## **Minimal Realization Problems for**

# Hidden Markov Models





Observe stationary random process  $y(t) \in [d] = \{1, 2, ..., d\}$ 

 The random process is characterized by the joint distribution (Probabilities of strings of any length N)

$$\mathcal{S}^{(\infty)} = \left\{ \mathbb{P}(y_1 = l_1, \cdots, y_N = l_N) : \quad \forall \mathbf{l}_1^N \in [d]^N, \ \forall N \in \mathbb{Z} \right\}$$



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Can we find a finite state system description of the process?



Randomness rightarrow? rightarrow Observed random process  $y(t) \in [d] = \{1, 2, ..., d\}$ 

+ Assume that the process can be described by a finite state system

$$\theta = (d, k, u \in \mathbb{R}^k, v \in \mathbb{R}^k, A^{(l)} \in \mathbb{R}^{k \times k} : l \in [d])$$

$$w_{t+1} = A^{(l_t)} w_t, \quad w_0 = v,$$
  
$$z_t = u' w_t, \quad \forall \mathbf{l}_1^N \in [d]^N, \forall N \in \mathbb{Z}$$

$$\mathbb{P}(y_1 = l_1, \cdots, y_N = l_N) = z_N(\mathbf{l}_1^N)$$
  
=  $u' A^{(l_n)} \dots A^{(l_1)} A^{(l_{-1})} \dots A^{(l_{-n})} v$ 

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State has no physical meaning $w_t \in \mathbb{R}^k$  $orall \mathbf{l}_1^N \in [d]^N, orall N \in \mathbb{Z}$ 

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$$\theta = (d, k, u \in \mathbb{R}^k, v \in \mathbb{R}^k, A^{(l)} \in \mathbb{R}^{k \times k} : l \in [d])$$

• Multi-linear system  $w_{t+1} = A^{(l_t)}w_t$ ,  $w_0 = v$ ,

$$z_t = u'w_t,$$

$$\theta = (d, k, u \in \mathbb{R}^k, v \in \mathbb{R}^k, A^{(l)} \in \mathbb{R}^{k \times k} : l \in [d])$$

- ▲ Multi-linear system w<sub>t+1</sub> = A<sup>(l<sub>t</sub>)</sup>w<sub>t</sub>, w<sub>0</sub> = v,
   z<sub>t</sub> = u'w<sub>t</sub>,
- Quasi- HMM realization

If 
$$\mathbb{P}(y_1 = l_1, \cdots, y_N = l_N) = z_N(\mathbf{l}_1^N)$$
 is a valid joint distribution  
and  $u' \left[ \sum_{j \in [d]} A^{(j)} \right] = u', \quad \left[ \sum_{j \in [d]} A^{(j)} \right] v = v.$  (stationarity)

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• HMM realization If in addition  $v = \mathbf{e}_k, \quad u \in \mathbb{R}^k_+, \sum_i u_i = 1,$  $A^{(j)} \in [0, 1]^{k \times k}, \forall j \in [d],$ 

$$\theta = (d, k, u \in \mathbb{R}^k, v \in \mathbb{R}^k, A^{(l)} \in \mathbb{R}^{k \times k} : l \in [d])$$

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 ★ HMM realization If in addition
  $v = \mathbf{e}_k$ ,  $u \in \mathbb{R}^k_+$ ,  $\sum_i u_i = 1$ ,  $A^{(j)} \in [0,1]^{k \times k}$ ,  $\forall j \in [d]$ ,
 1-1 mapping to Transition:  $Q \in \mathbb{R}^{k \times k}$ .
 Observation:  $O \in \mathbb{R}^{d \times k}$ 

#### **Realization problems**

+ Input: probabilities of length N strings of an HMM

$$\mathcal{S}^{(N)} = \{ \mathbb{P}(y_1 = l_1, \cdots, y_N = l_N) : \forall \mathbf{l}_1^N \in [d]^N \}$$

