An OOM Tutorial

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Overview

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Some Shorthand Notation

Let \( (X_n)_{n=0,1,2,...} \) be a discrete-time stochastic process.

- For \( P(X_0 = a_0, ..., X_N = a_N) \) write \( P(a_0...a_N) \) or \( P(\overline{a}) \).

- For \( P(X_{N+1} = b_1, ..., X_{N+M} = b_M \mid X_0 = a_0, ..., X_N = a_N) \) write \( P(b_{N+1}...b_{N+M} \mid a_0...a_N) \) or \( P(\overline{b} \mid \overline{a}) \).
1 From HMMs to OOMs

An HMM\(^1\):

\[
S = \{s_1, s_2\} \quad \text{hidden states}
\]
\[
O = \{a, b\} \quad \text{observable events}
\]

\[
M = \begin{bmatrix}
0.0 & 1.0 \\
0.5 & 0.5 \\
\end{bmatrix}
\]
\[
M^T = \begin{bmatrix}
0.0 & 0.5 \\
1.0 & 0.5 \\
\end{bmatrix} =: T_a
\]
\[
M^T O_a = \begin{bmatrix}
0.5 & 1.0 \\
0.5 & 0.5 \\
\end{bmatrix} =: T_b
\]

where \(w_0\) is the invariant vector of \(M^T\)

\[
P(ab) = 1T_bT_a w_0
\]

HMM: \( (\mathbb{R}^2, \{T_a, T_b\}, w_0) \)

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\(^1\) Graphics from slide of K. Kretschmar
HMM:

- HMM: \( (\mathbb{R}^m, \{T_a, T_b\}, w_0) \)
- \( T_a + T_b = M^T \) where \( M \) is a Markov matrix
- \( w_0 \) is an invariant P-vector with component sum = 1
- \( P(ab) = 1T_b T_a w_0 \)
- non-negative entries only

OOM:

- OOM: \( (\mathbb{R}^m, \{\tau_a, \tau_b\}, w_0) \)
- \( \tau_a + \tau_b = \mu \), where \( \mu \) has column sum = 1
- \( w_0 \) is an invariant vector with component sum = 1
- \( P(ab) = 1\tau_b \tau_a w_0 \)
- negative entries are permitted
Definition

An OOM is a structure \((\mathbb{R}^m, (\tau_a)_{a \in \Sigma}, w_0)\), where \(w_0 \in \mathbb{R}^m\), \(\tau_a : \mathbb{R}^m \to \mathbb{R}^m\) linear, such that

1. \(1 \mu = 1 \sum_{a \in \Sigma} \tau_a = 1\)
2. \(1 w_0 = 1\)
3. for every sequence \(a_1...a_n \in O^n:\ 1 \tau_{a_n} \cdots \tau_{a_1} w_0 \geq 0\)

Note. A formally more general, but equivalent, definition replaces the all-ones row vector \(1\) by any row vector \(\sigma\):

1. \(\sigma \mu = \sigma\)
2. \(\sigma w_0 = 1\)
3. for every sequence \(a_1...a_n \in O^n:\ \sigma \tau_{a_n} \cdots \tau_{a_1} w_0 \geq 0\)
Theorem

An OOM \((\mathbb{R}^m, (\tau_a)_{a \in \Sigma}, w_0)\) defines a stochastic process by putting

\[
P(a_1 \cdots a_n) = 1 \tau_{a_n} \cdots \tau_{a_1} w_0
\]

for every sequence \(a_1 \cdots a_n \in \Sigma^n\).

**Note.** The process is stationary iff \(\mu w_0 = w_0\).
2 OOMs as sequence generators

\[ A = (\mathbb{R}^2, \{\tau_a, \tau_b\}, w_0) \quad O = \{a, b\} \]

\[ t = 0 \]
- Compute \(1_{\tau_aw_0}, 1_{\tau_bw_0}\)
- \((1_{\tau_aw_0}, 1_{\tau_bw_0})\) is a P-vector

\[ t = 1 \]
- Select \(a\) vs. \(b\) according to P-vector
- Apply operator
- Renormalize to component sum 1 to obtain \(w_1\)

\(a\) is observed
3 Equivalence theorem

Two OOMs $A = (\mathbb{R}^m, (\tau_a)_{a \in O}, w_0)$, $B = (\mathbb{R}^m, (\tau'_a)_{a \in O}, w'_0)$, where $m$ is minimal, generate the same process iff there exists a coordinate transformation $\rho: \mathbb{R}^m \rightarrow \mathbb{R}^m$, that preserves component sums of vectors, with

$$\tau'_a = \rho \tau_a \rho^{-1} \text{ for all } a \in O.$$
Corollary 1

For a given OOM $A = (\mathbb{R}^m, (\tau_a)_{a \in O}, w_0)$ there exist infinitely many different but equivalent OOMs of same dimension.

Proof: every coordinate transformation $\rho: \mathbb{R}^m \rightarrow \mathbb{R}^m$, that preserves component sums of vectors, yields a new version of $A$ via $\tau'_a = \rho \tau_a \rho^{-1}$ for all $a \in O$. 
Corollary 2

For two OOMs $A = (\mathbb{R}^m, (\tau_a)_{a \in O}, w_0), B = (\mathbb{R}^{m'}, (\tau'_a)_{a \in O}, w'_0)$, it is decidable whether they are equivalent.

