Learning Automata with Hankel Matrices

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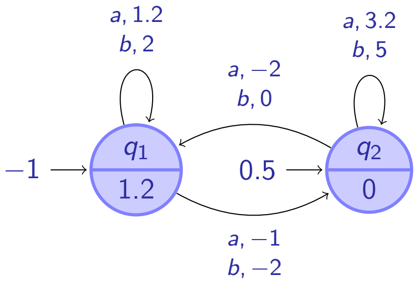
Highlights — London, September 2017

Weighted Finite Automata (WFA) (over $\mathbb{R}$)

Graphical Representation



Algebraic Representation

$$A = \langle \boldsymbol{\alpha}, \boldsymbol{\beta}, \{\mathbf{A}_a\}_{a \in \Sigma} \rangle$$

$$\boldsymbol{\alpha} = \begin{bmatrix} -1 \\ 0.5 \end{bmatrix} \qquad \mathbf{A}_a = \begin{bmatrix} 1.2 & -1 \\ -2 & 3.2 \end{bmatrix}$$

$$\boldsymbol{\beta} = \begin{bmatrix} 1.2 \\ 0 \end{bmatrix} \qquad \mathbf{A}_b = \begin{bmatrix} 2 & -2 \\ 0 & 5 \end{bmatrix}$$

Behavioral Representation

Each WFA A computes a function $A : \Sigma^\star \to \mathbb{R}$ given by $A(x_1 \cdots x_T) = \boldsymbol{\alpha}^\top \mathbf{A}_{x_1} \cdots \mathbf{A}_{x_T} \boldsymbol{\beta}$

In This Talk...

- Describe a core algorithm common to many algorithms for learning weighted automata
- Explain the role this core plays in three learning problems in different setups
- Survey extensions to more complex models and some applications

Outline

1. From Hankel Matrices to Weighted Automata
2. From Data to Hankel Matrices
3. From Theory to Practice

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Hankel Matrices and Fliess' Theorem

Given $f : \Sigma^\star \to \mathbb{R}$ define its Hankel matrix $\mathbf{H}_f \in \mathbb{R}^{\Sigma^\star \times \Sigma^\star}$ as

$$\mathbf{H}_f = \begin{array}{c} \\ \epsilon \\ a \\ b \\ \vdots \\ p \\ \vdots \end{array} \begin{array}{c} \begin{array}{cccccc} \epsilon & a & b & \cdots & s & \cdots \end{array} \\ \left[\begin{array}{cccccc} f(\epsilon) & f(a) & f(b) & & \vdots & \\ f(a) & f(aa) & f(ab) & & \vdots & \\ f(b) & f(ba) & f(bb) & & \vdots & \\ & & & & & \\ \cdots & \cdots & \cdots & & f(ps) & \\ & & & & & \end{array}\right] \end{array}$$

Theorem [Fli74]

1. The rank of $\mathbf{H}_f$ is finite if and only if f is computed by a WFA
2. The rank $\mathrm{rank}(f) = \mathrm{rank}(\mathbf{H}_f)$ equals the number of states of a minimal WFA computing f

The Structure of Hankel Matrices

$$A(p_1 \cdots p_T s_1 \cdots s_{T'}) = \alpha^\top \mathbf{A}_{p_1} \cdots \mathbf{A}_{p_T} \mathbf{A}_{s_1} \cdots \mathbf{A}_{s_{T'}} \beta$$

$$\mathbf{H} = \begin{array}{c c} & s \\ p & \left[\begin{array}{ccccc} & & \cdot & & \\ & & \cdot & & \\ & & \cdot & & \\ \cdot & \cdot & f(ps) & \cdot & \cdot \\ & & \cdot & & \end{array}\right] \end{array} = \left[\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \bullet & \bullet & \bullet \\ \cdot & \cdot & \cdot \end{array}\right] \left[\begin{array}{ccccc} \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \end{array}\right]$$