◆ Output:
 ✓ (d, k, u ∈ ℝ<sup>k</sup>, v ∈ ℝ<sup>k</sup>, A<sup>(l)</sup> ∈ ℝ<sup>k×k</sup> : l ∈ [d])
 ✓ Minimal order quasi-HMM realization
 ✓ Minimal order HMM realization

$$\mathcal{S}^{(\infty)} = \left\{ \mathbb{P}(\mathbf{y}_1^N = \mathbf{l}_1^N) : \quad \forall \mathbf{l}_1^N \in [d]^N, \ \forall N \in \mathbb{Z} \right\}$$
$$\mathbb{P}(\mathbf{y}_1^N = \mathbf{l}_1^N) = u' A^{(l_1)} A^{(l_1)} \dots A^{(l_N)} v, \quad \forall \mathbf{l}_1^N \in [d]^N$$

## **Realization problems**

#### + Informational complexity

✓ When is the minimal model identifiable from  $S^{(N)}$ ? window size N =?

#### + Computational complexity

✓ Can we compute the minimal realization with efficient algorithms?

#### + Statistical complexity

✓ Are the algorithms robust to estimation noise?

#### In general, learning HMMs is hard

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Main contribution 1:

Main contribution 2

+ Computational complexity



+ Statistical complexity

✓ Are the algorithms robust to estimation noise?

#### In general, learning HMMs is hard

# Quasi-HMM realization

## Quasi-HMM realization

- + Input: probabilities of length N = 2n + 1 strings  $y_{-n}, \dots, y_{-1} \ y_0 \ y_1, \dots, y_n$  $S^{(N)} = \{\mathbb{P}_{y_{-n}}, \dots, y_n\}$
- Output: a minimal quasi-HMM realization

$$\theta^o = (d, k, u, v, A^{(l)} : l \in [d])$$

#### + Key:

Arrange 
$$S^{(N)} = \{\mathbb{P}_{y_{-n}, \dots, y_n}\}$$
 into matrices:  
 $H^{(0)}, \{H^{(j)} : j \in [d]\} \in \mathbb{R}^{d^n \times d^n}$ 

Matrix rank decomposition of  $H^{(0)}$ equivalent minimal quasi realization up to linear transformation

**Complexity?** 

+ Input:  $\mathcal{S}^{(N)}$  arranged into  $H^{(0)}, \{H^{(j)}: j \in [d]\} \in \mathbb{R}^{d^n \times d^n}$ 

\* assume minimal realization  $\theta^o = (d, k, u, v, A^{(l)} : l \in [d])$ 

Enumerate all length n strings:  $L(\mathbf{l}_1^n) = (l_1 - 1)d^{n-1} + (l_2 - 1)d^{n-2} + \dots + l_n, \quad \forall \mathbf{l}_1^n = [d]_5^n$ 

+ Input:  $\mathcal{S}^{(N)}$  arranged into  $H^{(0)}, \{H^{(j)}: j \in [d]\} \in \mathbb{R}^{d^n \times d^n}$ 

$$\begin{split} [H^{(0)}]_{L(\mathbf{l}_{1}^{n}),L(\mathbf{l}_{-1}^{-n})} &= \mathbb{P}\Big(\mathbf{y}_{0}^{n-1} = \mathbf{l}_{1}^{n}, \ \mathbf{y}_{-1}^{-n} = \mathbf{l}_{-1}^{-n}\Big) \\ &= u'A^{(l_{n})} \dots A^{(l_{1})}A^{(l_{-1})} \dots A^{(l_{-n})}v \\ \end{split}$$
n letters now and future

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\* assume minimal realization  $\theta^o = (d, k, u, v, A^{(l)} : l \in [d])$ 

$$H^{(0)} = \begin{bmatrix} u'A^{(1)} \cdots A^{(1)} \\ u'A^{(1)} \cdots A^{(2)} \\ \vdots \\ u'A^{(d)} \cdots A^{(d)} \end{bmatrix} \begin{bmatrix} A^{(1)} \cdots A^{(1)}v, \cdots, A^{(d)} \cdots A^{(d)}v \end{bmatrix}$$

