An Automata Theory Perspective on Spectral Learning

Hankel Matrix Factorizations

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Outline

- Weighted Automata and Functions Over Strings
- A Spectral Method from Hankel Factorizations
- Survey on Recent Applications to Learning Problems
- Spectral Learning of Finite State Transducers

Precedents

- Subspace methods for identification of linear dynamical systems
  [Overschee–Moor '94]
- Results on identifiability and learning of HMM and phylogenetic trees
  [Chang '96, Mossel–Roch '06]
- Query learning algorithms for DFA and Multiplicity Automata
  [Angluin '87, Bergadano–Varrichio '94]

Notation

- Finite alphabet $\Sigma = \{\sigma_1, \sigma_2, \dots, \sigma_r\}$
- Free monoid $\Sigma^\star = \{\epsilon, a, b, aa, ab, ba, bb, aaa, \dots\}$
- Functions over strings $f : \Sigma^\star \to \mathbb{R}$
- Examples:

$$f(x) = \mathbb{P}[x] \qquad \text{(probability of a string)}$$

$$f(x) = \mathbb{P}[x\Sigma^\star] \qquad \text{(probability of a prefix)}$$

$$f(x) = \mathbb{I}[x \in L] \qquad \text{(characteristic function of language L)}$$

$$f(x) = |x|_a \qquad \text{(number of } a\text{'s in } x\text{)}$$

$$f(x) = \mathbb{E}[|w|_x] \qquad \text{(expected number of substrings equal to } x\text{)}$$

Weighted Automata

- Class of WA parametrized by alphabet Σ and number of states n

$$\mathbf{A} = \langle \alpha_1, \alpha_\infty, \{A_\sigma\}_{\sigma \in \Sigma} \rangle$$

$$\begin{aligned} \alpha_1 &\in \mathbb{R}^n && \text{(initial weights)} \\ \alpha_\infty &\in \mathbb{R}^n && \text{(terminal weights)} \\ A_\sigma &\in \mathbb{R}^{n \times n} && \text{(transition weights)} \end{aligned}$$

- Computes a function $f_{\mathbf{A}} : \Sigma^\star \to \mathbb{R}$

$$f_{\mathbf{A}}(x) = f_{\mathbf{A}}(x_1 \cdots x_t) = \alpha_1^\top A_{x_1} \cdots A_{x_t} \alpha_\infty = \alpha_1^\top A_x \alpha_\infty$$

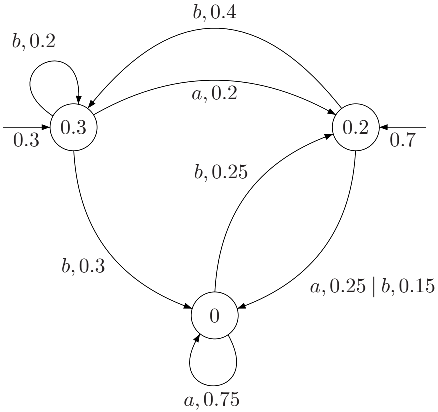
Examples – Probabilistic Finite Automata

- Compute / generate distributions over strings $\mathbb{P}[x]$

$$\alpha_1^\top = [0.3 \;\; 0 \;\; 0.7]$$

$$\alpha_\infty^\top = [0.2 \;\; 0 \;\; 0.2]$$

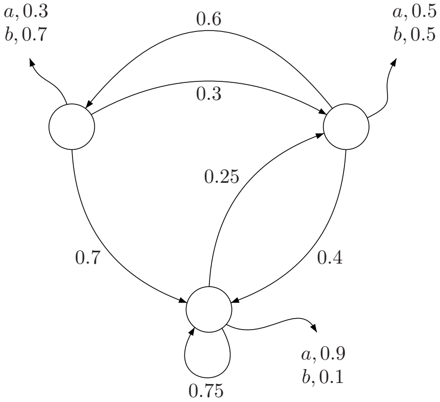
$$A_a = \begin{bmatrix} 0 & 0 & 0.2 \\ 0 & 0.75 & 0 \\ 0 & 0.25 & 0 \end{bmatrix}$$



