nz = 785$ nonzeros, $c = 8.4$ nonzeros per row,
$d = 9.1\%$ density

Matrix statistics

- Number of nonzeros is

$$nz = nz(A) = |\{a_{ij} : 0 \le i, j < n \wedge a_{ij} \neq 0\}|.$$

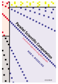
- Average number of nonzeros per row or column is

$$c = c(A) = \frac{nz(A)}{n}.$$

- Density is

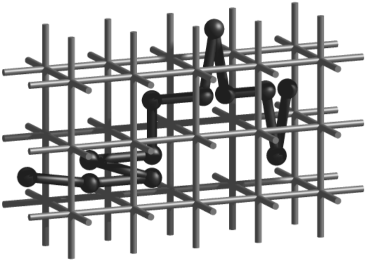
$$d = d(A) = \frac{nz(A)}{n^2}.$$

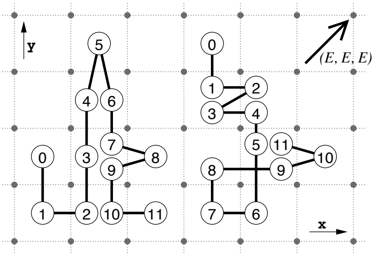
- Matrix is sparse if $nz(A) \ll n^2$, or $c(A) \ll n$, or $d(A) \ll 1$.



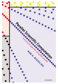
Application: cage model for DNA electrophoresis

(A. van Heukelum, G. T. Barkema, R. H. Bisseling,
Journal of Computational Physics **180** (2002) pp. 313–326.)

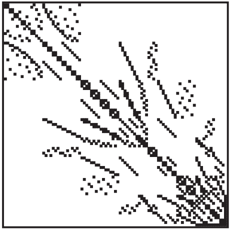




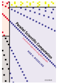
- 3D cubic lattice models a gel
- DNA polymer reptates (moves like a snake):
  kinks and end points move
- DNA sequencing machines: electric field E.
  Aim: study drift velocity $v(E)$.



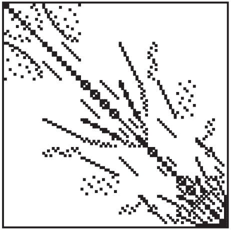
Transition matrix for cage model



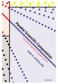
- Matrix element a_{ij} is the probability that a polymer in state j moves to a state i. Hence, $0 \leq a_{ij} \leq 1$.
- Polymer has 6 monomers for cage6. We can move only one monomer at a time. Hence, each state has only a few connected states and the matrix is sparse.



Sparsity structure of cage6

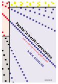


- Each move can be reversed, hence $a_{ij} \neq 0 \iff a_{ji} \neq 0$, i.e., the matrix is structurally symmetric.
- Move against the electric field has different probability than move with the field. Hence $a_{ij} \neq a_{ji}$, so that the matrix is unsymmetric.



Power method

- Let $\mathbf{x}$ be the vector of state frequencies: component x_i represents the relative frequency of state i, with $0 \leq x_i \leq 1$ and $\sum_i x_i = 1$.
- The power method computes $A\mathbf{x}, A^2\mathbf{x}, A^3\mathbf{x}, \ldots$, until convergence.
- Final component x_i represents the frequency of state i in the steady-state situation, where $A\mathbf{x} = \mathbf{x}$.
- Main operation: multiplication of sparse matrix A and dense vector $\mathbf{x}$.



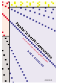
Sparse matrix–vector multiplication

- Let A be a sparse $n \times n$ matrix and $\mathbf{v}$ a dense input vector of length n.
- We consider the problem of computing the dense output vector $\mathbf{u}$,

$$\mathbf{u} := A\mathbf{v}.$$

- The components of $\mathbf{u}$ are

$$u_i = \sum_{j=0}^{n-1} a_{ij} v_j, \quad \text{for } 0 \le i < n.$$



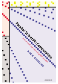
Sparse matrix–vector multiplication algorithm

input: A: sparse $n \times n$ matrix,
$\mathbf{v}$: dense vector of length n.
output: $\mathbf{u}$: dense vector of length n, $\mathbf{u} = A\mathbf{v}$.

for $i := 0$ **to** $n - 1$ **do**
    $u_i := 0;$

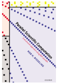
for all $(i, j) : 0 \le i, j < n \wedge a_{ij} \neq 0$ **do**
    $u_i := u_i + a_{ij} v_j;$

The sparsity of A is expressed by the test $a_{ij} \neq 0$. Such a test is never executed in practice, and instead a sparse data structure is used.