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$$H^{(0)} = \begin{bmatrix} u' & & & & & & \\ u' & & & & & \\ & & U & & \\ u' & & & & & \\ u' & & & & & & \end{bmatrix} \begin{bmatrix} A^{(1)} \cdots A & V' & {}^{l} \cdots A^{(d)} v \end{bmatrix}$$

Enumerate all length n strings:  $L(\mathbf{l}_{1}^{n}) = (l_{1}-1)d^{n-1} + (l_{2}-1)d^{n-2} + \dots + l_{n}, \quad \forall \mathbf{l}_{1}^{n} = [d]_{\mathbf{R}}^{n}$ 

+ Input:  $\mathcal{S}^{(N)}$  arranged into  $H^{(0)}, \{H^{(j)}: j \in [d]\} \in \mathbb{R}^{d^n \times d^n}$  $[H^{(j)}]_{L(\mathbf{l}_1^n), L(\mathbf{l}_{-1}^{-n})} = \mathbb{P}\left(\mathbf{y}_{-1}^{-n} = \mathbf{l}_{-1}^{-n}, y_0 = j, \mathbf{y}_1^n = \mathbf{l}_1^n\right),$ 

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$$H^{(j)} = \begin{bmatrix} u' & & & & & & & & & \\ u' & & & & & & & \\ u' & & & & & & & \\ u' & & & & & & & \\ u' & & & & & & & \\ \end{bmatrix} A^{(j)} A^{(1)} \cdot V' A^{(d)} \cdots A^{(d)} v \Big]$$



Algorithm 1 (Rank decomposition)  $H^{(0)} = UV'$ 



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 $H^{(0)} = UV'$  $\widetilde{A}^{(j)} = U^{\dagger}H^{(j)}(V^{\dagger})', \quad \forall j \in [d]$  $\widetilde{u} = U'\mathbf{e}$  $\widetilde{v} = V'\mathbf{e}$ 

Unique up to linear transformation

Require U V have column rank = k

How large N needs to be so that U, V have full column rank = k?

$$U = \begin{bmatrix} u'A^{(1)} \cdots A^{(1)} \\ u'A^{(1)} \cdots A^{(2)} \\ \vdots \\ u'A^{(d)} \cdots A^{(d)} \end{bmatrix} T \in \mathbb{R}^{d^{n} \times k}$$
  
In practice, used as a heuristic algorithm  
$$V = \begin{bmatrix} v'(A^{(1)} \cdots A^{(1)})' \\ v'(A^{(1)} \cdots A^{(2)})' \\ \vdots \\ v'(A^{(d)} \cdots A^{(d)})' \end{bmatrix} (T^{-1})' \in \mathbb{R}^{d^{n} \times k}$$

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Best hope:  
$$n \sim \mathcal{O}(\log_d k)$$
$$V = \begin{bmatrix} v'(A^{(1)} \cdots A^{(1)})' \\ v'(A^{(1)} \cdots A^{(2)})' \\ \vdots \\ v'(A^{(d)} \cdots A^{(d)})' \end{bmatrix} (T^{-1})' \in \mathbb{R}^{d^n \times k}$$

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Theorem 1:  
For almost all HMMs  
$$\mathbf{n} > 2 \log_{\mathbf{d}}(\mathbf{k})$$
  
guarantees U V full rank

 $\Theta^o_{(d,k)} = \{\theta^o : \text{ order } k, \text{ alphabet size } d\}$  N = 2n + 1

Theorem 1 (Information complexity for quasi-HMM realization).