Examples – Hidden Markov Models

- Generates infinite strings, computes probabilities of prefixes $\mathbb{P}[x\Sigma^\star]$
- Emission and transition are conditionally independent given state

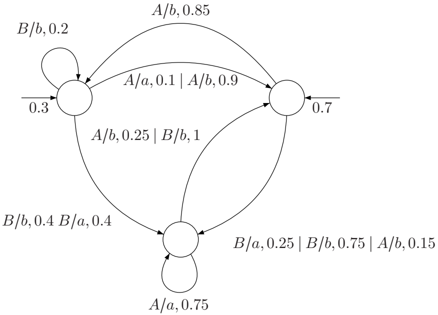
$$\alpha_1^\top = [0.3 \;\; 0.3 \;\; 0.4]$$
$$\alpha_\infty^\top = [1 \;\; 1 \;\; 1]$$
$$A_a = O_a \cdot T$$
$$T = \begin{bmatrix} 0 & 0.7 & 0.3 \\ 0 & 0.75 & 0.25 \\ 0 & 0.4 & 0.6 \end{bmatrix}$$
$$O_a = \begin{bmatrix} 0.3 & 0 & 0 \\ 0 & 0.9 & 0 \\ 0 & 0 & 0.5 \end{bmatrix}$$



Examples – Probabilistic Finite State Transducers

- Compute conditional probabilities $\mathbb{P}[y|x] = \alpha_1^\top A_x^y \alpha_\infty$ for pairs $(x, y) \in (\Sigma \times \Delta)^\star$, must have $|x| = |y|$
- Can also assume models factorized like in HMM

$$\alpha_1^\top = [0.3 \;\; 0 \;\; 0.7]$$
$$\alpha_\infty^\top = [1 \;\; 1 \;\; 1]$$
$$A_B^b = \begin{bmatrix} 0.2 & 0.4 & 0 \\ 0 & 0 & 1 \\ 0 & 0.75 & 0 \end{bmatrix}$$



WAs and Forward-Backward Recursions

Forward–Backward Factorization

- $\mathbf{A}$ defines *forward* and *backward* maps $f^F_{\mathbf{A}}, f^B_{\mathbf{A}} : \Sigma^\star \to \mathbb{R}^n$
- Such that for any splitting $x = y \cdot z$ one has $f_{\mathbf{A}}(x) = f^F_{\mathbf{A}}(y) \cdot f^B_{\mathbf{A}}(z)$

$$f^F_{\mathbf{A}}(y) = \alpha_1^\top A_y \qquad \text{and} \qquad f^B_{\mathbf{A}}(z) = A_z \alpha_\infty$$

Example

- For a PFA $\mathbf{A}$ and $i \in [n]$, one has
- $[f^F_{\mathbf{A}}(y)]_i = [\alpha_1^\top A_y]_i = \mathbb{P}[y \,,\, h_{|y|+1} = i]$
- $[f^B_{\mathbf{A}}(z)]_i = [A_z \alpha_\infty]_i = \mathbb{P}[z \,|\, h = i]$

Consequences

- String structure has direct relation to computation structure
- In particular, strings sharing prefixes or suffixes share computations
- Information on A_a can be recovered from $f_{\mathbf{A}}(yaz)$, $f^F_{\mathbf{A}}(y)$, and $f^B_{\mathbf{A}}(z)$:

$$f_{\mathbf{A}}(yaz) = f^F_{\mathbf{A}}(y) A_a f^B_{\mathbf{A}}(z)$$

The Hankel Matrix

- The *Hankel matrix* of $f : \Sigma^\star \to \mathbb{R}$ is $H_f \in \mathbb{R}^{\Sigma^\star \times \Sigma^\star}$
- For $y, z \in \Sigma^\star$, entries are defined by $H_f(y, z) = f(y \cdot z)$
- Given $\mathcal{P}, \mathcal{S} \subseteq \Sigma^\star$ will consider sub-blocks $H_f(\mathcal{P}, \mathcal{S}) \in \mathbb{R}^{\mathcal{P} \times \mathcal{S}}$
- Very *redundant* representation for f – $f(x)$ appears $|x| + 1$ times