Proof: first transform them into minimal-dimensional versions (effective algorithm exists), then check whether $\tau'_a = \rho \tau_a \rho^{-1}$ for all $a \in O$, for some $\rho$. 
4 OOMs and HMMs

The OOM

$$\tau_a = \begin{pmatrix} 0.645 & -0.395 & 0.125 \\ 0.355 & 0.395 & -0.125 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\tau_b = \begin{pmatrix} 0 & 0 & 0.218 \\ 0 & 0 & 0.329 \\ 0 & 0 & 0.452 \end{pmatrix}$$

generates/describes $aaaaabaaaaabaaaaabaaaabaa...$

$$P(a \mid ba^t)$$

a "probability clock"
How the probability clock works

- $\tau_b$ is a projection: every state vector is mapped on $\bullet$.

- $\tau_a$ is a rotation: iterated applications yield states on a circle.

- This gives rise to oscillation of $P(a \mid ba^n)$.

Probability clocks cannot be modelled by HMMs, "because" rotation operators need negative entries.
Consequence

The processes that can be modelled by HMMs are a proper subclass of the processes that can be modelled by OOMs:

\[ \text{HMM} \subsetneq \text{OOM} \]
5 Interpretable OOMs

Definition
1. Let $O$ be a finite set (alphabet) of observables, $k \geq 1$. A \textit{$k$-event} is a nonempty subset of $O^k$.
2. Let furthermore $m \geq 1$. A partitioning $O^k = A_1 \cup \ldots \cup A_m$ into $m$ disjoint nonempty $k$-events is a set of \textit{characteristic events} (of length $k$ and dimension $m$).

Example
$O = \{a,b\}$, $k = 2$, $m = 3$:
$A_1 = \{aa, ab\}$, $A_2 = \{ba\}$, $A_3 = \{bb\}$
Explanation of concept. Consider a 3-dim OOM, and let $A_1, A_2, A_3$ be characteristic events of dim 3 and some length $k$ (we don't care). Then this OOM is interpretable w.r.t. $A_1, A_2, A_3$, if the three components of state vectors = future probabilities of characteristic events $A_i$. 

$w = (P(A_1 | w), P(A_2 | w), P(A_3 | w))$
Example

Mary had...

P

=
Theorem

Let $A = (\mathbb{R}^m, (\tau_a)_{a \in \mathcal{O}}, w_0)$ be a minimal-dimensional OOM.

Let $\mathcal{O}^k = A_1 \cup \ldots \cup A_m$ be characteristic events of dim $m$ and some length $k$.

Then, generically, $A$ can be effectively transformed into an equivalent OOM that is interpretable w.r.t. $A_1, \ldots, A_m$.

Proof: define a transformation $\rho$ by $\rho(x) = (1\tau_{A_1} x, \ldots, 1\tau_{A_m} x)$, where $\tau_{A_i} = \sum_{a_1 \ldots a_k \in A_i} \tau_{a_k} \ldots \tau_{a_1}$. Then verify mechanically.
Application 1: visual comparison of OOMs

Given: two OOMs with same observables $S$. Both interpretable w.r.t. same characteristic events. If dim = 3, plot "fingerprints" immediately. If dim > 3, project on 3-dim subspace.
Application 2: Learning OOMs from data

Interpretable OOMs are at the core of efficient learning algorithms. It's so important that we will use a new section.
6 The basic learning algorithm

Core idea

• In an interpretable OOM:
  
  \[ w_0 = (P(A_1),...,P(A_m)) , \]
  
  \[ \tau_a w_0 = (P(aA_1),...,P(aA_m)) , \]
  
  \[ \tau_a \tau_b w_0 = (P(baA_1),...,P(baA_m)), \]
  
  etc.

• \( w_0, \tau_a w_0, \tau_a \tau_b w_0 \), etc, can be estimated from data by counting frequencies

• Basic linear algebra: obtain \( \tau_a \) from argument-value pairs

  \[ w_0 \rightarrow \tau_a w_0, \]
  
  \[ \tau_b w_0 \rightarrow \tau_a \tau_b w_0, \]
  
  etc.
Technical execution

• Assume $S = a_1a_2\ldots a_N$ is generated by $(\mathbb{R}^m, (\tau_a)_{a \in O}, w_0)$. 

• Task: get estimate $\tilde{\tau}_a$ from $S$.

Algorithm

• Choose $m$.

• Choose characteristic events $A_1, \ldots, A_m$.

• Count occurrences $\#(A_iA_j)$ and $\#(A_iaA_j)$ and put them into matrices $V = (\#(A_iA_j))$ and $W_a = (\#(A_iaA_j))$.

• Obtain estimate $\tilde{\tau}_a = W_a V^{-1}$.

• Do this for all operators.
Example

Given: $aabbabbbabababaabbbba$

Step 0: estimate model dim and choose characteristic events. Here: $\text{dim} = 2, A_1 = \{a\}, A_2 = \{b\}$.

Step 1: perform frequency counts of characteristic events:

$$V = \begin{pmatrix} #aa & #ba \\ #ab & #bb \end{pmatrix} = \begin{pmatrix} 3 & 4 \\ 5 & 6 \end{pmatrix}$$

$$W_a = \begin{pmatrix} #aaa & #baa \\ #aab & #bab \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ 3 & 2 \end{pmatrix}$$
Step 2 and finish:

\[ \tilde{\tau}_a = W_a V^{-1} = \begin{pmatrix} 5 & -3 \\ -4 & 3 \end{pmatrix} \]

(do the same for observable \( b \))
Two good properties of learning algorithm

If process is generated by $m$-dimensional OOM, and $m$ is estimated correctly, the learning algorithm...

- is asymptotically correct (= yields correct model as size of training sequence goes to infinity) regardless of choice of characteristic events,
- is constructive and computationally efficient with $O(N + |O| m^3 / p)$, where $p$ is degree of parallelization.