(1) Consider  $\Theta_{(d,k)}^h$ , the class of all HMMs with output alphabet size d and order k. There exists a measure zero set  $\mathcal{E} \in \Theta_{(d,k)}^h$ , such that for all the output process generated by HMMs in the set  $\Theta_{(d,k)}^h \setminus \mathcal{E}$ , the information in  $\mathcal{S}^{(N)}$  is sufficient for computing the minimal quasi-HMM realization, for N = 2n + 1 with

$$n > 2\log_d(k). \tag{16}$$

(2) For any (d,k) pair, randomly generated a HMM in  $\Theta_{(d,k)}^h$ . If for a given window size N = 2n + 1, the matrix  $H^{(0)} \in \mathbb{R}^{d^n \times d^n}$  constructed with  $\mathcal{S}^{(N)}$  is of the maximal rank k, then for all output processes generated by  $\Theta_{(d,k)}^o$ , excluding a measure zero set,  $\mathcal{S}^{(N)}$  is sufficient for computing the minimal quasi-HMM realization.

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Polynomial computational complexity

 $\mathcal{O}(d(d^n)^3) \sim \mathcal{O}(dk^6)$ 

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- For almost all HMM, min order quasi realization is easy
- + However, there exist information theoretic hard cases

#### Sketch of the proof

- We want to show for generic choices of Q and O, if N = 2n + 1 satisfies  $n > 2 \log_d(k)$ , the matrices U, V have full column rank k.
- Since the minors of U and V are nonzero polynomials in the elements of Q and O, it is enough to show for some specific choice of Q and O.
- $Q \in \mathbb{R}^{k \times k}$ : the state shifting matrix

$$Q_{i-1,i} = 1$$
, for  $2 \le i \le k$ , and  $Q_{k,1} = 1$ ,

 $O \in \mathbb{R}^{d \times k}$ : columns are independent unit-norm d-dimensional random vectors.

The *i*-th column of U is given by

$$U_{[:,i]} = O_{[:,i]} \odot \dots O_{[:,i+n-1]}.$$

• Show that with probability greater than 0 (random matrix, concentration ineq)

$$\sigma_{min}(U'U) > 0.$$
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## Minimal quasi-HMM realization (summary)

- Key to quasi-HMM realization:
  - ✓ conditional independence,
  - ✓ matrix decomposition, unique up to linear transformation
  - $\checkmark$  Minimal order is determined by the rank of  $H^{(0)}$

#### + For **almost all** HMM, minimal quasi-HMM realization is easy

- $\checkmark$  Informational:  $N \sim \log_d(k)$
- Computational : matrix factorization

 $\mathcal{O}(dk^6)$ 

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#### Smoothed analysis VS generic analysis

## Minimal HMM realization



## Minimal HMM realization

+ HMM conditional independence : probabilities in product form
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+ HMM conditional independence : probabilities in product form

$$\begin{array}{c} y_{-n}, \dots, y_{-1} \\ y_{0}, \dots, y_{n-1} \\ H^{(0)} \\ y_{0} = j \\ y_{1}, \dots, y_{n} \\ y_{1}, \dots, y_{n} \\ H^{(j)} \\ \{y_{-n}, \dots, y_{-1}\} \perp \{y_{0}, \dots, y_{n-1}\} \left| x_{0} \right. \end{array}$$

#### Minimal HMM realization

- + HMM conditional independence : probabilities in product form
- Exploit the uniqueness of tensor decomposition



#### Minimal HMM realization

- Input:  $S^{(N)} = \{ \mathbb{P}_{y_{-n}, \dots, y_n} \}$  N = 2n + 1
- + **Output**: a minimal HMM model  $\theta^h = (d, k, Q, O)$
- + Key:

Arrange  $\mathcal{S}^{(N)}$  into a three way tensor  $M \in \mathbb{R}^{d^n \times d^n \times d}$ 

Tensor rank decomposition recover minimal HMM realization up to state relabeling

#### Preliminaries on Tensor

- Tensor definition
  - ✓ Multi-way array
  - ✓ Multi-linear mapping



 $M_{j_1,j_2,j_3}, \quad j_1 \in [n_A], j_2 \in [n_B], j_3 \in [n_C]$ Compare to matrix  $H_{j_1,j_2}$ 

