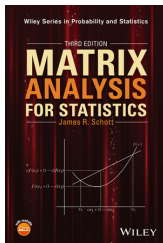


Forward-backward algorithm with matrix calculus

Alain Franc

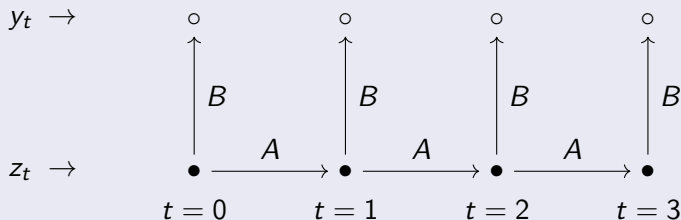
INRAE BioGeCo & INRIA Pleiade

INCA project, Masemo, Paris, July 1-3, 2025



Hidden Markov Chain: notations

Dependencies between hidden (●) and observed (○) variables



$$A[z, z'] = \mathbb{P}(Z_t = z \mid Z_{t-1} = z'); \quad B[y, z] = \mathbb{P}(Y_t = y \mid Z_t = z)$$

Joint law of hidden and observed variables: $p(\mathbf{z}, \mathbf{y})$

$$p(\mathbf{z}, \mathbf{y}) = \mathbb{P}(\mathbf{Z} = \mathbf{z}, \mathbf{Y} = \mathbf{y}) = \left[\prod_{t=1}^T B(y_t, z_t) A(z_t, z_{t-1}) \right] B(y_0, z_0) \pi_0(z_0)$$

Main issues for HMM (Rabiner, 1986)

knowing	compute or infer	algorithm
observations, parameters - id - - id - observations	probability of the observations smoothing, filtering most likely hidden states parameters	fw (-bw) fw-bw Viterbi ($\simeq$ fw) EM

Objective of this presentation

- ◇ provide a unified automatic approach (instead of case by case)
- ◇ to write a fw and fw-bw algorithm, compute their complexity
- ◇ for a diversity of HMM based models:
 - multichains,
 - semi-Markov,
 - their combinations.

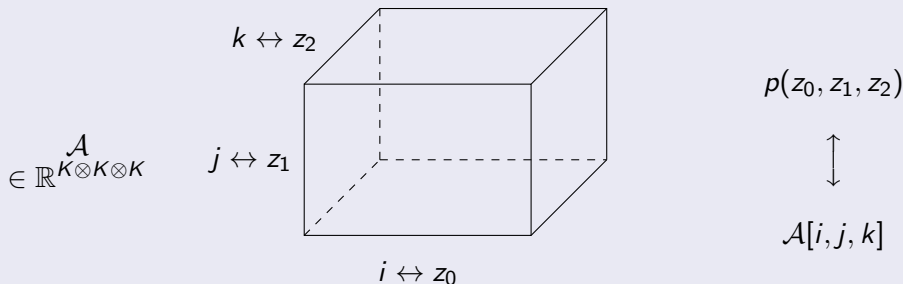
A probability distribution as a tensor

Distributions

$$p(z_0, \dots, z_T) \quad z_t \in \mathcal{K} \quad \mathcal{K} = \{1, \dots, K\} \subset \mathbb{N} \quad \Omega_Z = \mathcal{K}^{T+1}$$

Tensors as multi-ways arrays ($T = 2$)

$$p \longrightarrow \mathcal{A} \in \mathbb{R}^{K \times \dots \times K} = (\mathbb{R}^K)^{\otimes (T+1)}$$



New object:

Un-normalized Heterogeneous Markov based Distribution

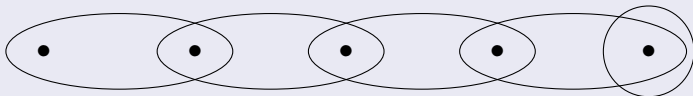
Definition: it is a tensor denoted $\mathcal{A}$

given $T \in \mathbb{N}^*$
 $K \in \mathbb{N}^*$
 $\pi_0 \in \mathbb{R}_+^K$
 $A_1, \dots, A_T \in \mathbb{R}^{K \times K}$

define $\mathcal{A} \in (\mathbb{R}^K)^{\otimes (T+1)}$

by $\mathcal{A}[z_0, \dots, z_T] = A_T[z_T, z_{T-1}] \dots A_1[z_1, z_0] \pi_0[z_0]$