$$
\begin{array}{cc}
 & \begin{array}{cccccc} \epsilon & a & b & aa & ab & \cdots \end{array} \\
\begin{array}{c} \epsilon \\ a \\ b \\ aa \\ ab \\ \vdots \end{array} &
\left[\begin{array}{cccccc}
 & & \vdots & & \vdots & \\
\cdots & \cdots & \vdots & \cdots & f(aab) & \\
 & & \vdots & & & \\
\cdots & \cdots & f(aab) & & & \\
 & & & & & \\
 & & & & &
\end{array}\right]
\end{array}
$$

Schützenberger's Theorem

Theorem: $\mathrm{rank}(H_f) \leqslant n$ if and only if $f = f_{\mathbf{A}}$ with $|\mathbf{A}| = n$

In particular, $\mathrm{rank}(H_f)$ is size of smallest WA for f

Proof ($\Leftarrow$)

- Write $F = f_{\mathbf{A}}^F(\Sigma^\star) \in \mathbb{R}^{\Sigma^\star \times n}$ and $B = f_{\mathbf{A}}^B(\Sigma^\star) \in \mathbb{R}^{n \times \Sigma^\star}$
- Note $H_f = F \cdot B$
- Then, $\mathrm{rank}(H_f) \leqslant n$

Proof ($\Rightarrow$)

- Assume $\mathrm{rank}(H_f) = n$
- Take *rank factorization* $H_f = F \cdot B$ with $F \in \mathbb{R}^{\Sigma^\star \times n}$ and $B \in \mathbb{R}^{n \times \Sigma^\star}$
- Let $\alpha_1^\top = F(\epsilon, [n])$ and $\alpha_\infty = B([n], \epsilon)$ (note $\alpha_1^\top \alpha_\infty = f(\epsilon)$)
- Let $A_\sigma = B([n], \sigma \cdot \Sigma^\star) \cdot B^+ \in \mathbb{R}^{n \times n}$ (note $A_\sigma \cdot B([n], x) = B([n], \sigma \cdot x)$)
- By induction on $|x|$ we get $\alpha_1^\top A_x \alpha_\infty = f(x)$

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The Spectral Method

Idea: Use SVD decomposition to obtain a factorization of H

- Given H and H_σ over basis $(\mathcal{P}, \mathcal{S})$
- Compute *compact* SVD as $\mathrm{H} = USV^\top$ with

$$U \in \mathbb{R}^{\mathcal{P} \times n} \qquad S \in \mathbb{R}^{n \times n} \qquad V \in \mathbb{R}^{\mathcal{S} \times n}$$

- Let $A_\sigma = (\mathrm{H}V)^+(\mathrm{H}_\sigma V)$ – corresponds to rank factorization $\mathrm{H} = (\mathrm{H}V)V^\top$

Properties

- Easy to implement: just linear algebra
- Fast to compute: $O(\max\{|\mathcal{P}|, |\mathcal{S}|\}^3)$
- Noise tolerant: $\hat{\mathrm{H}} \approx \mathrm{H}$ and $\hat{\mathrm{H}}_\sigma \approx \mathrm{H}_\sigma$ implies $\hat{A}_\sigma \approx A_\sigma$

Spetral Methods from the Automata-Theory Perspective

- Algorithmic and Miscellaneous Problems
  - Interpretation as an optimization problem - from linear algebra to convex optimization
  - Finding a basis via random sampling - knowing $(\mathcal{P}, \mathcal{S})$
- Direct Applications
  - Learning stochastic rational languages - any probability distribution computed by WA
  - Learning probabilistic finite state transducers
  - Learning tree distributions
- Composition with Other Methods
  - Combination with matrix completion for learning non-stochastic functions - when $f : \Sigma^* \to \mathbb{R}$ is not related to a probability distribution

