Scientific Computing I

Module 2: Population Modelling – Discrete Models

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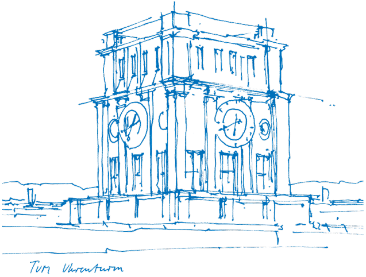


Outline – Algebraic Population Models

Fibonacci's Rabbits

PageRank

- Random Surfer Model
- Stochastic Matrices
- PageRank in Practice: Vector Iteration

Game of Life

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.

Rabbits and Matrices

Let $b^{(n)}$ the number of newborn rabbits and $g^{(n)}$ the number of grown-ups after n months, then:

$$\begin{pmatrix} b^{(n)} \\ g^{(n)} \end{pmatrix} = \begin{pmatrix} g^{(n-1)} \\ g^{(n-1)} + b^{(n-1)} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} b^{(n-1)} \\ g^{(n-1)} \end{pmatrix}$$

$\rightarrow$ tutorials (homework)

Challenge: “zombie” rabbits

- $r^{(n)}$ the number of rabbits, $z^{(n)}$ the number of zombie rabbits
- each month, rabbits get bitten by zombie rabbits and turn into zombies
- build your own model!
  Possible modeling questions: Do bitten rabbits immediately turn into zombies? What happens if no more rabbits are left? How about newborns?

Website Ranking and “Random Surfer” Models

The PageRank Algorithm

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

Graph Modeling with Adjacency Matrix:

- 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 the number of “visitors” of each node i
- how do visitors switch between websites?
  $\rightarrow$ “random surfer” assumption

A Random Surfer Model

Population of Web Surfers:

- each website/node i is "populated" by x_i web surfers
- total population shall be normalized: $\sum x_i = 1$
- population corresponds to page rank:
  how many surfer are expected to be on each site?

Assuming "Random Surfers"

- surfers randomly follow a link from the current page
  (and change to a different website)
- more exactly: from time step (n) to $(n+1)$, all surfers follow a random link

$$x_i^{(n+1)} = \rho_j x_j^{(n)} + \rho_k x_k^{(n)} + \ldots$$

- ρ_j the fraction of surfers on site j who change to site i
- number of outgoing links of page j is $n_j = \sum_l A_{jl}$
- thus assume $\rho_j := 1/n_j$ (each link has equal probability to be followed)

A Random Surfer Model (2)

Random Surfer Model and the Adjacency Matrix:

- recall $x_i^{(n+1)} = \rho_j x_j^{(n)} + \rho_k x_k^{(n)} + \ldots$
- surfers can only follow existing links (i.e., $A_{ji} \neq 0$):

$$x_i^{(n+1)} = \sum_j \frac{1}{n_j} A_{ji} x_j^{(n)} = \sum_j \frac{1}{n_j} (A^T)_{ij} x_j^{(n)}$$

- define **page rank matrix** $B_{ij} := \frac{1}{n_j}(A^T)_{ij}$ to obtain the following model:

$$x_i^{(n+1)} = \sum_{j \neq i} \frac{1}{n_j} (A^T)_{ij} x_j^{(n)} = \sum_{j \neq i} B_{ij} x_j^{(n)} \qquad \text{or} \quad x^{(n+1)} = Bx^{(n)}$$

What is the Expected Population?

- how does the sequence $x^{(n+1)} = Bx^{(n)}$ evolve for $n \to \infty$?
- is there an equilibrium? $\to$ can only happen for an x with

$$x_i = \sum_j \frac{1}{n_j} (A^T)_{ij} x_j \qquad \text{i.e.} \quad x = Bx$$

Page-Rank Matrix

- given: system of equations $x_i = \sum_{j \neq i} B_{ij} x_j$ with $B_{ij} := \frac{1}{n_j} (A^T)_{ij}$
- $x = Bx$ means: search an eigenvector for eigenvalue 1
- does such an eigenvalue/eigenvector pair exist?