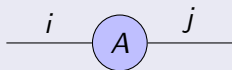
It is a pairwise graphical model along a line (ellipses are factors)



Why tensors? $\rightarrow$ Tensor networks, coupling by contractions

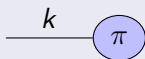
Nodes of the network

matrix



$$(a_{ij})_{i,j} \in \mathbb{R}^{K \times K}$$

vector



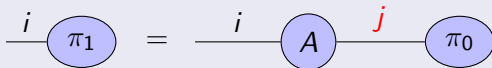
$$(\pi_k)_k \in \mathbb{R}^K$$

scalar



$$\alpha \in \mathbb{R}$$

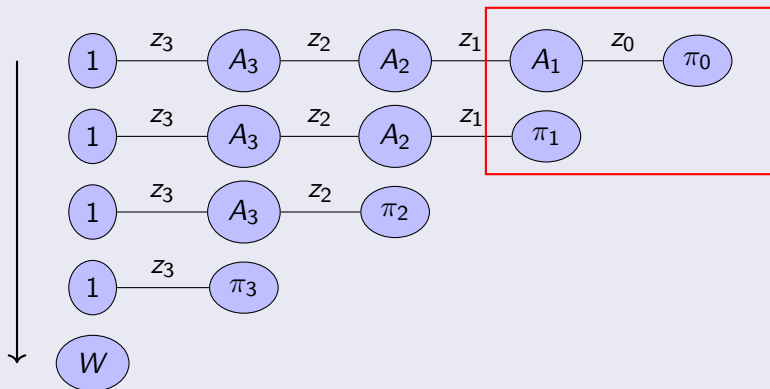
Matrix $\times$ vector product: i : free, j : summed upon (contracted)



$$\pi_1[i] = \sum_j A[i, j] \pi_0[j]$$

Computation of the normalizing constant

Variable elimination (visual)



Extensions

- on trees ("message passing")
- Dynamic Bayesian Networks ? Graphical models with low tree width?

Elimination as an algorithm on an UHMD

Objective

compute $W = \sum_{z_0=1}^K \dots \sum_{z_T=1}^K \mathcal{A}[z_0, \dots, z_T]$, K^{T+1} sums

Algorithm 1 Elimination algorithm elim() on an UHMD

```
1: input  $T, K, (A_t)_{1 \leq t \leq T}$  with  $A_t \in \mathbb{R}^{K \times K}$ ,  $\pi_0 \in \mathbb{R}^K$ 
2: for  $t \in \{1, \dots, T\}$  do
3:   compute  $\pi_t = A_t \pi_{t-1}$  with  $\pi_t[z] = \sum_{z'=1}^K A_t[z, z'] \pi_{t-1}[z']$ 
4: end for
5: compute  $W = \sum_{z \in \mathcal{K}} \pi_T[z]$ 
6: return  $W$ 
```

Complexity (as number of products)

lines 2 (loop on t) and 3 (matrix $\times$ vector product) $\implies \mathcal{O}(TK^2)$

What is behind: why selecting linear algebra

Main tool: matrix $\times$ vector product

The complexity of a matrix $\times$ vector product is on $\mathcal{O}(K^2)$

$$y = Ax$$
$$\begin{matrix} x_1 \\ \vdots \\ x_K \end{matrix}$$
$$i \rightarrow \begin{matrix} a_{i1} & \cdots & a_{iK} \end{matrix} \begin{matrix} y_i \end{matrix}$$

K^2 products

$$y_i = \sum_{j=1}^K a_{ij}x_j$$

Sparsity of transition matrix

A is a $K \times K$ matrix

Observation

if $\#A$ is the number of terms $a_{ij} \notin \{-1, 0, 1\}$
then $y = Ax$ has complexity $\mathcal{O}(\#A)$

Simple example with $K = 3$

$$A = \begin{pmatrix} a & 0 & 1 \\ -1 & 0 & b \\ c & 1 & 0 \end{pmatrix}, \quad x = \begin{pmatrix} u \\ v \\ w \end{pmatrix} \implies Ax = \begin{pmatrix} au + w \\ -u + bw \\ cu + v \end{pmatrix}$$

Complexity in $\mathcal{O}(\#A)$

$y = Ax$ costs 3 multiplications instead of 9: $\mathcal{O}(\#A)$ instead of $\mathcal{O}(K^2)$