Standard HMM learning via EM algorithm has neither property 1 nor 2.
Two bad properties of learning algorithm

The algorithm

- depends in its statistical efficiency crucially on the choice of characteristic events – the **statistical efficiency problem**.

- will often yield a set of operator matrices which violate the condition \( \sum_{i} \tau_{a_n} \cdots \tau_{a_1} w_0 \geq 0 \), i.e., the model will assign negative "probabilities" to some sequences – the **non-negativity problem**.

*The first of these two problems has prevented a practical use of OOMs for a long time, and the second has driven at least three people I know almost crazy.*
7 Statistically efficient learning algorithms
Characterizers

**Definition.** Let $k \geq 1$, and $b_1 \ldots b_k$ be the alphabetical enumeration of $O^k$. Let $A = (\mathbb{R}^m, (\tau_a)_{a \in O}, w_0)$ be an OOM of some process with distribution $P$ and states $w_{\bar{a}}$. Let $C \in \text{Mat}_{m \times k}$ have unit column sums. Then $C$ is a **characterizer** of length $k$ of $A$ iff for all $\bar{a} \in O^*$:

$$w_{\bar{a}} = C \begin{pmatrix} P(b_1 | \bar{a}) \\ \vdots \\ P(b_k | \bar{a}) \end{pmatrix}$$
Intuitive Interpretation

$$w_{\bar{a}} = C \begin{pmatrix} P(b_1 | \bar{a}) \\ \vdots \\ P(b_k | \bar{a}) \end{pmatrix}$$

A characterizer $C$ transforms the future distribution after initial history $\bar{a}$ (as represented by the probs $P(b_i | \bar{a})$) into the OOM state $w_{\bar{a}}$. 
Some Properties of Characterizers

1. Every OOM has characterizers of length $k$ for sufficiently large $k$.

2. Characteristic events, as introduced before, are a special case of characterizers. Example:

   $O = \{a,b\}$, $k = 2$, $m = 3$,

   Characteristic events $A_1 = \{aa, ab\}$, $A_2 = \{ba\}$, $A_3 = \{bb\}$:

   \[
   \begin{pmatrix}
   P(aa | \overline{c}) \\
   P(ab | \overline{c}) \\
   P(ba | \overline{c}) \\
   P(bb | \overline{c})
   \end{pmatrix}
   =
   \begin{pmatrix}
   P(A_1 | \overline{c}) \\
   P(A_2 | \overline{c}) \\
   P(A_2 | \overline{c})
   \end{pmatrix}
   = w_{\overline{c}}.
   \]
Learning Equation

Let $\mathcal{A} = (\mathbb{R}^m, (\tau_a)_{a \in O}, w_0)$ be an OOM of some process with distribution $P$ with characterizer $C$. Let

$$V = \begin{pmatrix} P(\bar{b}_1 | \bar{a}_1) & \cdots & P(\bar{b}_1 | \bar{a}_k) \\ \vdots & \ddots & \vdots \\ P(\bar{b}_k | \bar{a}_1) & \cdots & P(\bar{b}_k | \bar{a}_k) \end{pmatrix}, \quad W_a = \begin{pmatrix} P(ab_1 | \bar{a}_1) & \cdots & P(ab_1 | \bar{a}_k) \\ \vdots & \ddots & \vdots \\ P(ab_k | \bar{a}_1) & \cdots & P(ab_k | \bar{a}_k) \end{pmatrix}.$$

Then

$$\tau_a = CW_a (CV)^+$$
Generalized Learning Algorithm

1. Choose a characterizer $C$.

2. Estimate (by obvious frequency counting from data)

$$\hat{V} = \begin{pmatrix} \hat{P}(b_1 | \bar{a}_1) & \cdots & \hat{P}(b_1 | \bar{a}_k) \\ \vdots & \ddots & \vdots \\ \hat{P}(b_k | \bar{a}_1) & \cdots & \hat{P}(b_k | \bar{a}_k) \end{pmatrix}, \quad \hat{W}_a = \begin{pmatrix} \hat{P}(ab_1 | \bar{a}_1) & \cdots & \hat{P}(ab_1 | \bar{a}_k) \\ \vdots & \ddots & \vdots \\ \hat{P}(ab_k | \bar{a}_1) & \cdots & \hat{P}(ab_k | \bar{a}_k) \end{pmatrix}.$$ 

3. Compute $\hat{\tau}_a = CW_a (CV)^+$. 
Properties of General Learning Algorithm(s)

1. Yields asymptotically correct estimates $\hat{\tau}_a$ with any characterizer $C$.

2. Model variance (statistical efficiency) depends crucially on choice of $C$.

3. Search for "good" (low model variance, i.e. high statistical efficiency) learning algorithms boils down to optimizing $C$. 
Algorithms for characterizer optimizing on the market today


Notes on algorithms 1 & 2

- Algorithms 1 and 2 yield equivalent results (M. Thon, in preparation)
- Core idea: set $C = L_m^T$, where $L_m$ is made from the first $m$ singular vectors of $\hat{V}$ (i.e., $C\hat{V}$ is the PCA-transform of $\hat{V}$).
- Theory (M. Zhao 2007, 2009): this $C$ minimizes an upper bound on the relative error $e$ of estimated operators $\hat{\tau}$ over the true $\tau$:

$$e = \left\| \hat{T} - T \right\|_{Frob} \left\| T \right\|_{Frob}, \quad \text{where} \quad \hat{T} = (\hat{\tau}_{a_1} \ldots \hat{\tau}_{a_l}), \quad T = (\tau_{a_1} \ldots \tau_{a_l})$$