An Optimization Point of View

- Idea: Replace linear algebra with optimization primitives - make it possible to use the ML optimization toolkit.
- Algorithms
  - Spectral optimization: $\min_{\{A_\sigma\}, V_n^\top V_n = I} \sum_{\sigma \in \Sigma} ||H V_n A_\sigma - H_\sigma V_n||_F^2$
  - Convex relaxation: $\min_{A_\Sigma} ||H A_\Sigma - H_\Sigma||_F^2 + \tau ||A_\Sigma||_*$
- Properties
  - Equivalent in some situations and choice of parameters
  - Experiments show convex relaxation can be better in cases known to be difficult for the spectral method
- Open problems/ Future Work
  - Design problem-specific optimization algorithms
  - Constrain learned models imposing further regularizations, e.g. sparsity

Learning Probabilistic Finite State Transducers [BQC'11]

Idea: Learn a function $f : (\Sigma \times \Delta)^\star \to \mathbb{R}$ computing $\mathbb{P}[y|x]$ Learning Model

- Input is sample of aligned sequences (x^i, y^i), $|x^i| = |y^i|$
- Drawn i.i.d. from distribution $\mathbb{P}[x, y] = \mathbb{P}[y|x]\, D(x)$
- Want to assume as little as possible on D
- Performance measured against x generated from D

Properties

- Assuming independece $A_\sigma^\delta = O_\delta \cdot T_\sigma$, sample bound scales mildly with input alphabet $|\Sigma|$
- For applications, need to align sequences prior to learning – or use iterative procedures

Open problems / Current Work

- Deal with alignments inside the model

Learning PFST over very large input alphabets

- Goal: Learn a function $f : (\Sigma \times \Delta)^\star \to \mathbb{R}$ computing $\mathbb{P}[x, y]$ where Δ can be arbitrarily large.
- Idea: Transition function as a linear combination of basic transitions.
- Model
  - Assume a set of feature functions $\Phi(x) = [\phi_1(x), \dots, \phi_k(x)]$

$$
\begin{aligned}
f(x, y) &= \alpha_1^T A(\phi(x_1), y_1) \cdots, A(\phi(x_T), y_T)\alpha_\infty \\
&= \alpha_1^T \left(\sum_{l=1}^{k} \phi_l(x_1) O_l^{y_1} \right) \cdots \left(\sum_{l=1}^{k} \phi_l(x_T) O_l^{y_T} \right) \alpha_\infty
\end{aligned}
$$

Learning FST: Handling Missing Alignments

- Goal: Learn a function $g : (\Sigma^\star \times \Delta^\star) \to \mathbb{R}$ computing $\mathbb{P}[x, y]$
- Model:

$$\mathbb{P}(x, y) = \sum_{z \in \mathcal{Z}(x,y)} f(z)$$

- Aligned Sequences:

$$z = \begin{array}{ccc} y_1 & y_2 & y_3 \\ x_1 & x_2 & \end{array} \begin{bmatrix} y_4 \\ x_3 \end{bmatrix} \begin{bmatrix} y_5 \\ x_4 \end{bmatrix} \; y_6 \; \begin{bmatrix} y_7 \\ x_5 \end{bmatrix}$$

corresponds to a sequence of symbol pairs:

$$(x_1, \lambda)(x_2, \lambda)(\lambda, y_1)(\lambda, y_2)(\lambda, y_3)(x_3, y_4)(x_4, y_5)(\lambda, y_6)(x_5, y_7)$$

- WA over aligned sequences:

$$f(z) = \alpha_1^\top A_{x_1} A_{x_2} A^{y_1} A^{y_2} A^{y_3} A^{y_4}_{x_3} A^{y_5}_{x_4} A^{y_6} A^{y_7}_{x_5} \alpha_\infty$$

- Intuitively:
  - A_σ operators over $\Sigma^\star$
  - A^δ operators over $\Delta^\star$
  - A^σ_δ operators over $(\Sigma \times \Delta)^\star$