One among the three Rabiner's problem

Compute the probability of the observations knowing the parameters

$$p(\mathbf{y}) = \sum_{\mathbf{z}} p(\mathbf{z}, \mathbf{y})$$

Joint law as an UHMD

$\mathbf{y}$ fixed $\implies$ define $A_t[z_t, z_{t-1}] = B[y_t, z_t] A[z_t, z_{t-1}]$

joint law $p(\mathbf{z}, \mathbf{y}) = \left(\prod_{t=1}^T A_t[z_t, z_{t-1}] \right) \pi'_0[z_0]$

define UHMD $\mathcal{A}_{hmm}[z_0, \dots, z_T] = A_T[z_T, z_{T-1}] \dots A_1[z_1, z_0] \pi'_0[z_0]$

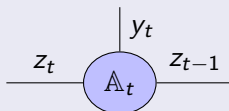
Proposition

- Algorithm `elim()` on the UHMD $\mathcal{A}_{hmm}$ permits to compute $p(\mathbf{y}) = W(\mathcal{A}_{hmm})$
- $\implies$ The complexity of the calculation is in $\mathcal{O}(TK^2)$

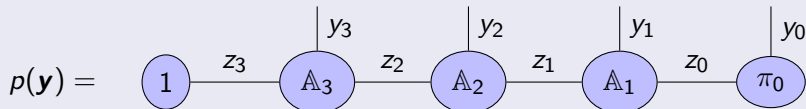
Probability of the observations as a tensor train

Define

$$\mathbb{A}_t[z_t, y_t, z_{t-1}] = B[y_t, z_t] A[z_t, z_{t-1}], \quad \mathbb{A}_t \in \mathbb{R}^{K \times O \times K}$$



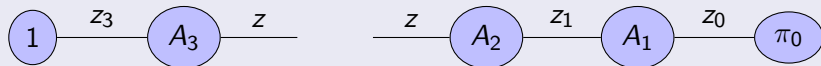
Probability of the observations as a tensor network: **tensor train**



Unary marginals (visual with tensor networks)

$$t = 2, \quad z_2 = z, \quad m(t, z) = \sum_{z_0, z_1, z_3} A[z_3, z] A[z, z_1] A[z_1, z_0] \pi_0[z_0]$$

Variable separation



$$\alpha_t[z] = \text{Diagram: } 1 \text{ --- } z_3 \text{ --- } A_3 \text{ --- } z$$

$$\beta_t[z] = \text{Diagram: } z \text{ --- } A_2 \text{ --- } z_1 \text{ --- } A_1 \text{ --- } z_0 \text{ --- } \pi_0$$

$$m(z, t) = \alpha_t[z] \beta_t[z]$$

Marginal's calculation for an UHMD (smoothing)

Definition: slicing for a tensor

$$m(t, z) = \sum_{\mathbf{z} : z_t = z} \mathcal{A}[\mathbf{z}]$$

Visualization of the algorithm (forward-backward)

$$\begin{array}{ccccccc} \alpha_0 & \xrightarrow{\times A_1} & \alpha_1 & \xrightarrow{\times A_2} & \alpha_2 & \xrightarrow{\times A_3} & \alpha_3 & \xrightarrow{\times A_4} & \alpha_4 \\ \odot & \xleftarrow{\times A_4^T} & \odot & \xleftarrow{\times A_3^T} & \odot & \xleftarrow{\times A_2^T} & \odot & \xleftarrow{\times A_1^T} & \odot \\ \beta_4 & & \beta_3 & & \beta_2 & & \beta_1 & & \beta_0 \\ = & & = & & = & & = & & = \\ m(0) & & m(1) & & m(2) & & m(3) & & m(4) \end{array}$$

$\alpha_0 \xrightarrow{\times A_1} \alpha_1$ means that $\alpha_1 = A_1 \alpha_0$; $\odot$ is the Hadamard product.
 $m(0) = \alpha_0 \odot \beta_4, \dots, \quad \alpha_0 = \pi_0, \quad \beta_0 = (1, \dots, 1)$

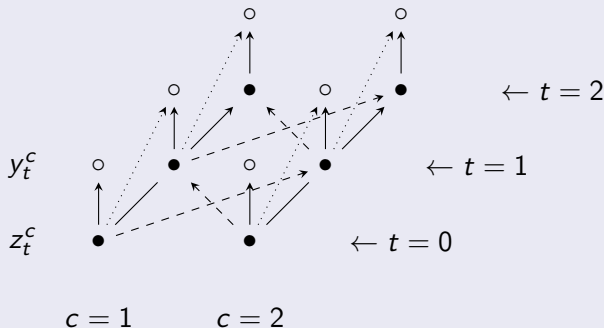
Pseudo-code for marginalisation: complexity in $\mathcal{O}(TK^2)$