- Resource problem: algorithms have time and space complexity that scales with $m N^3$ in the worst case, where $m$ is model dimension and $N$ training data length.
- Both algorithms are constructive.
Notes on algorithm 3

• Core idea: exploit a certain algebraic (!) characterization of the statistically maximally efficient characterizer $C_{\text{max-eff}}$. Approximate this precious $C_{\text{max-eff}}$ by an iterative re-estimation method.
• About 2-5 iterations usually suffice.
• One iteration has time and space cost scaling with $m^2 N$ (as opposed to worst-case $mN^3$ for algorithms 1 & 2).
• Algorithm does not necessarily converge (can jitter around terminal value). For too large assumed model dimensions prone to numerical instability. Iteration dynamics is not understood.
Notes on all three algorithms

• These algorithms are rooted in the OOM-typical translation of stochastic concepts into algebraic ones:
  • algorithm 1 exploits algebraic characterization of maximal statistical efficiency,
  • the other two minimize estimation error bound on metric distance between estimated and true model matrices.

• All algorithms are technically involved and need care when implementing them in space/time efficient ways.

• Model quality is empirically found similar for algorithms 1 & 2 vs. algorithm 3

• Model accuracy (statistical efficiency) is far superior to EM-trained HMMs

• All algorithms by design are insensitive to overfitting (test performance does not decrease when model dim is chosen too big)

• Computational cost of algorithm 3 is about 10 times less than EM-learning of HMMs due to low number of iterations

• Average cost of algorithms 1 & 2 appears to be much less than that of algorithm 3 (worst-case cost is however much higher), depends much on nature of process, needs analysis
Demo 1: logistic chaos process¹)

- Data from 16-bin discretized logistic process \( x(n+1) = 4 x(n) (1 - x(n)) \), which is strongly chaotic (max. Lyapunov exponent = 2)

- CPU times here were about 1:10 of algorithm 3 vs. EM-HMM, and again 1:10 of algorithm 1 vs. algorithm 3

¹) From Zhao/Jaeger/Thon, Neural Computation, forthcoming
Demo 2: some standard benchmarks from the PSR community\(^1\)

- These are input-output processes; OOMs can accommodate
- 2 out of 7 examples shown, others are similar
- Figures show average 1-step prediction error vs. training data length

\(^1\) From Zhao/Jaeger/Thon, Neural Computation, forthcoming
Efficient learning algorithms: summary

- The problem of finding statistically efficient versions of the basic OOM learning algorithm has essentially been solved.
- Algorithms starkly outperform EM-HMM in accuracy and cost.
- Algorithms use novel learning principles:
  - Algorithms 1 & 2: minimizing error bound on model parameters
  - Algorithm 3: optimizing statistical efficiency of asymptotically correct estimator
- More research needed:
  - Algorithms 1 & 2: improving worst-case cost
  - Algorithm 3: analysis of iteration dynamics and numerical stability
- Algorithms are much more complicated than EM-HMM.
- Overview and analytic comparison/unification paper (M. Thon) is in preparation.
8 The dreaded nonnegativity problem

1. Recall defining conditions of OOM \( (R^m, (\tau_a)_{a \in \Sigma}, w_0) \):
   1. \( \mu = \sum_{a \in \Sigma} \tau_a \) has column sums = 1
   2. \( \mathbf{1} w_0 = 1 \)
   3. for every sequence \( a_1...a_n \in O^n \) it holds that
      \[ \mathbf{1} \tau_{a_n} \cdots \tau_{a_1} w_0 \geq 0 \]

2. Conditions 1. and 2. are easy to check; the non-negativity condition 3. isn't.
3. Learnt models often (even typically, for nontrivial data) violate nonnegativity.
4. Utterly desirable: method to check for non-negativity condition; method to transform invalid learnt OOM into "closest" valid one.
5. Every OOM researcher I know has burnt lots of lifetime on this problem, aging prematurely in the process.
Three solutions to the dreaded problem

1. **Empirical workaround:** when an invalid model is used in prediction / generation, and invalid (negative-probability) states occur, **renormalize** them on the fly.
   - A recommended method is detailed in [1]

2. **Emphatic anti-solution:** it is **undecidable** whether a set of candidate operator matrices satisfies the nonnegativity condition.
   - Proof by E. Wiewora [2], by adaptation of a related proof by Denis and Esposito [3]

3. **Emperor's solution:** disallow non-negativity by using **norm-OOMs**, which are built around the idea to set

\[
P(a_1 \ldots a_n) = \left\| \tau_{a_n} \ldots \tau_{a_1} w_0 \right\|^2
\]

   - Introduced by M. Zhao [4,5], including a general stochastic framework and a basic learning algorithm.
4. M. Zhao, H. Jaeger (2007): **Norm observable operator models.** Jacobs University technical report Nr. 8
7 From stochastic processes to OOMs

So far, we introduced OOMs as generalizations of HMMs.

Now we will re-introduce OOMs in a very different way, starting from stochastic processes and showing that (basically) every stochastic process has an OOM.
What's a future?

For a robot, or anybody else modelling stochastic processes, the future is a probability distribution over possible future developments.
Dynamics of future distributions

- Observations update expectations, that is, future distributions.
- ... $E_t$, $E_{t+1}$, ... : observations. Formally, events in observation space s-algebra.
The basic idea

observable events = operators that change distributions

- set of all distributions is a (functional) vector space $V$
- for every event $E$ an "observable operator" $\tau_E$
- observable operators operate on $V$
Characterizing SD processes 1

The distribution of a stationary, discrete-valued process (SD process) is fully characterized by its conditioned continuation probabilities

\[ P(X_{n+1} = b_1, \ldots, X_{n+m} = b_m \mid X_1 = a_1, \ldots, X_n = a_n) \]

\[ =: P(b_1 \ldots b_m \mid a_1 \ldots a_n) \]

\[ =: P(\bar{b} \mid \bar{a}) \]

where \( m \geq 1, n \geq 0 \).