Forward-Backward Maps

$$z = \begin{array}{ccccc} y_1 & & y_2 & & y_3 \\ & x_1 & & x_2 & \end{array} \begin{bmatrix} y_4 \\ x_3 \end{bmatrix} \; y_5 \; \begin{bmatrix} y_6 \\ x_4 \end{bmatrix}$$

$$\begin{aligned}
f(z) &= \alpha_1^\top A_{x_{1:2}} A^{y_{1:3}} A_{x_3}^{y_4} A^{y_5} A_{x_4}^{y_6} \alpha_\infty \\
&= f^F\left(\begin{array}{ccccc} y_1 & & y_2 & & y_3 \\ & x_1 & & x_2 & \end{array} \begin{bmatrix} y_4 \\ x_3 \end{bmatrix} \right) \cdot f^B \left(y_5 \; \begin{bmatrix} y_6 \\ x_4 \end{bmatrix} \right) \\
&= f^F\left(\begin{array}{ccccc} y_1 & & y_2 & & y_3 \\ & x_1 & & x_2 & \end{array} \right) \cdot A_{x_3}^{y_4} \cdot f^B \left(y_5 \; \begin{bmatrix} y_6 \\ x_4 \end{bmatrix} \right)
\end{aligned}$$

Fully Observed Hankels

- Hankel over Aligned Sequences:

$$\begin{aligned}
H\left(\begin{smallmatrix} y_1 y_2 y_3 \\ x_1 x_2 \end{smallmatrix}, y_4 \begin{bmatrix} y_5 \\ x_3 \end{bmatrix}\right) &= f\left(\begin{smallmatrix} y_1 y_2 y_3 y_4 \\ x_1 x_2 \end{smallmatrix} \begin{bmatrix} y_5 \\ x_3 \end{bmatrix}\right) \\
H_{\sigma}\left(\begin{smallmatrix} y_1 y_2 y_3 \\ x_1 x_2 \end{smallmatrix}, y_4 \begin{bmatrix} y_5 \\ x_3 \end{bmatrix}\right) &= f\left(\begin{smallmatrix} y_1 y_2 y_3 y_4 \\ x_1 x_2 \sigma \end{smallmatrix} \begin{bmatrix} y_5 \\ x_3 \end{bmatrix}\right) \\
H^{\delta}\left(\begin{smallmatrix} y_1 y_2 y_3 \\ x_1 x_2 \end{smallmatrix}, y_4 \begin{bmatrix} y_5 \\ x_3 \end{bmatrix}\right) &= f\left(\begin{smallmatrix} y_1 y_2 y_3 \delta y_4 \\ x_1 x_2 \end{smallmatrix} \begin{bmatrix} y_5 \\ x_3 \end{bmatrix}\right) \\
H_{\sigma}^{\delta}\left(\begin{smallmatrix} y_1 y_2 y_3 \\ x_1 x_2 \end{smallmatrix}, y_4 \begin{bmatrix} y_5 \\ x_3 \end{bmatrix}\right) &= f\left(\begin{smallmatrix} y_1 y_2 y_3 \\ x_1 x_2 \end{smallmatrix} \begin{bmatrix} \delta \\ \sigma \end{bmatrix} y_4 \begin{bmatrix} y_5 \\ x_3 \end{bmatrix}\right)
\end{aligned}$$

- Hankel Factorizations:

$$H = FB$$

$$H_{\sigma}^{\delta} = F A_{\sigma}^{\delta} B$$

Hankel over Aligned Substrings

- A Hankel over aligned substrings:

$$H^\star\left(\begin{smallmatrix}\delta_1\\ \end{smallmatrix}\begin{bmatrix}\delta_2\\ \sigma_1\end{bmatrix}, \sigma_2\right) = H\left(\begin{smallmatrix}\Delta^\star\delta_1\\ \Sigma^\star\end{smallmatrix}\begin{bmatrix}\delta_2\\ \sigma_1\end{bmatrix}\ ,\ \begin{smallmatrix}\Delta^\star\\ \sigma_2\ \Sigma^\star\end{smallmatrix}\right)$$

- Problem: we do not observe aligned sequences!