#### Preliminaries on Tensor

- Tensor rank decomposition (CP/PARAFAC)
  - $\checkmark$  Sum of rank one tensors  $[\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}]_{j_1, j_2, j_3} = a_{j_1} b_{j_2} c_{j_3}$

Compare to matrix rank decomposition  $H = U \otimes V = \sum_{i=1}^{n} U_{[:,i]} V_{[:,i]}^{\top}$ 

#### Minimal HMM realization (intuition)

+ Key:  $\mathcal{S}^{(N)}$  arranged into a three way tensor  $M \in \mathbb{R}^{d^n \times d^n \times d}$ 

$$M_{L(\mathbf{l}_{-1}^{-n}), L(\mathbf{l}_{1}^{n}), l_{0}} = \mathbb{P}\left(\mathbf{y}_{-n}^{n} = \mathbf{l}_{-n}^{n}\right)$$

M relates to the model parameters via unique tensor factorization

$$M = A \otimes B \otimes C$$

$$A, B \in \mathbb{R}^{d^n \times k} \text{ and } C \in \mathbb{R}^{d \times k}$$
$$A = \mathbb{P}\left(y_1, y_2, \dots, y_n \middle| x_0\right)$$
$$B = \mathbb{P}\left(y_{-1}, y_{-2}, \dots, y_{-n} \middle| x_0\right)$$
$$C = \mathbb{P}\left(y_0, x_0\right)$$

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M relates to the model parameters via unique tensor factorization

$$M = A \otimes B \otimes C$$

$$A, B \in \mathbb{R}^{d^{n} \times k} \text{ and } C \in \mathbb{R}^{d \times k}$$

$$A = \mathbb{P}\Big(y_{1}, y_{2}, \dots, y_{n} \middle| x_{0}\Big) \qquad A = \underbrace{(O \odot (O \odot (O \odot \dots (O \odot O \underbrace{Q}) \dots)Q)Q)Q}_{n},$$

$$B = \mathbb{P}\Big(y_{-1}, y_{-2}, \dots, y_{-n} \middle| x_{0}\Big) \qquad B = \underbrace{(O \odot (O \odot (O \odot \dots (O \odot O \underbrace{Q}) \dots)Q)Q)Q}_{n},$$

$$C = \mathbb{P}\Big(y_{0}, x_{0}\Big) \qquad C = Odiag(\pi)$$

#### Minimal HMM realization (two-step approach)



Two-step realization algorithm

#### Minimal HMM realization (identifiability)

 $N \implies \mathcal{S}^{(N)} \implies (1) \quad M \Leftrightarrow A, B, C \implies (2) \quad A, B, C \Leftrightarrow (Q, O)$ 

# Minimal HMM realization ( identifiability ) $N \longrightarrow S^{(N)} \longrightarrow (1) \quad M \Leftrightarrow A, B, C \implies (2) \quad A, B, C \Leftrightarrow (Q, O)$

#### **Proposition 2:** sufficient conditions for invertibility of (1)

 $krank(A) + krank(B) + krank(C) \ge 2k + 2,$ 

# Minimal HMM realization ( identifiability ) $N \longrightarrow S^{(N)} \longrightarrow (1) \quad M \Leftrightarrow A, B, C \implies (2) \quad A, B, C \Leftrightarrow (Q, O)$

#### **Theorem 3:** sufficient conditions for invertibility of (1)

$$rank(A) = rank(B) = k$$



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$$rank(A) = rank(B) = k$$

Theorem: For almost all HMMs  $n > 2\log_d(k)$  guarantees A,B full rank



**Theorem 2**: sufficient conditions for invertability of (2)

1. If A has full column rank

2. Or if O has full column rank

# Minimal HMM realization (algorithm) $N \longrightarrow S^{(N)} \longrightarrow (1) \quad M \Leftrightarrow A, B, C \implies (2) \quad A, B, C \Leftrightarrow (Q, O)$