Algorithm 2 Marginalisation algorithm margin() in an UHMD

```
1: input  $T, K, (A_t)_{1 \leq t \leq T}$  with  $A_t \in \mathbb{R}^{K \times K}$ ,  $\pi_0 \in \mathbb{R}^K$ 
2: set  $\alpha_0 = \pi_0$ 
3: for  $t \in \{1, \dots, T\}$  do
4:   compute  $\alpha_t = A_t \alpha_{t-1}$ ,           (matrix  $\times$  vector product, in  $\mathcal{O}(K^2)$ )
5: end for
6: set  $\beta_T = 1$ 
7: for  $t \in \{T-1, \dots, 0\}$  do
8:   compute  $\beta_t = A_{t+1}^T \beta_{t+1}$        (matrix  $\times$  vector product, in  $\mathcal{O}(K^2)$ )
9: end for
10: for  $t \in \{0, \dots, T\}$  do
11:   compute  $\mathfrak{m}_t = \alpha_t \odot \beta_{T-t}$ 
12:   return  $\mathfrak{m}_t$ 
13: end for
```

Extension to multichain and richer dependency structures

An example



General Multichain HMM

Definition

- hidden variables $\mathbf{Z}_t \in \mathcal{K}^C$ C chains
- observed variables $\mathbf{Y}_t \in \mathcal{S}^O$ O observations

and $(\mathbf{Z}_t, \mathbf{Y}_t)_t$ is a Markov chain

$$A_G[(\mathbf{z}, \mathbf{y}); (\mathbf{z}', \mathbf{y}')] = \mathbb{P}(\mathbf{Z}_t = \mathbf{z}, \mathbf{Y}_t = \mathbf{y} \mid \mathbf{Z}_{t-1} = \mathbf{z}', \mathbf{Y}_{t-1} = \mathbf{y}')$$

Joint law

$$p(\mathbf{z}_{0:T}, \mathbf{y}_{0:T}) = A_G[(\mathbf{z}_T, \mathbf{y}_T); (\mathbf{z}_{T-1}, \mathbf{y}_{T-1})] \times \dots \times$$

$$A_G[(\mathbf{z}_1, \mathbf{y}_1); (\mathbf{z}_0, \mathbf{y}_0)] \times \pi'_0[\mathbf{z}_0, \mathbf{y}_0]$$

Emission and Transition

$$A_G[(\mathbf{z}, \mathbf{y}); (\mathbf{z}', \mathbf{y}')] = \underbrace{B[\mathbf{y}, (\mathbf{y}', \mathbf{z}, \mathbf{z}')] }_{\text{emission}} \times \underbrace{A[\mathbf{z}, (\mathbf{z}', \mathbf{y}')] }_{\text{transition}}$$

General approach for multichains

Reminder

$$A_G[(z, y); (z', y')] = \underbrace{B[y, (y', z, z')]}_{\text{emission}} \times \underbrace{A[z, (z', y')]}_{\text{transition}}$$

$y_{0:T}$ being fixed

- define $A_t[z_t, z_{t-1}] = B[y_t, (y_{t-1}, z_t, z_{t-1})] \times A[z_t, (z_{t-1}, y_{t-1})]$
- Then the joint law is $\pi'_0[z_0] \prod_{t=1}^T A_t[z_t, z_{t-1}]$
- define an UHMD $\mathcal{A}_G$ with $\mathcal{A}[z_{0:T}] = p(z_{0:T}, y_{0:T})$
- run elimination and marginalisation algorithm on it.