$$A(p_1 \cdots p_T a s_1 \cdots s_{T'}) = \alpha^\top \mathbf{A}_{p_1} \cdots \mathbf{A}_{p_T} \mathbf{A}_a \mathbf{A}_{s_1} \cdots \mathbf{A}_{s_{T'}} \beta$$

$$\mathbf{H}_a = \begin{array}{c c} & s \\ p & \left[\begin{array}{ccccc} & & \cdot & & \\ & & \cdot & & \\ & & \cdot & & \\ \cdot & \cdot & f(pas) & \cdot & \cdot \\ & & \cdot & & \end{array}\right] \end{array} = \left[\begin{array}{ccc} \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot \\ \bullet & \bullet & \bullet \\ \cdot & \cdot & \cdot \end{array}\right] \left[\begin{array}{ccc} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{array}\right] \left[\begin{array}{ccccc} \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \\ \cdot & \cdot & \bullet & \cdot & \cdot \end{array}\right]$$

Algebraically: Factorizing $\mathbf{H}$ lets us solve for $\mathbf{A}_a$

$$\mathbf{H} = \mathbf{P}\ \mathbf{S} \quad \Longrightarrow \quad \mathbf{H}_\sigma = \mathbf{P}\ \mathbf{A}_a\ \mathbf{S} \quad \Longrightarrow \quad \mathbf{A}_a = \mathbf{P}^+\ \mathbf{H}_a\ \mathbf{S}^+$$

SVD-based Reconstruction [HKZ09; Bal+14]

Inputs

- Desired number of states r
- Basis $\mathcal{B} = (\mathcal{P}, \mathcal{S})$ with $\mathcal{P}, \mathcal{S} \subset \Sigma^\star$, $\epsilon \in \mathcal{P} \cap \mathcal{S}$
- Finite Hankel blocks indexed by prefixes and suffixes in $\mathcal{B}$:
  - $\mathbf{H}^{\mathcal{B}} \in \mathbb{R}^{\mathcal{P} \times \mathcal{S}}$
  - $\mathbf{H}^{\mathcal{B}}_{\Sigma} = \{\mathbf{H}^{\mathcal{B}}_a \in \mathbb{R}^{\mathcal{P} \times \mathcal{S}} : a \in \Sigma\}$

Algorithm: Spectral$(\mathbf{H}^{\mathcal{B}}, \mathbf{H}^{\mathcal{B}}_{\Sigma}, r)$

1. Compute the rank r SVD of $\mathbf{H}^{\mathcal{B}} \approx \mathbf{U}\mathbf{D}\mathbf{V}^\top$
2. Let $\mathbf{A}_a = \mathbf{D}^{-1}\mathbf{U}^\top \mathbf{H}_a \mathbf{V}$
3. Let $\boldsymbol{\alpha} = \mathbf{V}^\top \mathbf{H}^{\mathcal{B}}(\epsilon, -)$ and $\boldsymbol{\beta} = \mathbf{D}^{-1}\mathbf{U}^\top \mathbf{H}^{\mathcal{B}}(-, \epsilon)$
4. Return $A = \langle \boldsymbol{\alpha}, \boldsymbol{\beta}, \{\mathbf{A}_a\} \rangle$

Running time:

1. SVD takes $O(|\mathcal{P}||\mathcal{S}|r)$
2. Matrix multiplications take $O(|\Sigma||\mathcal{P}||\mathcal{S}|r)$

Properties of Spectral [HKZ09; Bal13; BM15a]