Special case \( n = 0 \): \( P(\bar{b} \mid \varepsilon) = P(\bar{b}) \) would suffice.
Characterizing SD processes 2

Consider the vector space of all numerical functions on finite sequences, 
\[ \mathcal{D} = \{ d : O^* \to \mathbb{R} \} \]

For each antecedent \( \bar{a} \), define a predictor function 
\[ g_{\bar{a}} : O^* \to \mathbb{R}, \quad g_{\bar{a}}(\bar{b}) = P(\bar{b} \mid \bar{a}) \]

Shorthand: \( g_{\bar{a}} = P(\cdot \mid \bar{a}) \)

The set of all such predictor functions, 
\[ \{ g_{\bar{a}} \mid \bar{a} \in O^* \} \subset \mathcal{D} \]

describes all \( P(\bar{b} \mid \bar{a}) \) and thus characterizes the process.
Consider the linear subspace spanned by all predictor functions \( g_{\bar{a}} \),
\[
\mathcal{G} = \left\{ g_{\bar{a}} \mid \bar{a} \in \Sigma^* \right\}.
\]

Let \( t_\alpha : \mathcal{G} \to \mathcal{G} \) be a linear mapping satisfying
\[
t_\alpha (g_{\bar{c}}) = P(a \mid \bar{c}) g_{\bar{c}a}
\]
for all \( a \in O, \bar{c} \in O^* \). (They exist!)

Let \( g_\varepsilon : O^* \to \mathbb{R}, \ g_\varepsilon (\bar{b}) = P(\bar{b} \mid \varepsilon) = P(\bar{b}) \)

Let \( 1 : \mathcal{G} \to \mathbb{R} \) be a linear mapping satisfying \( 1g_{\bar{c}} = 1 \)
for all \( \bar{c} \in O^* \). (exists!)
Characterizing SD processes 4

| SD process  | \( \{g_{\bar{a}} | \bar{a} \in \Sigma^* \} \) |
|-------------|--------------------------------------|
| \( G = \)   | \([\{g_{\bar{a}} | \bar{a} \in O^* \}]_D \) |
| \( t_a(g_{\bar{c}}) = \) | \( P(a \, | \, \bar{c}) g_{\bar{c}a} \) |
| \( g_{\epsilon}(\bar{b}) = P(\bar{b}) \) | |
| \( 1g_{\bar{c}} = 1 \) | |

**Theorem.** For any \( a_1...a_n \in O^* \) it holds that

\[
P(a_1...a_n) = 1t_{a_n} \cdots t_{a_1} g_{\epsilon}
\]

Compare:

\[
P(a_1...a_n) = 1\tau_{a_n} \cdots \tau_{a_1} w_0
\]

**Definition.** \( \dim(G) \) is the dimension of the process.

**Corollary.** A finite-dimensional process of dimension \( m \) has a "matrix" OOM

\[
(\mathbb{R}^m,(\tau_a)_{a \in \Sigma},w_0) \equiv (G,(t_a)_{a \in \Sigma},g_{\epsilon}).
\]
Characterizing SD processes 5

Every SD process has an "abstract" OOM \((G, (t_a)_{a \in \Sigma}, g_\varepsilon)\).

These abstract OOMs are unique ("coordinate-free representation").

The dimension of a process may be infinite.

Abstract OOMs are needed for proving the equivalence theorem.
Theorem. Let \((X_t)_{t \geq 0}\) be a process with values in \((\mathcal{B}, \mathcal{B})\), not necessarily stationary. Then there exists an OOM
\[
(R^K, (\tau_{A,t})_{A \in \mathcal{B}, t > 0}, w_0)
\]
such that
\[
P(X_{t_1} \in A_1, \ldots, X_{t_n} \in A_n)
= \mathbf{1} \tau_{A_n, t_n - t_{n-1}} \cdots \tau_{A_1, t_1} w_0.
\]
Furthermore, it holds that
\[
(1) \quad \tau = \sum_{n} \tau_{A_n, t}
\]
\[
(2) \quad \tau_{A, t_1 + t_2} = \tau_{A, t_2} \tau_{B, t_1}
\]
Decomposing OOMs 1

Recall: observable operators of OOMs derived from HMMs have the form

\[ T_a = M^\top O_a \]

where \( M \) is the transition matrix of a Markov chain and \( O_a \) is a (diagonal) observation matrix containing emission probabilities of \( a \).
**Theorem.** Let \((X_t)_{t \geq 0}\) be a process with values in \((B, \mathcal{B})\), not necessarily stationary. Then there exists an OOM with

- evolution operators \((\mu_r)_{r > 0}\)
- observation operators \((\eta_A)_{A \in B}\)

such that

\[
P(X_0 \in A_0, X_{t_1} \in A_1, \ldots, X_{t_{n-1}} \in A_{n-1})
\]

\[
= 1 \eta_{A_{n-1}} \mu_{t_{n-1}-t_{n-2}} \cdots \eta_{A_2} \mu_{t_2-t_1} \eta_{A_1} \mu_{t_1} \eta_{A_0} \psi_0.
\]
Decomposing OOMs 3

Visualization of evolution operators $\mu_{\Delta t}$ and observation operators $\eta_A$
From linear algebra back to processes