#### **Theorem 2**: algorithm for inverting (2)

Obtain the observation probabilities by:  $O_{[:,i]} = C_{[:,i]}/(\mathbf{e}'C_{[:,i]}), \quad \forall i \in [k].$ Given the matrix A, i.e.,  $\mathbb{P}(\mathbf{y}_1^n | x_0)$ , we can marginalize to obtain the matrices:

$$\widetilde{A}^{(1)} = \mathbb{P}(y_1 | x_0) \quad \widetilde{A}^{(n-1)} = \mathbb{P}(\mathbf{y}[1:n-1] | x_0),$$

- 1. If A has full column rank:  $Q = (O \odot \widetilde{A}^{(n-1)})^{-1}A';$
- 2. if O has full column rank:  $Q = O^{\dagger} \widetilde{A}^{(1)}$ .

#### Minimal HMM realization (algorithm)

 $N \implies \mathcal{S}^{(N)} \implies (1) \quad M \Leftrightarrow A, B, C \implies (2) \quad A, B, C \Leftrightarrow (Q, O)$ 

- Unique tensor decomposition to invert (1)
  - In general tensor decomposition is hard (Alternating least square)
- Have efficient algorithm if
  - ✓ A and B have full column rank
  - $\checkmark$  C is full rank, A $\odot$ B is full rank and ...  $\leftarrow$  Algorithm 3
  - ✓ The two cases apply to *almost all* HMMs for large enough N

← Algorithm 2

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+ Take 2 random projections along the 3<sup>rd</sup> dim





- + Take 2 random projections along the  $3^{rd}$  dimension  $\rightarrow$  2 matrix slices
- Simultaneous diagonalization is unique almost surely



• Take 2 random projections along the 3<sup>rd</sup> dimension  $\widetilde{M}_1 = M(I_{d^n \times d^n}, I_{d^n \times d^n}, \mathbf{v}_1), \quad \widetilde{M}_2 = M(I_{d^n \times d^n}, I_{d^n \times d^n}, \mathbf{v}_2).$ 

> $\widetilde{\widetilde{M}}_{1}\widetilde{\widetilde{M}}_{2}^{-1} = A\Lambda A^{-1},$   $\widetilde{\widetilde{M}}_{2}\widetilde{\widetilde{M}}_{1}^{-1} = B\Lambda^{-1}B^{-1}.$   $\Rightarrow$  pair up eigenvalues to get A, Bsolve linear eqn to obtain C

(1)  $M = A \otimes B \otimes C$ 

A,B are rank degenerate But if A • B has full column rank

• Degenerate case: Q is not full rank, set N = 3



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 $\overline{M} = C \otimes (A \odot B)'$ 

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Can be converted to solving linear equations and simultaneous diagonalization

rank decomposition  $\overline{M} = UV'$ such that: each column of V is a rank 1 matrix

# Algorithm 3 (correctness)

 $\Theta_{(d,k,r)}^{h} = \{\theta^{h} : \text{ order } k, \text{ alphabet size } d, Q \text{ is of rank } r < k\}$ 

#### **Theorem 4**: Correctness of Algorithm 3

Pick a random instance from the model class  $\Theta_{(d,k,r)}^{h}$ If Algorithm 3 works correctly to recover the minimal HMM Then it works for almost all instances in  $\Theta_{(d,k,r)}^{h}$ 

#### Minimal HMM realization (summary)

- Key to HMM realization:
  - ✓ conditional independence: current, past and future
  - ✓ tensor decomposition, unique up to column permutation

- + For almost all HMM, minimal HMM realization is easy
  - ✓ Informational:  $N \sim \log_d(k)$
  - $\checkmark$  Computational : simultaneous diagonalization  $\mathcal{O}(dk^6)$
- A class of degenerate cases can also be efficiently realized