This leads, in a systematic and unified way, to:

- how to write the fw and fw-bw algorithm
- compute their complexity

an example: 1to1-MHMM-CI model

Structure

- | | |
|---|------|
| • A HMM model | HMM |
| • multichain | M |
| • with conditional independence | CI |
| • bijection between hidden and observed variables | 1to1 |

Conditional independence (simplified)

$$p(z_t^1, z_t^2 \mid z_{t-1}^1, z_{t-1}^2) = p_1(z_t^1 \mid z_{t-1}^1, z_{t-1}^2) \times p_2(z_t^2 \mid z_{t-1}^1, z_{t-1}^2)$$

written as

$$A[(z_t^1, z_t^2); (z_{t-1}^1, z_{t-1}^2)] = A^1[z_t^1; (z_{t-1}^1, z_{t-1}^2)] \times A^2[z_t^2; (z_{t-1}^1, z_{t-1}^2)]$$

leading to

$$A[\mathbf{z}_t, \mathbf{z}_{t-1}] = \prod_{c=1}^C A^c[\mathbf{z}_t^c; \mathbf{z}_{t-1}] \Rightarrow A_t[\mathbf{z}_t, \mathbf{z}_{t-1}]$$

Forward algorithm for a 1to1-MHMM-CI

Algorithm 3 Forward algorithm for a 1to1-MHMM-CI

```
1: input  $T, K, C, \pi_0 \in \mathbb{R}^{K^C}, \quad \pi_0[\mathbf{z}] = \mathbb{P}(\mathbf{Z}_0 = \mathbf{z})$ 
2: input  $A_t^c, B_t^c$  for  $1 \leq t \leq T$  and  $1 \leq c \leq C$ , with  $A_t^c, B_t^c \in \mathbb{R}^{K \times K^C}$ ,
3: # preparation
4: for  $t \in \{1, \dots, T\}$  do
5:   compute  $A_t^{ci} \in \mathbb{R}^{K^C \times K^C}$   $\mathcal{O}(T(C-1)K^{2C})$ 
6:     with  $A_t^{CI}[\mathbf{z}_t, \mathbf{z}_{t-1}] = \prod_{c=1}^C B_t^c[\mathbf{z}_t, \mathbf{z}_{t-1}] A_t^c[\mathbf{z}_t^c, \mathbf{z}_{t-1}^c]$ 
7: end for
8: # elimination
9: compute  $W = \text{elim}(T, K^C, (A_t^{CI})_t, \pi_0)$ ,  $\mathcal{O}(TK^{2C})$ 
10: return  $W$ 
```

Complexity: preparation + elimination

$$\mathcal{O}(T(C-1)K^{2C}) + \mathcal{O}(TK^{2C}) = \mathcal{O}(TCK^{2C})$$

A Semi-Markov Model as a Markov Model

SMM (reminder)

SMM: $(J_n, X_{n+1})_n$ is a Markov chain with

- J_n is state z at jump n
- X_{n+1} is sojourn duration in state J_n

$(Z_t, R_t, E_t)_t$ is a MM with

- R_t is the remaining time until next jump
- E_t is the elapsed time since last jump

if $r_t > 0$	no jump	$z \rightarrow z$	$r_t \rightarrow r_t - 1$	$e_t \rightarrow e_t + 1$
if $r_t = 0$	jump	$z \rightarrow z' \neq z$	$r_{t+1} = A_J(.. z_t, e_t)$	$e_{t+1} = 1$

HSMM

$\Rightarrow$ A HSMM can be translated into a HMM

- hidden state space $\mathcal{K} \times \mathcal{D} \times \mathcal{D} \Rightarrow$ transition matrix is $KD^2 \times KD^2$

fw and fw-bw algorithm for a HSMM

naively ...

- Hidden state space has cardinality KD^2
- so elimination algorithm is in $\mathcal{O}(T(KD^2)^2)$

Sparsity

A_{zre} : transition matrix $(z_t, r_t, e_t) \longrightarrow (z_{t+1}, r_{t+1}, e_{t+1})$

- at a jump: $A_{zre}[(z_t, r_t, 1), (z_{t-1}, 0, e_{t-1})] = A_j[(z_t, r_t + 1), (z_{t-1}, e_{t-1})]$
- out of a jump: $A_{zre}[(z_t, r_t, e_t), (z_{t-1}, r_{t-1}, e_{t-1})] \in \{0, 1\}$

$\Rightarrow \#A_{zre} = K^2 D^2$

$\Rightarrow$ complexity of fw or fw-bw algorithm

$\mathcal{O}(T(KD)^2)$ instead of $\mathcal{O}(T(KD^2)^2)$

Challenge

How to write an efficient algorithm for computing $\pi_t = A_{zre}\pi_{t-1}$

$A_{zr} := A_{zre}$ on an example: ED-HMM, $K = 3$, $D = 3$

$\cdot := 0$; $\times := \neq 0, 1$; $ij := (z = i \in \{1, 2, 3\}, r = j \in \{0, 1, 2\})$

	10	11	12	20	21	22	30	31	32
10	.	1	.	×	.	.	×	.	.
11	.	.	1	×	.	.	×	.	.
12	.	.	.	×	.	.	×	.	.
20	×	.	.	.	1	.	×	.	.
21	×	.	.	.	.	1	×	.	.
22	×	.	.	.	.	.	×	.	.
30	×	.	.	×	.	.	.	1	.
31	×	.	.	×	.	.	.	.	1
32	×	.	.	×	.	.	.	.	.