Hankel over Aligned Substrings

- A Hankel over aligned substrings:

$$H^\star\left({}^{\delta_1}\begin{bmatrix}\delta_2\\ \sigma_1\end{bmatrix}, {}_{\sigma_2}\right) = H\left(\begin{smallmatrix}\Delta^\star\\ \Sigma^\star\end{smallmatrix}{}^{\delta_1}\begin{bmatrix}\delta_2\\ \sigma_1\end{bmatrix}\ ,\ {}_{\sigma_2}\begin{smallmatrix}\Delta^\star\\ \Sigma^\star\end{smallmatrix}\right)$$

- Problem: we do not observe aligned sequences!

Observable Statistics

$$\begin{aligned}
\mathbb{E}\left[|x,y|^{\delta_1\delta_2}_{\sigma_1\sigma_2}\right] &= \sum_{\substack{x_s,x_p\in\Sigma^\star \\ y_s,y_p\in\Delta^\star}} \mathbb{P}[x_p\,\sigma_1\sigma_2 x_s,\, y_p\,\delta_1\delta_2 y_s] \\
&= \begin{smallmatrix}\cdots\delta_1\delta_2\cdots\cdots\cdots\cdots\cdots \\ \cdots\cdots\cdots\cdots\cdots\sigma_1\sigma_2\cdots\end{smallmatrix} \quad + \quad \ldots \\
&+ \begin{smallmatrix}\cdots\cdots\delta_1 \\ \cdots\cdots\cdots\end{smallmatrix}\begin{bmatrix}\delta_2\\\sigma_1\end{bmatrix}\begin{smallmatrix}\cdots\cdots\cdots \\ \sigma_2\cdots\cdots\end{smallmatrix} \quad + \quad \begin{smallmatrix}\cdots\cdots \\ \cdots\cdots\end{smallmatrix}\begin{bmatrix}\delta_1\\\sigma_1\end{bmatrix}\begin{bmatrix}\delta_2\\\sigma_2\end{bmatrix}\begin{smallmatrix}\cdots\cdots \\ \cdots\cdots\end{smallmatrix} \\
&+ \quad \ldots \quad + \quad \begin{smallmatrix}\cdots\cdots\cdots\cdots\cdots\delta_1\delta_2\cdots \\ \cdots\sigma_1\sigma_2\cdots\cdots\cdots\cdots\cdots\end{smallmatrix}
\end{aligned}$$

where:

$$\begin{smallmatrix}\cdots\cdots\delta_1 \\ \cdots\cdots\cdots\end{smallmatrix}\begin{bmatrix}\delta_2\\\sigma_1\end{bmatrix}\begin{smallmatrix}\cdots\cdots\cdots \\ \sigma_2\cdots\cdots\end{smallmatrix} = H^\star\left(\delta_1\begin{bmatrix}\delta_2\\\sigma_1\end{bmatrix}, \sigma_2\right)$$

Guessing a good Hankel

- Idea:
  - Guess the entries in the Hankel
  - Use rank constraints and observables to guide your guess
- Observable Constraints:
  - $\mathbb{E}[|x, y|^{\delta_1 \delta_2}_{\sigma_1 \sigma_2}] =$ sums of entries in $H^\star$
- Optimization:

$$\min_{H^\star} ||\, H^\star||_* \quad \text{subject to: linear constraints on observables}$$

- Number of Variables in $H^\star$: $C \cdot |\Sigma \times \Delta|^4$

Conclusion

- Summary:
  - Spectral algorithms follow directly from classical algebraic methods for learning automata
  - Automata Theory Perspective in a Nutshell: the Hankel trick
    - Recipe to derive learning algorithms for many models.
    - Convex optimization + Hankel trick
  - Extensions: guess missing Hankel entries
- Future Directions:
  - Can we learn subclasses of PCFG?
- A reference:
  - R. Gavaldà and J. Castro, Learning Probability Distributions Generated by Finite-State Machines, tutorial at ICGI-2012