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# Summary & Discussions



#### Discussions

- Hardness of worst cases
  - Reduction to parity of noise
- + Learning via realization algorithms
  - Statistical complexity
- Ongoing works
  - ✓ Smoothed analysis
  - ✓ Agnostic learning
  - V HMM model reduction

#### Hardness results

- We showed for almost all HMM, operator model and HMM model both are easy to learn (poly time algorithm, poly sample complexity)
- There exist information theoretic hard cases [Abe,Warmuth] [Kearns]
  - $\checkmark$  Given order k, cannot learn  $\theta^h = (d, k, Q, O)$  in poly time, unless RP=NP
  - ✓ Unknown k, HMM is not efficiently PAC learnable, under noisy parity assumption
- + Example: reduction to parity of noise
  - $\checkmark$  Number of states = 4T-1, observation alphabet = 2
  - $\checkmark$  required window size = T
  - $\checkmark$  There exists an  $\eta$  such that there is no efficient algorithm for learning parity under uniform distribution in the PAC framework with classification noise  $\eta$

#### State = (Emission, Parity sum, Stage)

#### Skip stage for parity sum



#### HMM learning problems

- + Observe: sample sequences of the output process of an HMM
- + Goal: an operator / HMM model to fit the process



**Statistics matching** 

# HMM learning problems

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#### Sample complexity

# Ongoing works

- Smoothed analysis perturbation based
   Understand the polynomial time algorithm in practice
- Agnostic HMM learning

If the underlying model is not a HMM...

which class of models have better fitting power?

HMM model reduction
# Appendix

#### Quasi-HMM realization ( correctness of the algorithm )

**Proposition 1.** Let  $\theta^o = (d, k, u, v, A^{(j)} : j \in [d])$  be a minimal order quasi realization for the output process. If the matrix  $H^{(0)}$  has rank k, then the Algorithm returns an operator model  $\tilde{\theta}^o$  that is equivalent to  $\theta^o$  up to linear transformation. Assume the output process can be realized by an HMM model of order  $k^h$ . The order  $k^h$  is always lower bounded by the order of the minimal order quasi realization k.

Sketch of the proof

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 $H^{(0)} = UV', \quad U, V$  both of full rank k

$$U = \begin{bmatrix} u'A^{(1)}\cdots A^{(1)} \\ u'A^{(1)}\cdots A^{(2)} \\ \vdots \\ u'A^{(d)}\cdots A^{(d)} \end{bmatrix} T = \begin{bmatrix} \widetilde{u}'\widetilde{A}^{(1)}\cdots \widetilde{A}^{(1)} \\ \widetilde{u}'\widetilde{A}^{(1)}\cdots \widetilde{A}^{(2)} \\ \vdots \\ \widetilde{u}'\widetilde{A}^{(d)}\cdots \widetilde{A}^{(d)} \end{bmatrix}$$

$$\widetilde{A}^{(j)} = T^{-1}AT$$
$$\widetilde{u} = T'u$$
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$$V' = T^{-1} \left[ A^{(1)} \cdots A^{(1)} v, \cdots, A^{(d)} \cdots A^{(d)} v \right] = \left[ \widetilde{A}^{(1)} \cdots \widetilde{A}^{(1)} v, \cdots, \widetilde{A}^{(d)} \cdots \widetilde{A}^{(d)} \widetilde{v} \right]$$

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Unique up to linear transformation

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**Theorem 3**: (1)  $M = A \otimes B \otimes C$ 

If both A and B have full column rank, then with probability one (over random projections), Algorithm 1 uniquely recovers the factors A, B, C up to state permutation. Moreover, Theorem 2.1 can be applied to recover (Q, O).

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Q needs to be of full rank k Increasing n can boost the rank of A,B How large N=2n+1 needs to be?