Properties of the page-rank matrix:

- all column sums of B are 1 (due to definition of n_j)
- all $B_{ij} \geq 0$, diagonal elements $B_{ii} = 0$
  (links to your own page are not followed)
- 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 $x^{[m]} = Bx^{[m-1]} = \cdots = B^m x^{[0]}$, 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: $x^{[m]} = B^m x^{[0]} = \sum_j \gamma_j \lambda_j^m b^{(j)}$
- assume $\lambda_1 = 1$ and all other $0 \leq |\lambda_j| < 1$, then:

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

Comment on notation:

- upper index in square brackets $[m]$ denotes a sequence of vectors, $x^{[m]}$
- upper index in parentheses (j) denotes different eigenvectors, $b^{(j)}$

PageRank in Practice

- use a start vector $x^{[0]}$ with element sum 1
- stochastic matrix property #3 plus normalisation of $b^{(1)}$ ensure that $\gamma_1 = 1$ ($|\lambda_j| < 1$, thus element sum of $b^{(j)}$ is 0)
- vector iteration $x^{[m]} = Bx^{[m-1]}$ converges to eigenvector $\gamma_1 b^{(1)} = b^{(1)}$
- element sum 1 always maintained (stochastic matrix property #2)

How about efficiency?

- 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 depends on the largest eigenvalue except $\lambda_1 = 1$
  $\rightarrow$ faster convergence for smaller "largest not 1" eigenvalue

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?
  $\rightarrow$ independent rating of partitions I and II

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 B are ≤ 1
  $\Rightarrow$ 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

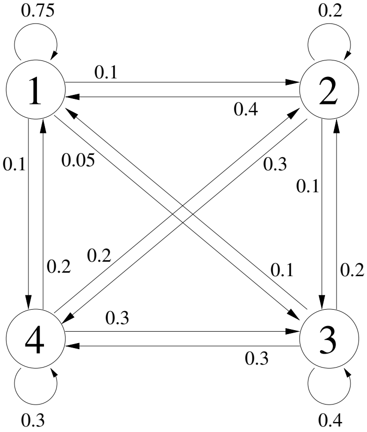
- Vector iteration converges faster for smaller α
- solution is better, the closer α is to 1
  (then $\tilde{B} \approx B$)
- task: find an optimal α
  (common page-rank choice: $\alpha = 0.85$)
- regularisation parameter balances between exact solution and "well-behaved" problem
- regularisation therefore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

Regularisation and "Random Surfer"

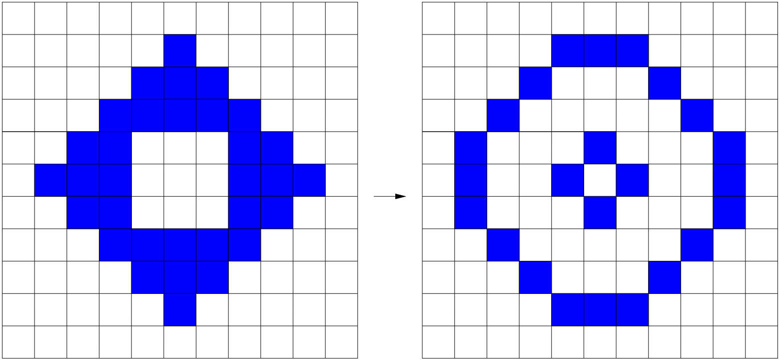
- with probability $(1 - \alpha)$, a surfer will jump to another (random) page in the internet

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”)



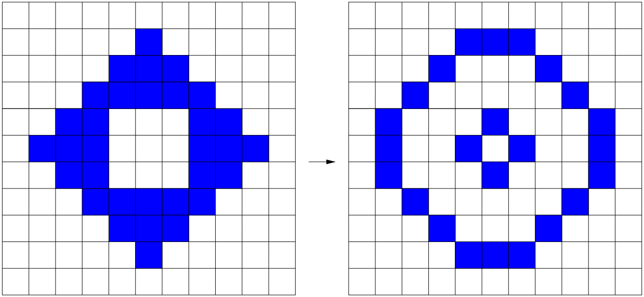
Conway's Game of Life



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



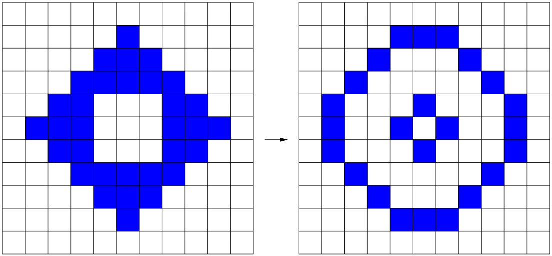
A living cell:

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