**Recall:** in an abstract OOM \((\mathbb{R}^K, (\tau_{A,t})_{A \in \mathcal{B}, t > 0}, w_0)\) we obtain

\[
P(\{X_{t_1} \in A_1, \ldots, X_{t_n} \in A_n\}) = \mathbf{1}_{\tau_{A_n, t_n-t_{n-1}}} \cdots \mathbf{1}_{\tau_{A_1, t_1}} w_0.
\]

**Theorem.** Let \((B, \mathcal{B})\) be a polish measure space, \(V\) a real vector space with basis \(E\), \(w_0 \in V\), \((\tau_{A,t})_{A \in B, t > 0}\) a family of linear operators on \(V\), \(V\) be generated by the vectors \(\tau_{A_n, t_n-t_{n-1}} \cdots \tau_{A_1, t_1} w_0\) and the numerical function \(P : (\mathcal{B} \times [0, +\infty))^* \to \mathbb{R}\) be defined by

\[
P((A_1, t_1), \ldots, (A_n, t_n)) = \mathbf{1}_{\tau_{A_n, t_n-t_{n-1}}} \cdots \mathbf{1}_{\tau_{A_1, t_1}} w_0.
\]

Then \(P\) can be extended to the distribution of a stochastic process iff

1. \(\mathbf{1} w_0 = 1\)
2. \(\mathbf{1}_{\tau_{(B,t)}} e = 1\) for all basis vectors \(e\) and times \(t\)
3. \(\mathbf{1}_{\tau_{A_n, t_n-t_{n-1}}} \cdots \mathbf{1}_{\tau_{A_1, t_1}} w_0 \geq 0\) for all \(\tau\) sequences
4. \(\tau_{\bigcup_{n} A_n, t} = \sum_{n} \tau_{A_n, t}\)
5. \(\tau_{A, t_1+t_2} = \tau_{A, t_2} \tau_{B, t_1}\)
From processes to linear algebra and back to processes

\[ P(X_{t_1} \in A_1, \ldots, X_{t_n} \in A_n) = 1_{\tau_{A_n, t_n-t_{n-1}}} \cdots 1_{\tau_{A_1, t_1}} \mathcal{W}_0. \]

The theory of distributions of stochastic processes (with polish measure spaces and real or discrete time) becomes a subtheory of linear algebra.
## Historical notes / related approaches

<table>
<thead>
<tr>
<th>Year</th>
<th>Event</th>
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<tbody>
<tr>
<td>1957-1970</td>
<td>A long series of investigations in mathematical probability theory concerning the question when two HMMs are equivalent (overviews in [1] [2])</td>
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<tr>
<td>... - 1969</td>
<td>A Roumanian school of probability theory develops theory to describe stochastic processes by observable operators (although it is not recognized that they can always be chosen linear) [5]</td>
</tr>
<tr>
<td>2001</td>
<td>Littman/Sutton/Singh [9] introduce <strong>predictive state representations</strong> (PSRs) for input-driven processes, unaware of IO-OMMs described earlier by Jaeger [10].</td>
</tr>
<tr>
<td>1969</td>
<td>Schützenberger [11] introduces <strong>multiplicity automata</strong> (MAs), which are equivalent to finite-dimensional OOMs, expressed in a context of automata theory.</td>
</tr>
<tr>
<td>1980's - present</td>
<td>A series of investigations in statistical learning theory and stochastic languages on learnability and decidability issues concerning MAs. Among other, it is found that the non-negativity problem is undecidable [12][13]</td>
</tr>
<tr>
<td>antiquity - present</td>
<td>Ancient idea in quantum mechanics, information theory [14] and statistical physics [15]: the state of a physical system is that which contains all information about the future</td>
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Norm OOMs [1,2]

• Motivation: avoid the non-negativity problem of standard linear OOMs
• Approach: keep basic structure of OOMs: \((\mathbb{R}^m, (\tau_a)_{a \in O}, w_0)\), but compute probabilities from states by

\[
P(a_1 \ldots a_n) = \left\| \tau_{a_n} \ldots \tau_{a_1} w_0 \right\|^2.
\]

• This avoids the non-negativity problem by design.
Norm OOMs, cont'd

Definition. Let $O = \{a_1, \ldots, a_k\}$ be a finite set of observables, and let $E$ be a real vector space with an inner product (and hence, a norm). Let $w_0 \in E$ and for each $a \in O$, let $\tau_a$ be a linear map on $E$, and $\tau_a^*$ its adjoint operator (i.e., $\langle \tau_a^* u, v \rangle = \langle u, \tau_a v \rangle \forall u, v \in E$).

Then $(E, (\tau_a)_{a \in O}, w_0)$ is a norm-OOM, if

1. $\|w_0\| = 1$,
2. $\sum_{a \in O} \tau_a^* \tau_a = id_E$.

Theorem. If $(E, (\tau_a)_{a \in O}, w_0)$ is a norm-OOM, then the prescription

$$P(a_1 \ldots a_n) = \|\tau_a \ldots \tau_a w_0\|^2$$

describes the distribution of a stochastic process.

Theorem. Every stochastic process with observables $O = \{a_1, \ldots, a_k\}$ has a norm-OOM $(E, (\tau_a)_{a \in O}, w_0)$ which describes the distribution of the process by the above formula.
Norm OOMs, notes

• Mingjie Zhao [2] found a constructive, asymptotically correct learning algorithm for norm-OOMs.

• This algorithm is computationally prohibitively expensive. Mingjie explores tractable versions.

• Mingjie also has found another, iterative, EM-based learning algorithm (manuscript in preparation).