Consistency

- If $\mathcal{P}$ is prefix-closed, $\mathcal{S}$ is suffix-closed, and $r = \text{rank}(\mathbf{H}^{\mathcal{B}}) = \text{rank}([\mathbf{H}^{\mathcal{B}} | \mathbf{H}_{\Sigma}^{\mathcal{B}}])$
- Then $\forall p \in \mathcal{P}$, $\forall s \in \mathcal{S}$, $\forall a \in \Sigma$, the WFA $A = \text{Spectral}(\mathbf{H}^{\mathcal{B}}, \mathbf{H}_{\Sigma}^{\mathcal{B}}, r)$ satisfies $A(p \cdot s) = \mathbf{H}^{\mathcal{B}}(p, s)$ and $\tilde{A}(p \cdot a \cdot s) = \mathbf{H}_{a}^{\mathcal{B}}(p, s)$

Recovery

- If $\mathbf{H}^{\mathcal{B}}$ and $\mathbf{H}_{\Sigma}^{\mathcal{B}}$ are sub-blocks of $\mathbf{H}_f$ with $r = \text{rank}(f) = \text{rank}(\mathbf{H}^{\mathcal{B}})$
- Then the WFA $A = \text{Spectral}(\mathbf{H}^{\mathcal{B}}, \mathbf{H}_{\Sigma}^{\mathcal{B}}, r)$ satisfies $A \equiv f$

Robustness

- If $r = \text{rank}(\mathbf{H}^{\mathcal{B}}) = \text{rank}([\mathbf{H}^{\mathcal{B}} | \mathbf{H}_{\Sigma}^{\mathcal{B}}])$ and $\|\mathbf{H}^{\mathcal{B}} - \hat{\mathbf{H}}^{\mathcal{B}}\| \leqslant \varepsilon$ and $\|\mathbf{H}_{a}^{\mathcal{B}} - \hat{\mathbf{H}}_{a}^{\mathcal{B}}\| \leqslant \varepsilon$ for all $a \in \Sigma$
- Then $\langle \boldsymbol{\alpha}, \boldsymbol{\beta}, \{\mathbf{A}_a\} \rangle = \text{Spectral}(\mathbf{H}^{\mathcal{B}}, \mathbf{H}_{\Sigma}^{\mathcal{B}}, r)$ and $\langle \hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}}, \{\hat{\mathbf{A}}_a\} \rangle = \text{Spectral}(\hat{\mathbf{H}}^{\mathcal{B}}, \hat{\mathbf{H}}_{\Sigma}^{\mathcal{B}}, r)$ satisfy $\|\boldsymbol{\alpha} - \hat{\boldsymbol{\alpha}}\|$, $\|\boldsymbol{\beta} - \hat{\boldsymbol{\beta}}\|$, $\|\mathbf{A}_a - \hat{\mathbf{A}}_a\| \leqslant \varepsilon$

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Learning Models

1. Exact query learning: membership + equivalence queries [BV96; BBM06; BM15a]
2. Distributional PAC learning: samples from a stochastic WFA [HKZ09; BDR09; Bal+14]
3. Statistical learning: optimize output predictions wrt a loss function [BM12; BM15b]

Exact Learning of WFA with Queries

Setup:

- Unknown $f : \Sigma^\star \to \mathbb{R}$ with $\mathrm{rank}(f) = n$
- Membership oracle: $\mathrm{MQ}_f(x)$ returns $f(x)$ for any $x \in \Sigma^\star$
- Equivalence oracle: $\mathrm{EQ}_f(A)$ returns $\mathtt{true}$ if $f \equiv A$ and $(\mathtt{false}, z)$ if $f(z) \neq A(z)$

Algorithm:

1. Initialize $\mathcal{P} = \mathcal{S} = \{\epsilon\}$ and maintain $\mathcal{B} = (\mathcal{P}, \mathcal{S})$
2. Let $A = \mathrm{Spectral}(\mathbf{H}^{\mathcal{B}}, \mathbf{H}^{\mathcal{B}}_{\Sigma}, \mathrm{rank}(\mathbf{H}^{\mathcal{B}}))$
3. While $\mathrm{EQ}(A) = (\mathtt{false}, z)$
   3.1 Let $z = p \cdot a \cdot s$ with p the longest prefix of z in $\mathcal{P}$
   3.2 Let $\mathcal{S} = \mathcal{S} \cup \mathrm{suffixes}(s)$
   3.3 While $\exists p \in \mathcal{P}$ and $\exists a \in \Sigma$ such that $\mathbf{H}^{\mathcal{B}}_a(p, -) \notin \mathrm{rowspan}(\mathbf{H}^{\mathcal{B}})$, add $p \cdot a$ to $\mathcal{P}$
   3.4 Let $A = \mathrm{Spectral}(\mathbf{H}^{\mathcal{B}}, \mathbf{H}^{\mathcal{B}}_{\Sigma}, \mathrm{rank}(\mathbf{H}^{\mathcal{B}}))$

Analysis:

- At most $n + 1$ calls to EQ_f and $O(|\Sigma| n^2 L)$ calls to MQ_f, where $L = \max |z|$
- Can be improved to $O((|\Sigma| + \log L) n^2)$ calls to MQ_f; can reduce calls to EQ_f by increasing calls to MQ_f

PAC Learning Stochastic WFA

Setup:

- Unknown $f : \Sigma^\star \to \mathbb{R}$ with $\mathrm{rank}(f) = n$ defining probability distribution on $\Sigma^\star$
- Data: $x^{(1)}, \dots, x^{(m)}$ i.i.d. strings sampled from f
- Parameters: n and $\mathcal{B} = (\mathcal{P}, \mathcal{S})$ such that $\mathrm{rank}(\mathbf{H}^{\mathcal{B}}) = n$ and $\epsilon \in \mathcal{P} \cap \mathcal{S}$

Algorithm:

1. Estimate Hankel matrices $\hat{\mathbf{H}}^{\mathcal{B}}$ and $\hat{\mathbf{H}}_a^{\mathcal{B}}$ for all $a \in \Sigma$ using empirical probabilities

$$\hat{f}(x) = \frac{1}{m} \sum_{i=1}^{m} 1[x^{(i)} = x]$$

2. Return $\hat{A} = \mathrm{Spectral}(\hat{\mathbf{H}}^{\mathcal{B}}, \hat{\mathbf{H}}_\Sigma^{\mathcal{B}}, n)$

Analysis:

- Running time is $O(|\mathcal{P} \cdot \mathcal{S}| m + |\Sigma||\mathcal{P}||\mathcal{S}| n)$
- With high probability $\sum_{|x| \leqslant L} |f(x) - \hat{A}(x)| = O\left(\frac{L^2 |\Sigma| \sqrt{n}}{\sigma_n(\mathbf{H}_f^{\mathcal{B}})^2 \sqrt{m}}\right)$

Statistical Learning of WFA

Setup:

- Unknown distribution $\mathcal{D}$ over $\Sigma^\star \times \mathbb{R}$
- Data: $(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})$ i.i.d. string-label pairs sampled from $\mathcal{D}$
- Parameters: n, convex loss function $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}_+$, convex regularizer R, regularization parameter $\lambda > 0$, and $\mathcal{B} = (\mathcal{P}, \mathcal{S})$ with $\epsilon \in \mathcal{P} \cap \mathcal{S}$

Algorithm:

1. Build $\mathcal{B}' = (\mathcal{P}', \mathcal{S})$ with $\mathcal{P}' = \mathcal{P} \cup \mathcal{P} \cdot \Sigma$
2. Find the Hankel matrix $\hat{\mathbf{H}}^{\mathcal{B}'}$ solving $\min_{\mathbf{H}} \frac{1}{m} \sum_{i=1}^m \ell(\mathbf{H}(x^{(i)}), y^{(i)}) + \lambda R(\mathbf{H})$
3. Return $\hat{A} = \mathrm{Spectral}(\hat{\mathbf{H}}^{\mathcal{B}}, \hat{\mathbf{H}}_{\Sigma}^{\mathcal{B}}, n)$, where $\hat{\mathbf{H}}^{\mathcal{B}}$ and $\hat{\mathbf{H}}_{\Sigma}^{\mathcal{B}}$ are submatrices of $\hat{\mathbf{H}}^{\mathcal{B}'}$