$\left. \begin{array}{l} KD \text{ rows} \\ \text{per row: } K - 1 \text{ terms } \notin \{0, 1\} \end{array} \right\} \implies K(K - 1)D \text{ products}$

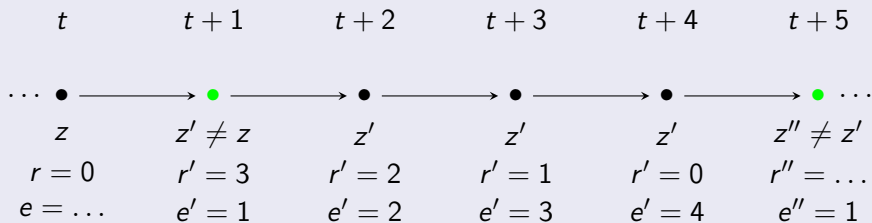
$\implies$ Complexity in $\mathcal{O}(TK^2D)$

Multichain HSMM

Setting: J-MHSMM

Interactions between chains occur at jumps ● only

For one chain c



- ◇ At time $t + 1$, (z', r') depends on the states $z_{t+1}^{c'}$ of other chains
 - ◇ At times $t + 2, t + 3, t + 4$, the transitions are compulsory
 $(z', r', e') \rightarrow (z', r' - 1, e' + 1)$
- ⇒ the transition matrix is sparse

Forward algorithm for a J-MHSMM

States

$(\mathbf{z}_t, \mathbf{r}_t, \mathbf{e}_t)_t$ with $\mathbf{z}_t = (z_t^1, \dots, z_t^C)$, $\mathbf{r}_t = (r_t^1, \dots, r_t^C)$ and $\mathbf{e}_t = (e_t^1, \dots, e_t^C)$

Transition matrix

$$A[(\mathbf{z}_t, \mathbf{r}_t, \mathbf{e}_t), (\mathbf{z}_{t-1}, \mathbf{r}_{t-1}, \mathbf{e}_{t-1})] = p(\mathbf{z}_t, \mathbf{r}_t, \mathbf{e}_t \mid \mathbf{z}_{t-1}, \mathbf{r}_{t-1}, \mathbf{e}_{t-1})$$

$z_t^c \in \mathcal{K}$ and $|\mathcal{K}| = K$

$r_t^c \in \mathcal{D}$ and $|\mathcal{D}| = D$

$e_t^c \in \mathcal{D}^*$ and $|\mathcal{D}^*| = D$

$\implies A$ is a $(KD^2)^C \times (KD^2)^C$ matrix

Complexity

- ◇ expected complexity $\mathcal{O}(T(K^2 D^4)^C)$
- ◇ because of sparsity $\mathcal{O}(T(K^2 D^2)^C)$
- ◇ for a J-M-ED-HMM $\mathcal{O}(T(K^2 D)^C)$

UHMD on semi-rings

Observation

- Matrix $\times$ vector product ($y_i = \sum_{j=1}^K a_{ij}x_j$) does not imply any inversion ($x \rightarrow \frac{1}{x}$)
 $\Rightarrow$ it can be developed on semi-rings

Semi-ring $(\mathbb{R} \cup \{-\infty\}, \max, \times)$

- $+$ $\mapsto$ $\max$
- $\times$ $\mapsto$ $\times$
- $a + 0 = a$ $\mapsto$ $\max(a, -\infty) = a$
- $a(b + c) = ab + ac$ $\mapsto$ $a(\max(b, c)) = \max(ab, ac)$