• Unlike the deplorable case of linear OOMs, it is decidable whether a structure \((\mathbb{R}^m, (\tau_a)_{a \in O}, w_0)\) is a norm-OOM.

• Every finite-dimensional norm-OOM \((\mathbb{R}^m, (\tau_a)_{a \in O}, w_0)\) can be effectively transformed into an equivalent (higher-dimensional) linear OOM. It appears that processes obtained from randomly generated norm-OOMs are generically non-HMM.

• It is unknown whether finite-dim HMM processes are a subclass of finite-dim norm-OOM processes. All that is known is that \(m\)-state Markov Chains have an \(m\)-dimensional norm-OOM.
1. M. Zhao, H. Jaeger (2007): **Norm observable operator models**. Jacobs University technical report Nr. 8

9 Beginnings of a Hilbert space theory 1

Consider a $K$-dimensional process $\left(\Omega, \mathcal{A}, P, X_t\right)$ with discrete values and one of its OOMs $\left(\mathbb{R}^K, (\tau_a)_{a \in \Sigma}, \omega_0\right)$.

For every $x \in \mathbb{R}^K$, one can construct a $P$-measurable function $\gamma(x) : \Omega \to \mathbb{R}$ where $\gamma(\omega_0) \equiv 1$, such that the following holds:

Theorem. (i) $\forall x \in \mathbb{R}^K : \gamma(x) \in L^\infty(P)$

(ii) $\langle x, y \rangle := \int_\Omega \gamma(x)\gamma(y) dP$ defines an inner product and thereby a norm on $\mathbb{R}^K$

(iii) The operators $(\tau_a)_{a \in \Sigma}$ are continuous w.r.t. this norm
Hilbert space theory 2: construction of \( \gamma \)

1. For every \( w = \tau_b w_0 / 1 \tau_b w_0 \), where \( P(\bar{b}) > 0 \),
we obtain a measure \( \mu_w \) on \((\Omega, \mathcal{A})\) by extending
\[
\mu_w(a_1...a_n) = 1 \tau_{a_n} ... \tau_{a_1} w
\]

2. For every such \( w \), \( \gamma(w) \) is defined as the density of \( \mu_w \) w.r.t. \( P \).

3. There exists a basis of \( \mathbb{R}^K \) consisting of such \( w \)'s.
For \( x \in \mathbb{R}^K \), \( x = \sum_{i=1}^{k} \alpha_i w_i \), define
\[
\gamma(x) = \sum \alpha_i \gamma(w_i)
\]
Open question\textsuperscript{1)}: it is not clear under which conditions the metric space $\mathbb{R}^K$ (where the metric is the one induced by $\langle x, y \rangle := \int_{\Omega} \gamma(x)\gamma(x) dP$) is complete.

If we had a complete vector space, it would be a Hilbert space and we could develop an approximation theory (of infinite-dimensional operators by finite-dimensional).
10 Research topics

- Algebraic characterization of OOM matrices
- Characterization of OOMs that are HMMs
- Recovery of discrete "hidden" event structure from observation sequences
- Learning nonstationary OOMs
- Online learning algorithms
- Spatio-temporal OOMs, "Bayesian network" OOMs
- OOM and quantum mechanics
- OOMs in speech processing and biosequence modeling
- Efficient "direct" and online learning algorithms for input-output OOMs
- Incorporating prior knowledge into learning
- Learning with missing values and unequal observation intervals
- Characterization of standard processes
- Development of Hilbert space theory
11 A survey of further results
11.1 Input-output OOMs and Predictive State Representations
Controlled stochastic processes

• In open systems, future distributions depend on input.

Formally, a **controlled stochastic process** [1] is defined by conditional probabilities of the kind

\[
P(X_{n+1} = a | X_{n-k} = a_0, \ldots, X_n = a_k, U_{n-k} = u_0, \ldots, U_n = u_k, U_{n+1} = u)\]
Input-Output OOMs (IO-OOMs)

- An IO-OOM [2] is essentially a set of OOMs of same dimension; these OOMs are indexed by possible inputs; input switches between them.
- IO-OOMs standardly use $\sigma$, not $1$, for projection of states on probabilities.
- If at time $n$ the IO-OOM state is $w_n$, the probability to observe $a$ at time $n+1$, given that input at time $n+1$ is $u$, is
  $$P(X_{n+1} = a \mid w_n) = \sigma \tau_a^u w_n.$$  
- The probability to see observations $a_1, \ldots, a_n$, given control input $u_1, \ldots, u_n$, is
  $$P(X_1 = a_1, \ldots, X_n = a_n \mid U_1 = u_1, \ldots, U_n = u_n) = \sigma \tau_{a_n}^{u_n} \cdots \tau_{a_1}^{u_1} w_n.$$  

$$(\mathbb{R}^m, (\tau_a^u)_{a \in O, \ u \in U, \ \sigma, w_0})$$
Learning IO-OOMs

\((\mathbb{R}^m, (\tau^u_a)_{a \in O, u \in U}, \sigma, W_0)\)

**Given:** training sequence \(u_1a_1 \ldots u_Na_N\).

1. Choose \(\kappa\) indicative & characteristic sequences, typically \((U \times O)^l\).
2. Let \(\hat{V} = \left(\hat{P}(\bar{q}^j \bar{c}^{i})\right)_{i,j}\) and \(\hat{W}_{ua} = \left(\hat{P}(q^j u a c^{i})\right)_{i,j}\) and \(\hat{c} = \left(\hat{P}(\bar{c}^{i})\right)_{i}\) and \(\hat{q}^T = \left(\hat{P}(\bar{q}^i)\right)_{j}\).