Analysis:

- Running time is polynomial in n, m, $|\Sigma|$, $|\mathcal{P}|$, and $|\mathcal{S}|$
- With high probability

$$\mathbb{E}_{(x,y)\sim\mathcal{D}}[\ell(\hat{A}(x), y)] \leqslant \frac{1}{m} \sum_{i=1}^m \ell(\hat{A}(x^{(i)}), y^{(i)}) + O\left(\frac{1}{\sqrt{m}}\right)$$

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Extensions

1. More complex models
   - Transducers and taggers [BQC11; Qua+14]
   - Grammars and tree automata [Luq+12; Bal+14; RBC16]
   - Reactive models [BBP15; LBP16; BM17a]
2. More realistic setups
   - Multiple related tasks [RBP17]
   - Timing data [BBP15; LBP16]
   - Single trajectory [BM17a]
   - Probabilistic models [BHP14]
3. Deeper theory
   - Convex relaxations [BQC12]
   - Generalization bounds [BM15b; BM17b]
   - Approximate minimisation [BPP15]
   - Bisimulation metrics [BGP17]

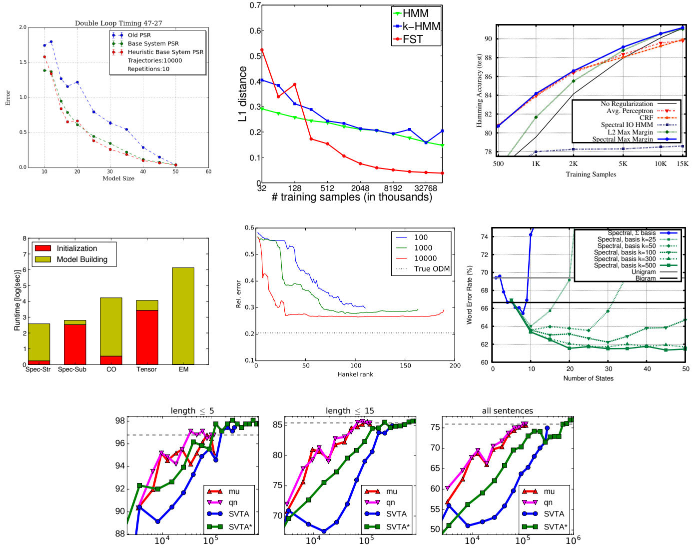
And It Works Too!

Spectral methods are competitive against traditional methods:

- Expectation maximization
- Conditional random fields
- Tensor decompositions

In a variety of problems:

- Sequence tagging
- Constituency and dependency parsing
- Timing and geometry learning
- POS-level language modelling



Open Problems and Current Trends

- Optimal selection of $\mathcal{P}$ and $\mathcal{S}$ from data
- Scalable convex optimization over sets of Hankel matrices
- Constraining the output WFA (eg. probabilistic automata)
- Relations between learning and approximate minimisation
- How much of this can be extended to WFA over semi-rings?
- Spectral methods for initializing non-convex gradient-based learning algorithms

Conclusion

Take home points

- A single building block based on SVD of Hankel matrices
- Implementation only requires linear algebra
- Analysis involves linear algebra, probability, convex optimization
- Can be made practical for a variety of models and applications

Want to know more?

- EMNLP'14 tutorial (with slides, video, and code)
  `https://borjaballe.github.io/emnlp14-tutorial/`
- Survey papers [BM15a; TJ15]
- Python toolkit Sp2Learn [Arr+16]
- Neighbouring literature: Predictive state representations (PSR) [LSS02] and Observable operator models (OOM) [Jae00]

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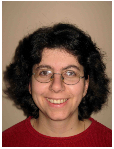

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