Scientific Computing I

Module 2: Population Modelling – Discrete Models

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Outline – Algebraic Population Models

Fibonacci's Rabbits

Game of Life

PageRank

- Ranking of Websites
- Stochastic Matrices, Markov Chains
- PageRank in Practice: Vector Iteration
- Random Surfer Model

Fibonacci's Rabbits

A pair of rabbits are put in a field.
If rabbits take a month to become mature
and then produce a new pair every month,
how many pairs will there be in twelve months time?

Leonardo Pisano ("Fibonacci"), A.D. 1202

Model Assumptions

Which assumptions or simplifications have been made?

- we consider pairs of rabbits
- rabbits reproduce exactly once a month
- female rabbits always give birth to a pair of rabbits
- newborn rabbits require one month to become mature
- rabbits don't die
- . . . ?

The Fibonacci Numbers

How many pairs of rabbits are there?

- we start with a newborn pair of rabbits
- after one month: still 1 pair of rabbits (now mature)
- after two months: 2 pairs of rabbits (one mature)
- after three months: 3 pairs of rabbits (two mature)
- after n months:

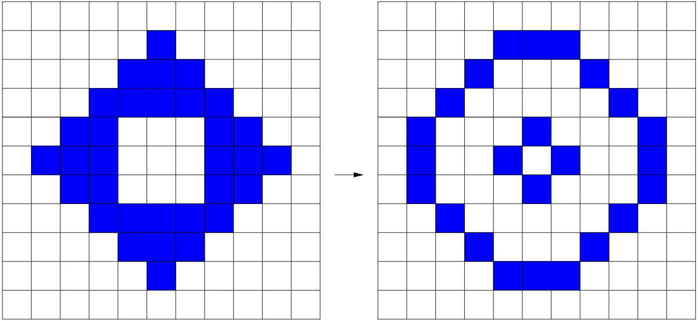
$$f_n = f_{n-1} + f_{n-2}, \qquad f_0 = f_1 = 1$$

- exponential growth of rabbits (see tutorials):

$$f_n = \frac{1}{\sqrt{5}} \left(\phi^n - (1-\phi)^n\right),$$

where $\phi = \frac{1}{2}\left(1 + \sqrt{5}\right) \approx 1.61\ldots$ is the golden section number.

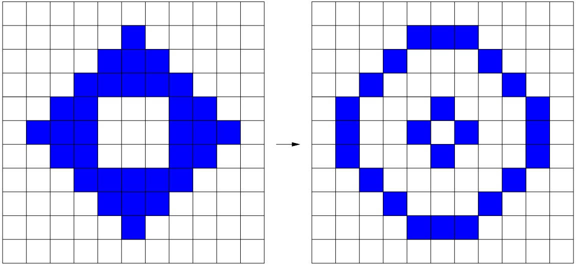
Conway's Game of Life



Cellular Automaton:

- cells are either "alive" or "dead"
- synchronous status update of all cells
- depending on the status of the neighbour cells

Game of Life – Update Rules



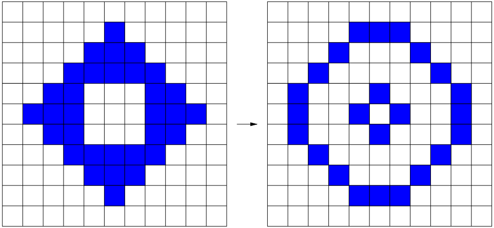
A living cell:

- stays alive, if it has exactly 2 or 3 living neighbours
- dies, if it has more or less neighbours

A dead cell:

- comes alive, if it has exactly 3 living neighbours

Game of Life – Modelling Questions



Modelling Questions:

- are there any stable states? (or cycles?)
- is extinction or infinite growth of the population possible?
- how do such scenarios look like?
- is it possible to explicitly compute such scenarios?

PageRank: Website Ranking and “Random Surfer” Models

- 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

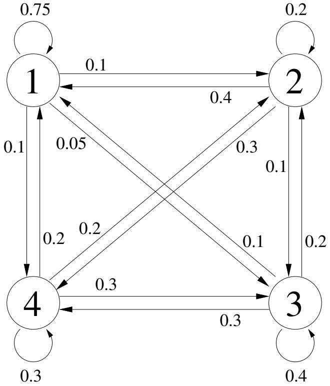
B a stochastic matrix, then:

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)

Compare: Markov Chain

- finite set of states with certain possible state transitions
- change of states subject to given probability
- probability only depends on current state (“memoryless”)



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: $\gamma_1 = 1$ can be assumed via normalisation of $b^{(1)}$)
- 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: 2 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 and 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