   Note: \(\hat{P}(u_1 a_1 \ldots u_l a_l) = \prod_{n=1, \ldots, l} \frac{\# u_1 a_1 \cdots u_n a_n}{\# u_1 a_1 \cdots u_{n-1} a_{n-1} u_n}\).

3. Estimate dimension \(m\) of IO-OOM as \(\text{numrank}(\hat{V})\).
4. Scale columns of \(\hat{V}\) and \(\hat{W}_{ua}\) by \(\sqrt{\# q_j}\).
5. Choose characterizer \(C \in \mathbb{R}^{m \times \kappa}\) such that \(C \hat{V}\) is invertible.
6. Set \(\hat{\tau}_a^u = CW_{ua}(C \hat{V})\)
   \(\hat{w}_0 = C \hat{c}\)
   \(\hat{\sigma}^T = \hat{q}^T (C \hat{V})^{-1}\)

Note: step 5 is where all the effort and quality lies. Re-use the efficient OOM-learning algorithms here.
Predictive state representations (PSR)

- PSRs are equivalent to IO-OOMs, using a slightly different formalism.

- Basic concept: tests. A test $t$ is any sequence $u_1a_1 ... u_la_l$ of input/observation pairs.

- For an $m$-dimensional (in the sense of IO-OOMs) controlled stochastic process, there exist $m$ core tests $t_1,..., t_m$, s.th. for any history $h = u_1a_1 ... u_Na_N$, the predictive state $p(h) = (P(t_1|h),..., P(t_m|h))^\top$ – i.e., an $m$-dimensional column vector – is a sufficient statistic of the future distribution of the process.

- This amounts to the following. For every history $h$, next input $u$ and observation $a$, one can compute from $p(h)$ the probability $P(a \mid h, u)$ to see $a$ under this input, by

$$P(a \mid h, u) = m_{ua} p(h),$$

where $m_{ua}$ is an $m$-dimensional row vector which depends only on $u$ and $a$.

- PSRs amount thus to IO-OOMs whose states are interpretable w.r.t. the core tests.
11.2 Mixture OOMs

Problem:
Continuous-valued processes have continuously many observable operators.

A solution [1]:
Combine observable operators from finite number of basis operators through membership functions.

\[ \tau_x = 0.3 \tau_b + 0.7 \tau_c \]
Mixture OOMs, Results 1

- Fundamental equation transfers

\[ P(X_1 \in I_1, \ldots, X_k \in I_k) = \sigma \circ \tau_{I_k} \circ \cdots \circ \tau_{I_1} \nu_0 \]

where \( \tau_I = \int_I \sum_{a \in E} \nu_a(x) \tau_a \, dx \).

- When membership functions are fixed, basic learning algorithms transfer.
Blended OOMs, results 2

Learning algorithm adapted:

- Example: learning a continuous-valued version of the probability clock - an almost white-noise process
11.3 Optimal decision making

Setup

- reward delayed for uncertain time up to time horizon $h$
- stochasticity in sensing, acting, environment
Optimal decision making 2

A quick recap of interpretable OOMs:

\[ w = P(A_1 A_2 A_3) \]

state components = probabilities of characteristic events
Optimal decision making 3

**Approach [1]:** Merge into characteristic event $A^+$ all futures which yield reward within $h$
Optimal decision making 4

- Assume agent has a "self-and-world-OOM" $S$ of how it acts and how the world reacts.

- Let $U = \{u_1, \ldots, u_k\}$ and $A = \{a_1, \ldots, a_l\}$ be the actions and world (sensed) observables. Let $O = U \times A$. Then $S = (\mathbb{R}^m, (\tau_{ua})_{ua \in O}, w_0)$.

- Put $\tau_u = \sum_{a \in A} \tau_{au}$.

- In non-deliberate mode, agent acts and updates OOM state $w_n$ as follows:
  1. Choose action $u_i$ according to probabilities $1 \tau_{u_i} w_n$.
  2. Execute chosen action $u_i$ and observe world sensor feedback $a_j$.
  3. Update state $w_{n+1} = \tau_{u_i a_j} w_n / 1 \tau_{u_i a_j} w_n$.

- If $S$ models world feedback correctly, $P(a_j | w_n, u_i) = 1 \tau_{u_i a_j} w_n / 1 \tau_{u_i} w_n$. 
Optimal decision making 5

• Recall from previous slide: $S = (\mathbb{R}^m, (\tau_{ua})_{ua \in O}, w_0)$, $P(a_j | w_n, u_i) = 1 \tau_{ua_j} w_n / 1 \tau_{u_i} w_n$.

• Assume $S$ is interpretable w.r.t. characteristic events $A_i$, where $A_1 = A^+$. Then the agent knows that the probability $P(+, h | w_n)$ to get a reward within horizon $h$, when the current state is $w_n$, is the first component $w_n[1]$ of $w_n$. This is subject to the condition that the agent continues operating in non-deliberative mode.

• The agent may want to do better than this, by switching to a deliberated action. That is, it would be advantageous to deliberately use action $u$ at time $n$, if $P(+, h - 1 | w_n, u) > P(+, h | w_n)$.

• $P(+, h - 1 | w_n, u)$ can be computed cheaply:
  • Let $B^+ = \{u_1 a_1 ... u_{h-1} a_{h-1} | u_1 a_1 ... u_{h-1} a_{h-1} contains a reward\}$, and let $t_u = 1 \tau_{B^+} \tau_u$.
  • Then, $P(+, h - 1 | w_n, u) = t_u w_n$. 
Thank you.