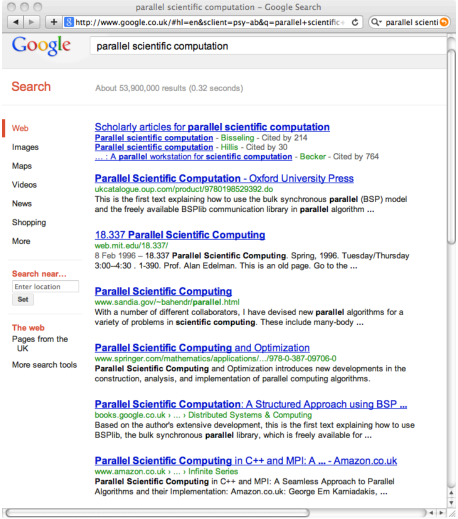


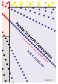
Iterative solution methods

- Sparse matrix–vector multiplication is the main computation step in iterative solution methods for linear systems or eigensystems.
- Iterative methods start with an initial guess $\mathbf{x}^0$ and then successively improve the solution by finding better approximations $\mathbf{x}^k$, $k = 1, 2, \ldots$, until the error is tolerable.
- Examples:
  - Linear systems $A\mathbf{x} = \mathbf{b}$, solved by the conjugate gradient (CG) method or MINRES, GMRES, QMR, BiCG, Bi-CGSTAB, IDR, SOR, FOM, ...
  - Eigensystems $A\mathbf{x} = \lambda\mathbf{x}$ solved by the Lanczos method, Jacobi–Davidson, ...



Web searching: which page ranks first?





The link matrix A

- Given n web pages with links between them.
  We can define the sparse $n \times n$ link matrix A by

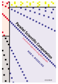
$$a_{ij} = \begin{cases} 1 & \text{if there is a link from page } j \text{ to page } i \\ 0 & \text{otherwise.} \end{cases}$$

- Let $\mathbf{e} = (1, 1, \ldots, 1)^T$, representing an initial uniform importance (rank) of all web pages. Then

$$(A\mathbf{e})_i = \sum_j a_{ij} e_j = \sum_j a_{ij}$$

  is the total number of links pointing to page i.

- The vector $A\mathbf{e}$ represents the importance of the pages; $A^2\mathbf{e}$ takes the importance of the pointing pages into account as well; and so on.

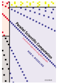


The Google matrix

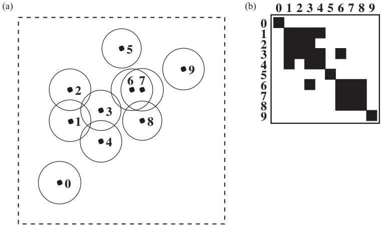
- A web surfer chooses each of the outgoing N_j links from page j with equal probability. Define the $n \times n$ diagonal matrix D with $d_{jj} = 1/N_j$.
- Let α be the probability that a surfer follows an outlink of the current page. Typically $\alpha = 0.85$. The surfer jumps to a random page with probability $1 - \alpha$.
- The Google matrix is defined by (Brin and Page 1998)

$$G = \alpha A D + (1 - \alpha)\mathbf{e}\mathbf{e}^T / n.$$

- The PageRank of a set of web pages is obtained by repeated multiplication by G, involving sparse matrix–vector multiplication by A, and some vector operations.



Insight into other applications



- (a) A 2D molecular dynamics domain of size 1.0×1.0 with 10 particles.
- The cut-off radius for the interaction between particles is $r_{\mathrm{c}} = 0.2$. The circles shown have radius $r_{\mathrm{c}}/2 = 0.1$.
- (b) The corresponding sparse 10×10 force matrix F. If the circles of radius $r_{\mathrm{c}}/2$ of particles i and j overlap, then i and j interact, so that nonzero forces f_{ij} and f_{ji} appear in F.

Summary

- Sparse matrices are the rule, rather than the exception. In many applications, variables are connected to only a few others, leading to sparse matrices.
- Sparse matrices occur in various application areas:
  - transition matrices in Markov models;
  - finite-element matrices in engineering;
  - linear programming matrices in optimisation;
  - weblink matrices in Google PageRank computation.
- We often express computation costs in the matrix size n and the average number of nonzeros per row c.
- Sparse matrix–vector multiplication is important for iterative solvers. It can also capture other applications such as molecular dynamics.
- The sequential computation is simple, but its parallelisation is a big challenge.