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$$\Theta_{(d,k)}^h = \{\theta^h : \text{ order } k, \text{ alphabet size } d\}$$

There exists a measure zero set  $\mathcal{E} \in \Theta_{(d,k)}^h$  such that for all HMMs in the set  $\Theta_{(d,k)}^h \setminus \mathcal{E}$ , for N = 2n + 1, with

$$n > 2\log_d(k),$$

the matrices A and B have full column rank, thus  $\mathcal{S}^{(N)}$  is sufficient for learning the minimal order HMM of the output process.

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$$\begin{split} \Theta^{h}_{(d,k)} &= \{\theta^{h}: \text{ order } k, \text{ alphabet} \\ \\ \mathbb{O}(d(d^{n})^{3}) \sim \mathcal{O}(dk^{6}) \\ \\ \\ \\ \\ \mathbb{O}(d(d^{n})^{3}) \sim \mathcal{O}(dk^{6}) \\ \\ \\ \\ \\ \\ \mathbb{O}(d(d^{n})^{3}) \sim \mathcal{O}(dk^{6}) \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$$

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# Minimal HMM realization ( identifiability ) $N \implies S^{(N)} \implies (1) \quad M \Leftrightarrow A, B, C \implies (2) \quad A, B, C \Leftrightarrow (Q, O)$

#### **Proposition 2:** sufficient conditions for invertability of (1)

Consider the matrices A, B, C parameterized by a minimal realization (Q, O). If the following deterministic conditions on the Kruskal rank are satisfied:

$$krank(A) + krank(B) + krank(C) \ge 2k + 2,$$
(1)

then M can be uniquely (up to common column permutation) decomposed into A, B, C, and k can be determined thereby.

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$$A = \underbrace{(O \odot (O \odot (O \odot \dots (O \odot O Q) \dots)Q)Q)Q}_{n},$$

$$B = \underbrace{(O \odot (O \odot (O \odot \dots (O \odot O Q) \dots)\widetilde{Q})\widetilde{Q})\widetilde{Q}}_{n},$$

$$C = Odiag(\pi)$$

### Algorithm 4 (random instance check)

 $\Theta_{(d,k,r)}^{h} = \{\theta^{h} : \text{ order } k, \text{ alphabet size } d, Q \text{ is of rank } r < k\}$ 

- 1. Randomly pick an HMM model  $(d, k, Q, O) \in \Theta_{(d,k,r)}^h$ .
- 2. Construct matrices A = OQ,  $B = O\widetilde{Q}$ ,  $C = ODiag(\pi)$ , where  $\pi$  is the stationary distribution, and  $\widetilde{Q} = Diag(\pi)Q'Diag(\pi)^{-1}$ .
- 3. Run Algorithm 2.a with input  $M = A \otimes B \otimes C$ .
- 4. Return "yes" if the algorithm recovers A, B, C up to state permutation, and "no" otherwise.

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#### **Theorem 4**: Correctness of Algorithm 3

For given  $d \ge k$  and n = 1, if Algorithm 2.b returns "yes", then there exists a measure zero set  $\mathcal{E} \in \Theta_{(d,r,k)}^h$  such that Algorithm 2.a can identify all minimal HMM realizations in the set  $\Theta_{(d,r,k)}^h \setminus \mathcal{E}$ .

Moreover, if the latter is true, Algorithm 2.b returns "yes" with probability 1. Theorem 1 (2) can be applied to recover (Q, O) for this class of HMMs.

## Minimal HMM realization (summary)

 $N \implies \mathcal{S}^{(N)} \implies (1) \quad M \Leftrightarrow A, B, C \implies (2) \quad A, B, C \Leftrightarrow (Q, O)$ 

- Identifiability: if (1) (2) are bijective mappings
  - $\checkmark$  How large N is so that the minimal HMM is identifiable from  $\mathcal{S}^{(N)}$ ?
- Algorithms: efficiently invert (1) (2)
  - ✓ For (1): Algorithm 2 (Simultaneous diagnolization)
     If Q is full rank

Algorithm 3 (Foobi)

If O has full column rank, and check a random

instance

✓ For (2): Theorem 2 (Linear inversion)
 If Q or O has full column rank