$W(\mathcal{A})$ of an UHMD $\mathcal{A}$ on a semi-ring

On $\mathbb{R}$,

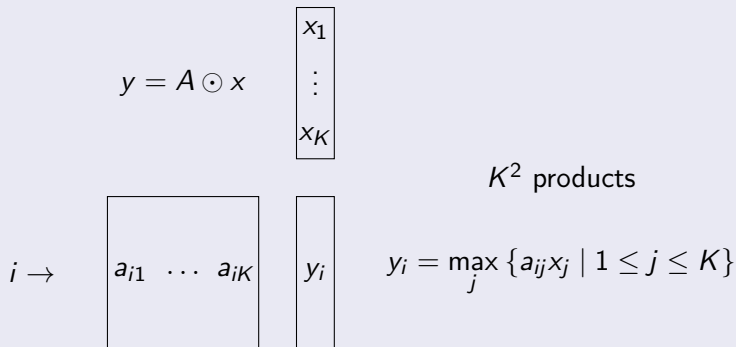
$$W(\mathcal{A}) = \sum_{z \in \Omega_Z} \mathcal{A}[z_0, \dots, z_T]$$

On semi-ring $(\mathbb{R} \cup \{-\infty\}, \max, \times)$

$$W(\mathcal{A}) = \max_{z \in \Omega_Z} \mathcal{A}[z_0, \dots, z_T]$$

Matrix product $y = A \odot x$ in $(\mathbb{R} \cup \{-\infty\}, \max, \times)$

$$y = A \odot x \implies y_i = \bigoplus_{j=1}^K (a_{ij} \odot x_j) = \max_{1 \leq j \leq K} a_{ij} x_j$$



Complexity

The complexity of computing $y = A \odot x$ is in $\mathcal{O}(K^2)$.

Elimination algorithm in $(\mathbb{R} \cup \{-\infty\}, \max, \times)$

Algorithm 4 Elimination algorithm for an UHMD in $(\mathbb{R} \cup \{-\infty\}, \max, \times)$

```
1: input  $T, K, (A_t)_{1 \leq t \leq T}$  with  $A_t \in \mathbb{R}^{K \times K}, \pi_0 \in \mathbb{R}^K$ 
2: for  $t \in \{1, \dots, T\}$  do
3:   compute  $\pi_t = A_t \odot \pi_{t-1}$    with    $\pi_t[z] = \max_{1 \leq z' \leq K} A_t[z, z'] \pi_{t-1}[z']$ 
4: end for
5: compute  $W = \max_{1 \leq z \leq K} \pi_T[z]$ 
6: return  $W$ 
```

Complexity

Its complexity is in $\mathcal{O}(TK^2)$ as well (lines 2 and 3)

Viterbi algorithm for a HMM

Finding the most likely hidden state of a HMM knowing the observations and the parameters.

How to ...

- 1 Let $p(\mathbf{z}, \mathbf{y})$ be the joint law between hidden and observed variables
- 2 write $p(\mathbf{z}, \mathbf{y})$ as an UHMD $\mathcal{A}[z_0, \dots, z_T]$
- 3 compute $M = \max_{\mathbf{z}} \mathcal{A}[\mathbf{z}]$ with elimination algorithm on $\mathcal{A}$ in $(\mathbb{R} \cup \{-\infty\}, \max, \times)$
- 4 run the traceback

Can be extended as a procedure to

- 1 Multichain HMM
- 2 HSMM
- 3 Multichain HSMM with interactions at jumps

What can be next?

∃ different models for a MHMM

- 1 general MHMM
- 2 MHMM with conditional independence
- 3 one to one MHMM with CI

∃ different models for a HSMM

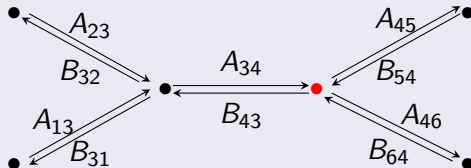
- 1 general HSMM
- 2 standard HSMM
- 3 ED-HMM

What is reachable

- 1 develop fw and fw-bw algorithm as a unified procedure for all these models
- 2 cross together choices for MHMM and for HSMM
- 3 extend to EM

Message passing on a tree

an example (the hidden layer only is shown)



How to associate incoming messages

$$\begin{array}{c} \pi_a \xrightarrow{A} \\ \pi_b \xrightarrow{B} \end{array} \pi_c = (A\pi_a) \odot (B\pi_b)$$

Acknowledgements (warm ones ...)

Working groups on monochain HSMM
and multichain HMM & HSMM of INCA project

Hanna, Irène, Jean-Baptiste, Nathalie, Nicolas, Régis, Sandra, Vlad

Anwar PhD's thesis

Nathalie, Anwar, Olivier for links between tensor algebra and statistical models (on WSBM) and the use of tensor networks

Last but not least ... Inca project

